MSG No. 155.46 $R321'$ [Type II, trigonal]

Table 1: Wyckoff site: 3a, site symmetry: 32.1'

No.	position	mapping
1	$[0, 0, 0]$	[1,2,3,4,5,6,19,20,21,22,23,24]
2	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right]$	[7,8,9,10,11,12,25,26,27,28,29,30]
3	$\left[\frac{1}{3}, \frac{2}{3}, \frac{2}{3}\right]$	[13,14,15,16,17,18,31,32,33,34,35,36]

Table 2: Wyckoff site: 3b, site symmetry: 32.1'

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[1,2,3,4,5,6,19,20,21,22,23,24]
2	$\left[\frac{2}{3}, \frac{1}{3}, \frac{5}{6}\right]$	[7,8,9,10,11,12,25,26,27,28,29,30]
3	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{6}\right]$	[13,14,15,16,17,18,31,32,33,34,35,36]

Table 3: Wyckoff site: 6c, site symmetry: 3..1'

No.	position	mapping
1	$[0, 0, z]$	[1,2,3,19,20,21]
2	$[0, 0, -z]$	[4,5,6,22,23,24]
3	$\left[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}\right]$	[7,8,9,25,26,27]
4	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z\right]$	[10,11,12,28,29,30]
5	$\left[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}\right]$	[13,14,15,31,32,33]
6	$\left[\frac{1}{3}, \frac{2}{3}, \frac{2}{3} - z\right]$	[16,17,18,34,35,36]

Table 4: Wyckoff site: 9d, site symmetry: .2.1'

No.	position	mapping
1	$[x, 0, 0]$	[1,4,19,22]
2	$[0, x, 0]$	[2,5,20,23]
3	$[-x, -x, 0]$	[3,6,21,24]
4	$\left[x + \frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right]$	[7,10,25,28]
5	$\left[\frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}\right]$	[8,11,26,29]
6	$\left[\frac{2}{3} - x, \frac{1}{3} - x, \frac{1}{3}\right]$	[9,12,27,30]
7	$\left[x + \frac{1}{3}, \frac{2}{3}, \frac{2}{3}\right]$	[13,16,31,34]
8	$\left[\frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}\right]$	[14,17,32,35]
9	$\left[\frac{1}{3} - x, \frac{2}{3} - x, \frac{2}{3}\right]$	[15,18,33,36]

Table 5: Wyckoff site: `9e`, site symmetry: `.2.1'`

No.	position	mapping
1	$\left[x,\, 0,\, \frac{1}{2}\right]$	`[1,4,19,22]`
2	$\left[0,\, x,\, \frac{1}{2}\right]$	`[2,5,20,23]`
3	$\left[-x,\, -x,\, \frac{1}{2}\right]$	`[3,6,21,24]`
4	$\left[x+\frac{2}{3},\, \frac{1}{3},\, \frac{5}{6}\right]$	`[7,10,25,28]`
5	$\left[\frac{2}{3},\, x+\frac{1}{3},\, \frac{5}{6}\right]$	`[8,11,26,29]`
6	$\left[\frac{2}{3}-x,\, \frac{1}{3}-x,\, \frac{5}{6}\right]$	`[9,12,27,30]`
7	$\left[x+\frac{1}{3},\, \frac{2}{3},\, \frac{1}{6}\right]$	`[13,16,31,34]`
8	$\left[\frac{1}{3},\, x+\frac{2}{3},\, \frac{1}{6}\right]$	`[14,17,32,35]`
9	$\left[\frac{1}{3}-x,\, \frac{2}{3}-x,\, \frac{1}{6}\right]$	`[15,18,33,36]`

Table 6: Wyckoff site: `18f`, site symmetry: `11'`

No.	position	mapping
1	$[x,\, y,\, z]$	`[1,19]`
2	$[-y,\, x-y,\, z]$	`[2,20]`
3	$[-x+y,\, -x,\, z]$	`[3,21]`
4	$[x-y,\, -y,\, -z]$	`[4,22]`
5	$[y,\, x,\, -z]$	`[5,23]`
6	$[-x,\, -x+y,\, -z]$	`[6,24]`
7	$\left[x+\frac{2}{3},\, y+\frac{1}{3},\, z+\frac{1}{3}\right]$	`[7,25]`
8	$\left[\frac{2}{3}-y,\, x-y+\frac{1}{3},\, z+\frac{1}{3}\right]$	`[8,26]`
9	$\left[-x+y+\frac{2}{3},\, \frac{1}{3}-x,\, z+\frac{1}{3}\right]$	`[9,27]`
10	$\left[x-y+\frac{2}{3},\, \frac{1}{3}-y,\, \frac{1}{3}-z\right]$	`[10,28]`
11	$\left[y+\frac{2}{3},\, x+\frac{1}{3},\, \frac{1}{3}-z\right]$	`[11,29]`
12	$\left[\frac{2}{3}-x,\, -x+y+\frac{1}{3},\, \frac{1}{3}-z\right]$	`[12,30]`
13	$\left[x+\frac{1}{3},\, y+\frac{2}{3},\, z+\frac{2}{3}\right]$	`[13,31]`
14	$\left[\frac{1}{3}-y,\, x-y+\frac{2}{3},\, z+\frac{2}{3}\right]$	`[14,32]`
15	$\left[-x+y+\frac{1}{3},\, \frac{2}{3}-x,\, z+\frac{2}{3}\right]$	`[15,33]`
16	$\left[x-y+\frac{1}{3},\, \frac{2}{3}-y,\, \frac{2}{3}-z\right]$	`[16,34]`
17	$\left[y+\frac{1}{3},\, x+\frac{2}{3},\, \frac{2}{3}-z\right]$	`[17,35]`
18	$\left[\frac{1}{3}-x,\, -x+y+\frac{2}{3},\, \frac{2}{3}-z\right]$	`[18,36]`