



FOUNDATIONS
ADVANCES

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Supporting information for article:

An algebraic approach to cooperative rotations in networks of interconnected rigid units

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Supplementary Information

Algebraic detection of
cooperative-rotational rigid-unit modes
in the HTB and TTB structures

TTB modes: $Z_5^+(2)$, $A_5^-(2)$, $R_1(4)$

HTB modes: $A_3^+(1)$, $A_6^+(2)$, $L_2^-(3)$

Amplitudes -> number of free and independent SUPA parameters (rotational and displacive vector components) allowed by the space-group symmetry; also the number of rotational and displacive symmetry-mode amplitudes of the SUPAs.

SADPs -> the number of shared atom coordinates

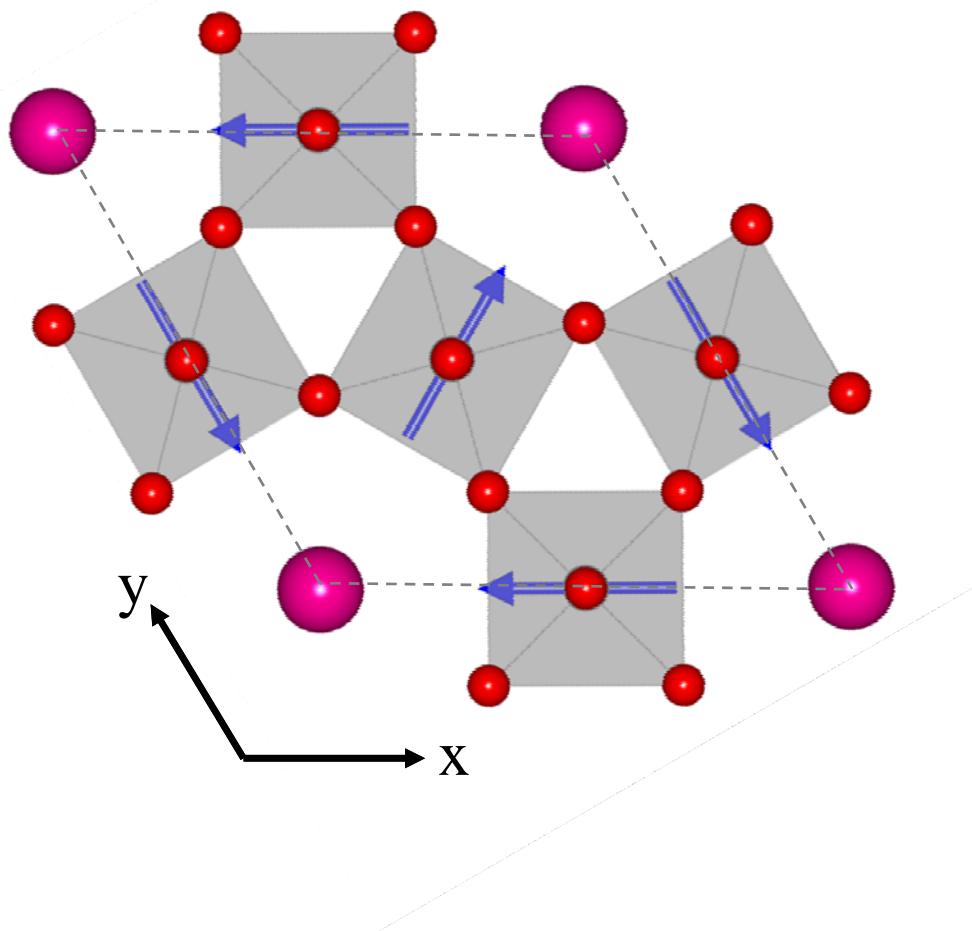
Equations -> the number equations constructed (two for each component since each shared atom is shared by two pivots).

Variables -> the number of variables in each equation (SADPs + amplitudes).

Independent modes -> the number of symmetry-mode amplitudes that lead to independent RUM patterns.

Dependent modes -> the number of symmetry-mode amplitudes that depend on the independent symmetry-mode amplitudes.

HTB A3+ P1(a)



HTB A3+ P1(a)

194 P6_3/mmc, basis={(1,0,0),(0,1,0),(0,0,2)}, origin=(0,0,0), s=2, i=2,
k-active= (0,0,1/2)

Amplitudes = 1, SADPs = 6, Equations = 6 X 2 = 12, Variables = 6 + 1 = 7

All modes:

1 P6/mmm[0,0,1/2]A3+(a)[W:f:rot]B3g(a)

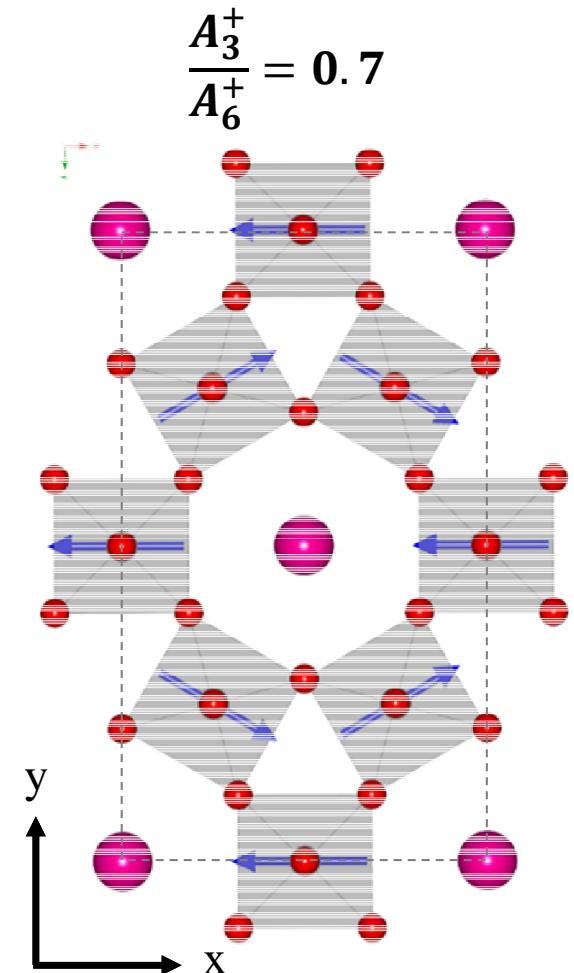
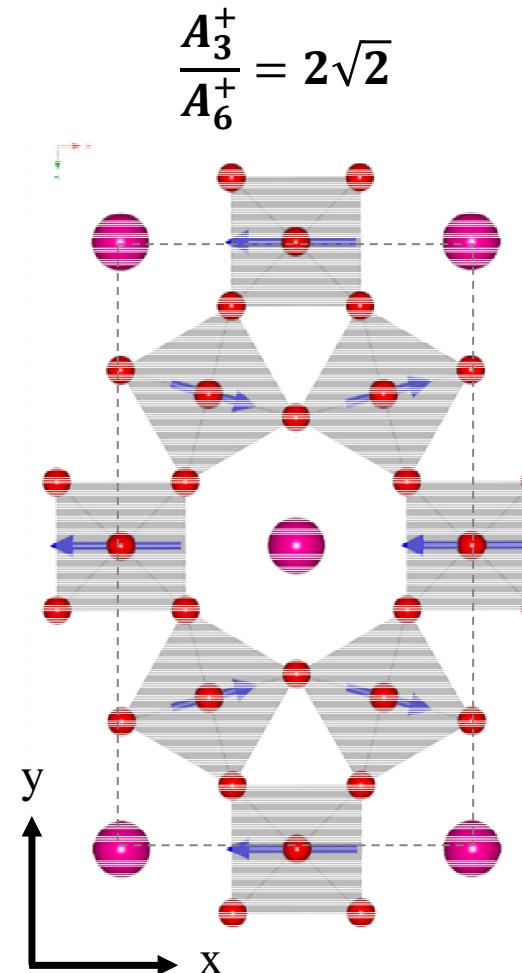
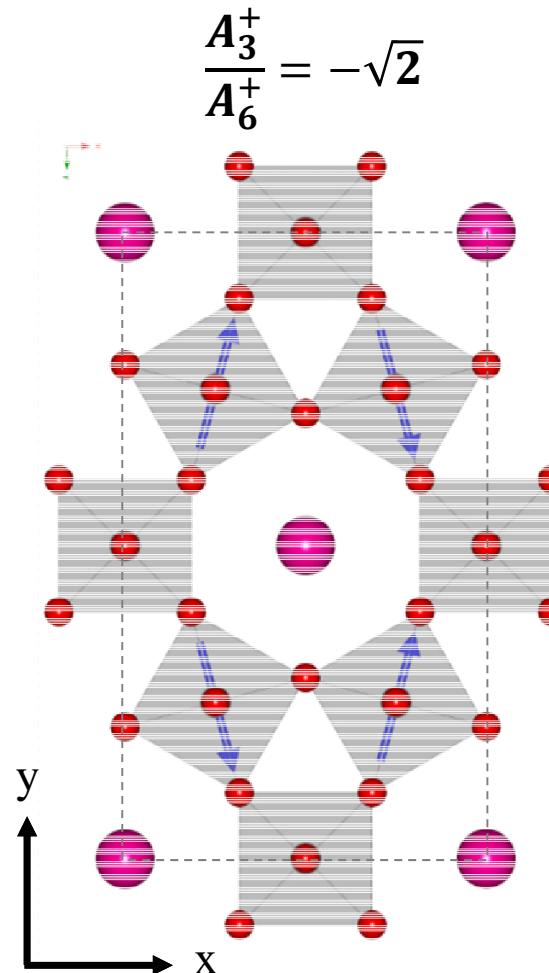
Independent modes:

1 P6/mmm[0,0,1/2]A3+(a)[W:f:rot]B3g(a)

Dependent modes: { }

HTB A6+ P1(a,0)

Because A6+(a,0) has A3+(a) as an independent secondary mode, we illustrate this RUM at three different A3+/A6+(B_{3g}) amplitude ratios.



HTB A6+ P1(a,0)

63 Cmcm, basis={(1,0,0),(1,2,0),(0,0,2)}, origin=(0,0,0), s=2, i=6,
k-active= (0,0,1/2)
Amplitudes = 4, SADPs = 12, Equations = 12 x 2 = 24, Variables = 12 + 4 = 16

All modes:

1 P6/mmm[0,0,1/2]A6+(a,0)[W:f:rot]B3g(a)
2 P6/mmm[0,0,1/2]A6+(a,0)[W:f:rot]B2g(a)
3 P6/mmm[0,0,0]GM5+(a,0)[W:f:rot]B1g(a)
4 P6/mmm[0,0,1/2]A3+(a)[W:f:rot]B3g(a)

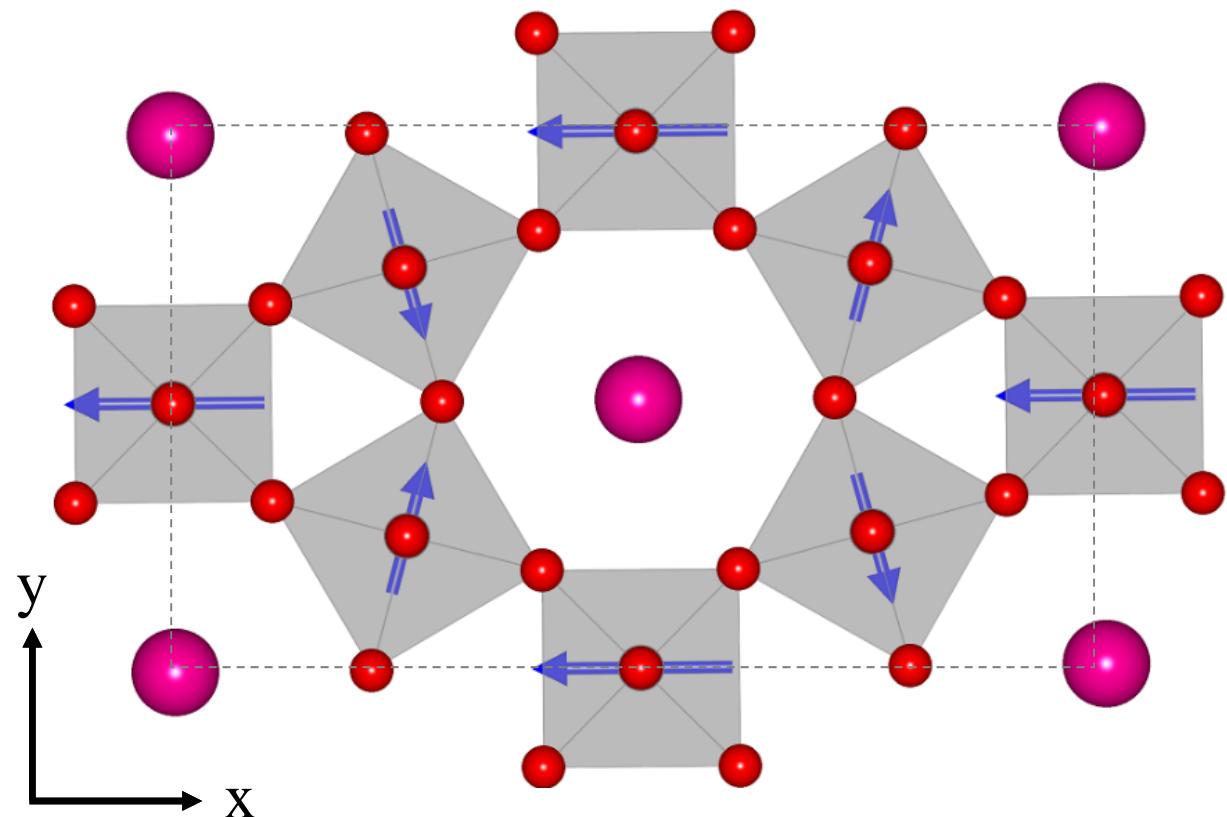
Independent modes:

2 P6/mmm[0,0,1/2]A6+(a,0)[W:f:rot]B2g(a)
4 P6/mmm[0,0,1/2]A3+(a)[W:f:rot]B3g(a)

Dependent modes:

1 P6/mmm[0,0,1/2]A6+(a,0)[W:f:rot]B3g(a) a[1] -> 0.579755 a[2]

HTB A6+ P2(0,a)



HTB A6+ P2(0,a)

```
63 Cmcm, basis={(1,2,0),(-1,0,0),(0,0,2)}, origin=(0,0,0), s=2, i=6,
k-active= (0,0,1/2)
Amplitudes = 4, SADPs = 12, Equations = 12 X 2 = 24, Variables = 12 + 4 = 16
```

All modes:

```
1 P6/mmm[0,0,1/2]A6+(0,a)[W:f:rot]B3g(a)
2 P6/mmm[0,0,1/2]A6+(0,a)[W:f:rot]B2g(a)
3 P6/mmm[0,0,0]GM5+(a,0)[W:f:rot]B1g(a)
4 P6/mmm[0,0,1/2]A4+(a)[W:f:rot]B2g(a)
```

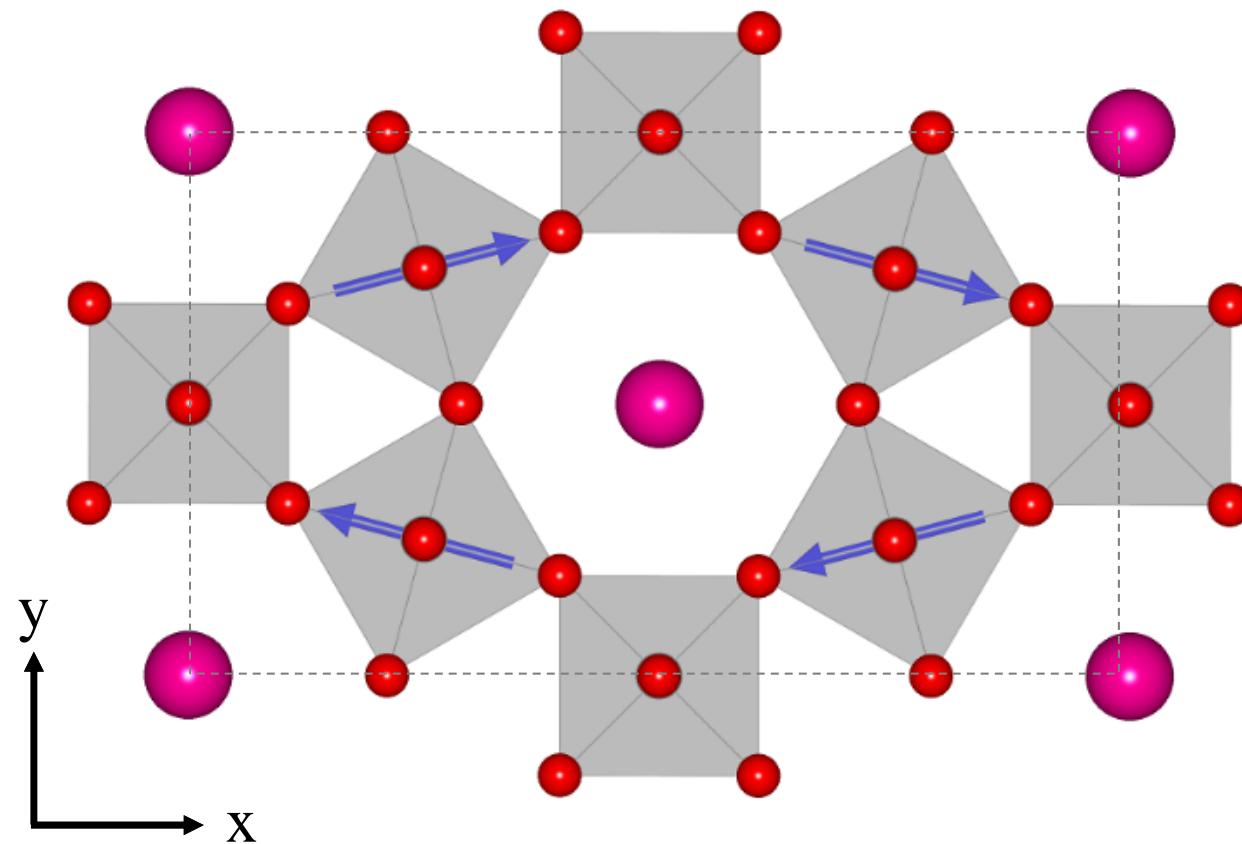
Independent modes:

```
2 P6/mmm[0,0,1/2]A6+(0,a)[W:f:rot]B2g(a)
```

Dependent modes:

```
1 P6/mmm[0,0,1/2]A6+(0,a)[W:f:rot]B3g(a) a[1] -> 0.579736 a[2]
```

HTB L2- P1($a, 0, 0$)



HTB L2- P1(a,0,0)

71 Immm, basis={(2,1,0),(0,1,0),(0,0,2)}, origin=(0,0,1/2), s=2, i=6,
k-active= (1/2,0,1/2)
Amplitudes = 3, SADPs = 15, Equations = 15 x 2 = 30, Variables = 15 + 5 = 18

All modes:

1 P6/mmm[1/2,0,1/2]L2-(a,0,0)[W:f:rot]B3g(a)
2 P6/mmm[1/2,0,1/2]L2-(a,0,0)[W:f:rot]B2g(a)
3 P6/mmm[0,0,0]GM5+(a,-1.732a)[W:f:rot]B1g(a)

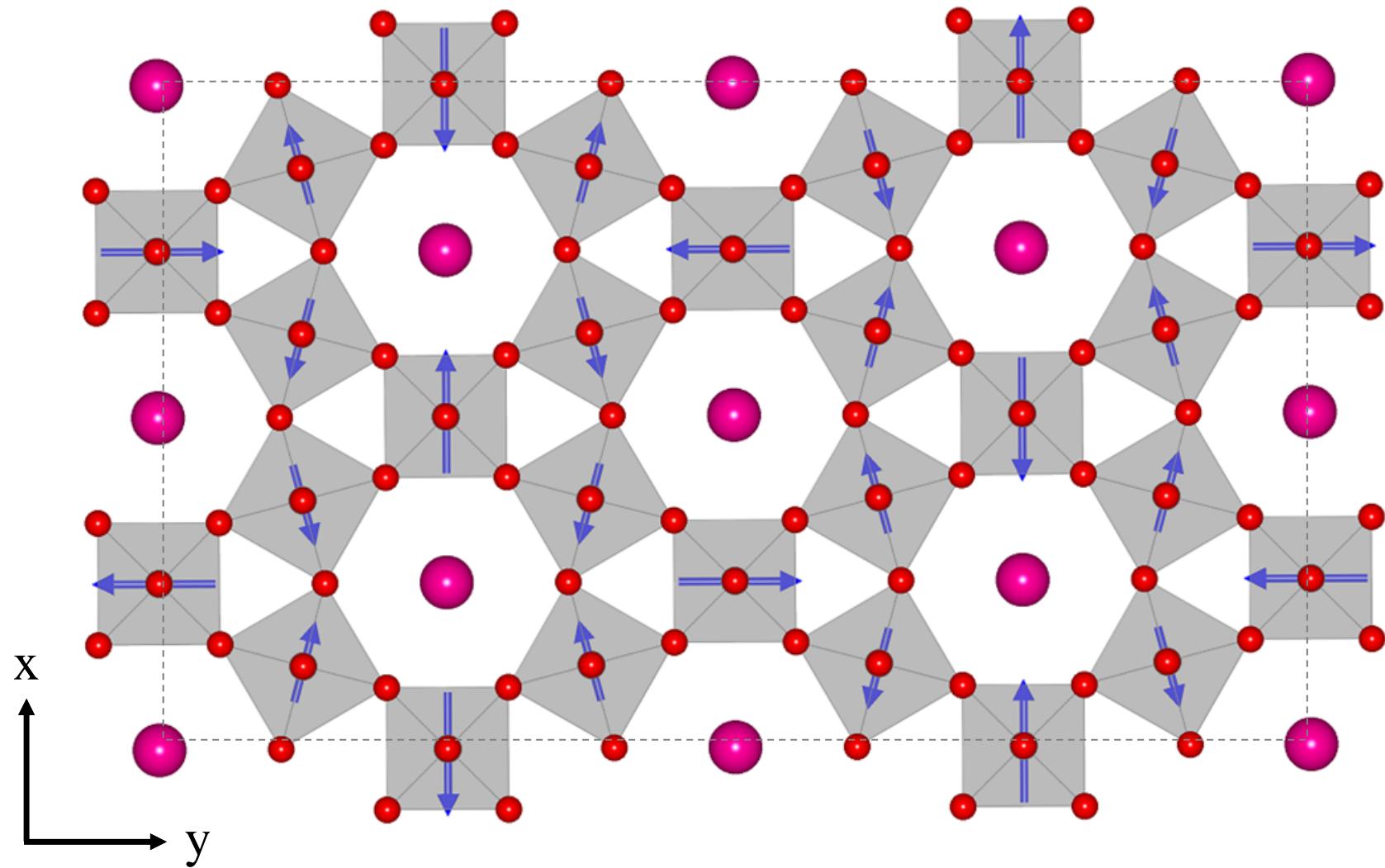
Independent modes:

2 P6/mmm[1/2,0,1/2]L2-(a,0,0)[W:f:rot]B2g(a)

Dependent modes:

1 P6/mmm[1/2,0,1/2]L2-(a,0,0)[W:f:rot]B3g(a) a[1] -> 1.004 a[2]

HTB L2- P2($a, 0, a$)



HTB L2- P2(a,0,a)

69 Fmmm, basis={(2,0,0),(2,4,0),(0,0,2)}, origin=(0,0,1/2), s=4, i=12,
k-active= (1/2,0,1/2),(1/2,1/2,1/2)
Amplitudes = 5, SADPs = 24, Equations = 24 X 2 = 48, Variables = 24 + 5 = 29

All modes:

1 P6/mmm[1/2,0,1/2]L2-(a,0,a)[W:f:rot]B3g(a)
2 P6/mmm[1/2,0,1/2]L2-(a,0,a)[W:f:rot]B2g(a)
3 P6/mmm[0,0,0]GM5+(a,0)[W:f:rot]B1g(a)
4 P6/mmm[1/2,0,1/2]L1-(a,0,-a)[W:f:rot]B3g(a)
5 P6/mmm[1/2,0,1/2]L1-(a,0,-a)[W:f:rot]B2g(a)

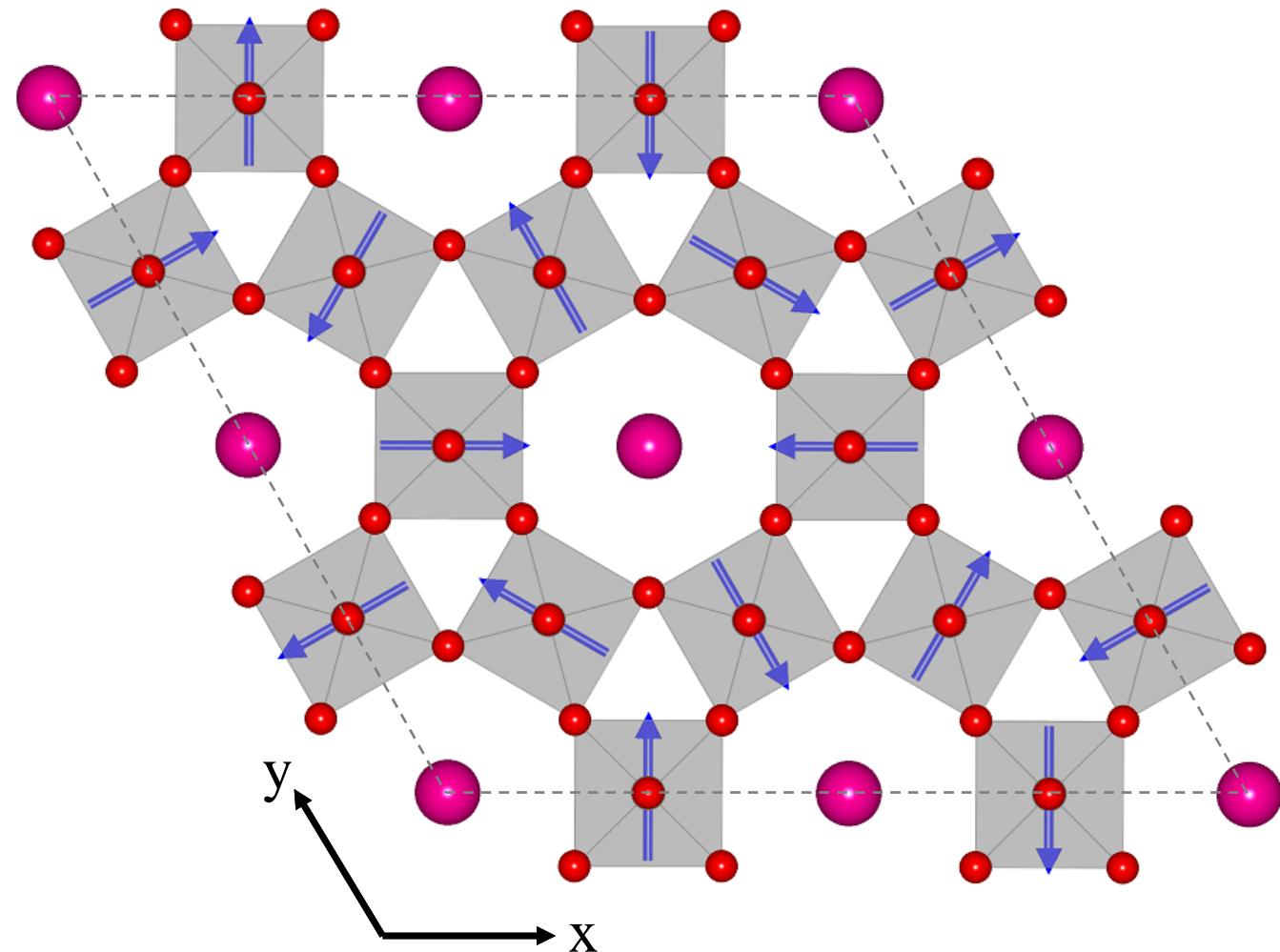
Independent modes:

2 P6/mmm[1/2,0,1/2]L2-(a,0,a)[W:f:rot]B2g(a)

Dependent modes:

1 P6/mmm[1/2,0,1/2]L2-(a,0,a)[W:f:rot]B3g(a) a[1] -> 1.00417 a[2]

HTB L2- P3(a, a, a)



HTB L2- P3(a,a,a)

191 P6/mmm, basis={(2,0,0),(0,2,0),(0,0,2)}, origin=(0,0,1/2), s=8, i=8,
k-active= (1/2,0,1/2),(0,1/2,1/2),(1/2,1/2,1/2)
Amplitudes = 2, SADPs = 21, Equations = 21 x 2 = 42, Variables = 21 + 2 = 23

All modes:

1 P6/mmm[1/2,0,1/2]L2-(a,a,a)[W:f:rot]B3g(a)
2 P6/mmm[1/2,0,1/2]L2-(a,a,a)[W:f:rot]B2g(a)

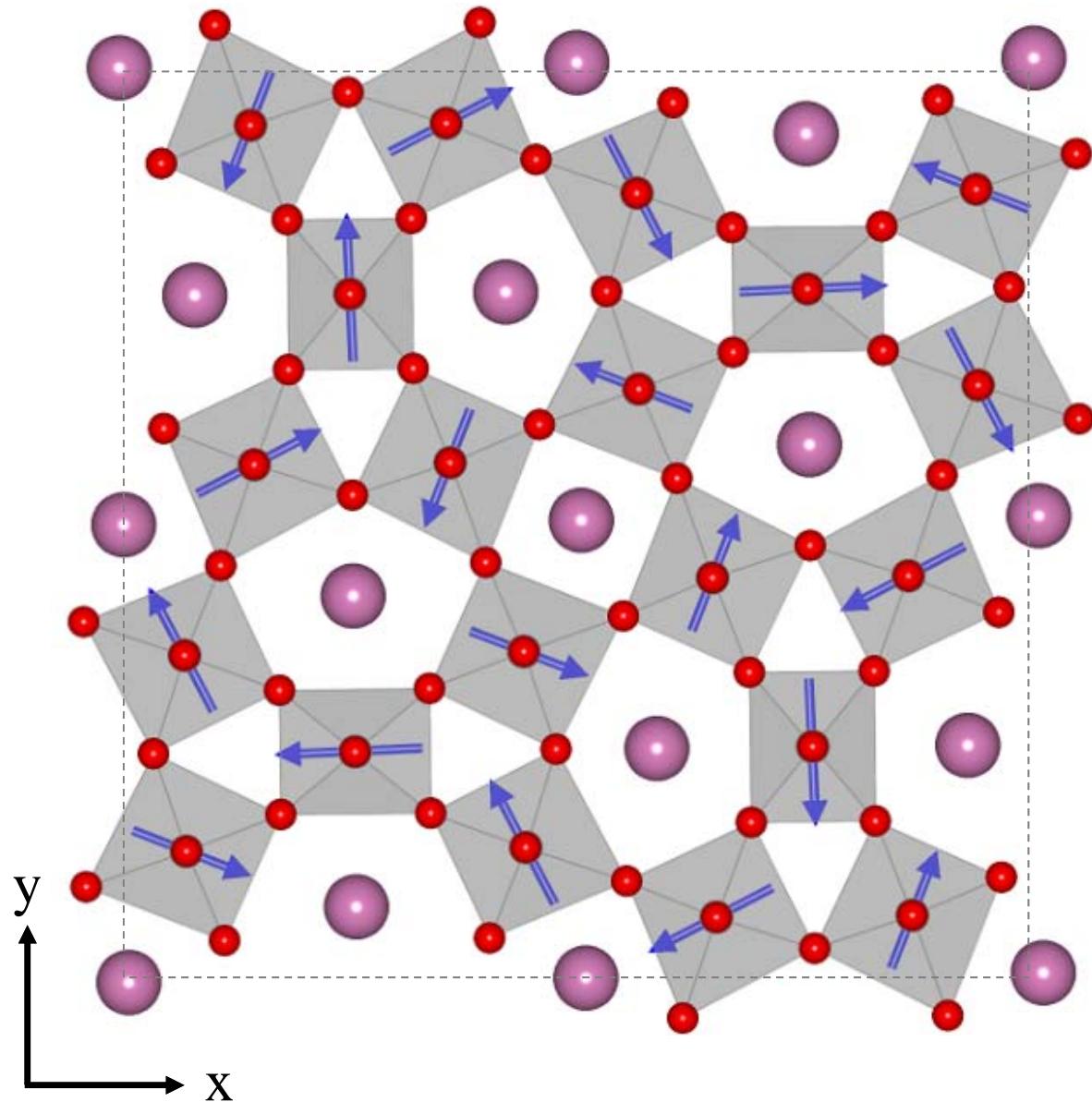
Independent modes:

2 P6/mmm[1/2,0,1/2]L2-(a,a,a)[W:f:rot]B2g(a)

Dependent modes:

1 P6/mmm[1/2,0,1/2]L2-(a,a,a)[W:f:rot]B3g(a) a[1] -> 1.00394 a[2]

TTB A5- P1($a, 0$)



TTB A5- P1(a,0)

87 I4/m, basis={(1,1,0),(-1,1,0),(0,0,2)}, origin=(0,0,1/2), s=2, i=4,
k-active= (1/2,1/2,1/2)
Amplitudes = 9, SADPs = 30, Equations = 30 X 2 = 60, Variables = 30 + 9 = 39

All modes:

- 1 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W1:d:rot]B3g(a)
- 2 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W1:d:rot]B2g(a)
- 3 P4/mbm[0,0,0]GM3+(a)[W1:d:rot]B1g(a)
- 4 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_1(a)
- 5 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_2(a)
- 6 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_3(a)
- 7 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_4(a)
- 8 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)
- 9 P4/mbm[0,0,0]GM3+(a)[W2:i:rot]A'(a)

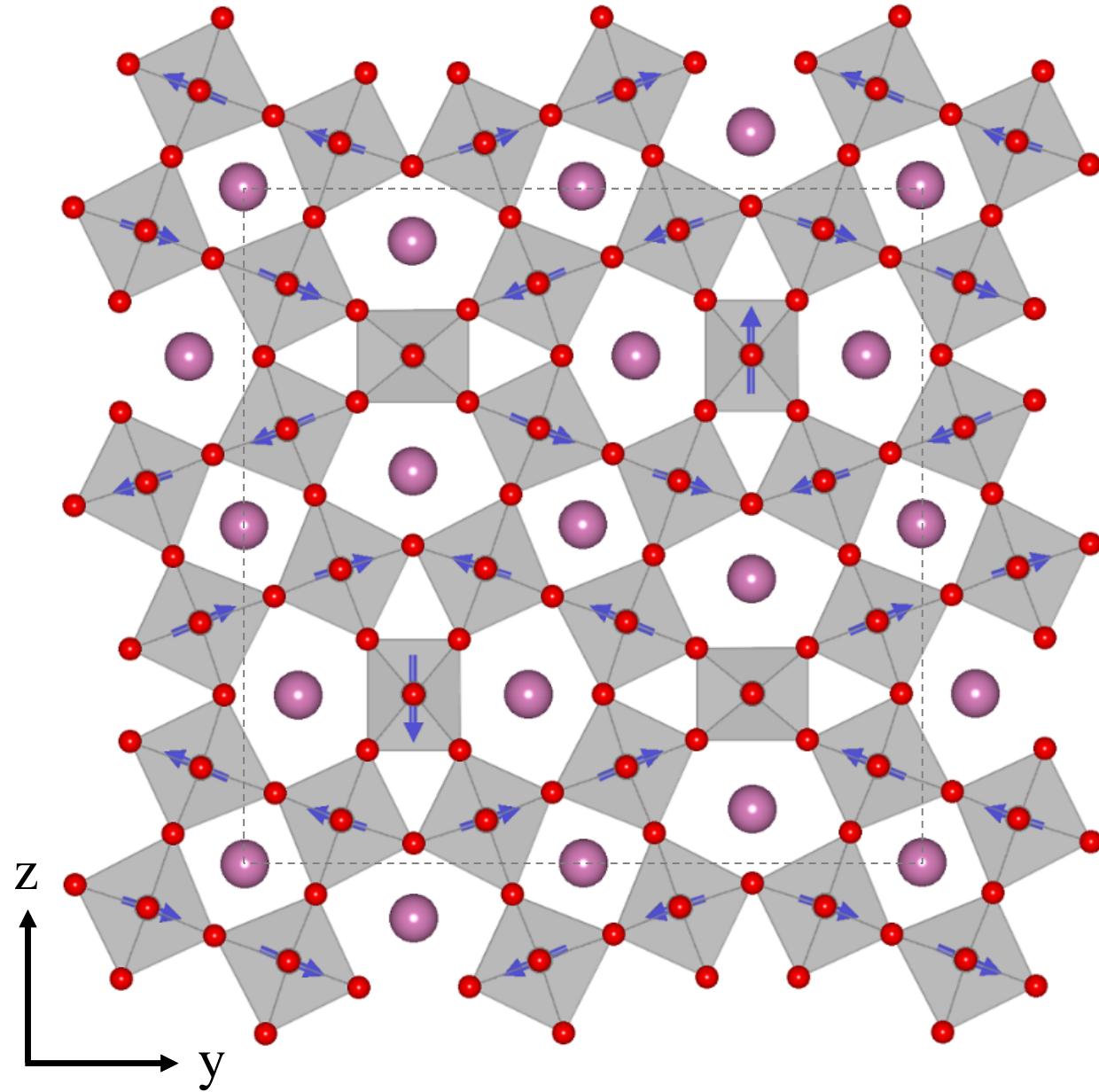
Independent modes:

- 7 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_4(a)

Dependent modes:

- 1 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W1:d:rot]B3g(a) a[1] -> 0.027935 a[7]
- 2 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W1:d:rot]B2g(a) a[2] -> -0.784535 a[7]
- 4 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_1(a) a[4] -> 0.884715 a[7]
- 5 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_2(a) a[5] -> 0.326172 a[7]
- 6 P4/mbm[1/2,1/2,1/2]A5-(a,0)[W2:i:rot]A''_3(a) a[6] -> -0.379164 a[7]

TTB A5- P3(a,a)



TTB A5- P3(a,a)

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74 Imma, basis={(0,0,2),(1,-1,0),(1,1,0)}, origin=(0,0,1/2), s=2, i=4,  
k-active= (1/2,1/2,1/2)  
Amplitudes = 8, SADPs = 36, Equations = 36 x 2 = 72, Variables = 36 + 8 = 44
```

All modes:

```
1 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W1:d:rot]B3g(a)  
2 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W1:d:rot]B2g(a)  
3 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_1(a)  
4 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_2(a)  
5 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_3(a)  
6 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_4(a)  
7 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)  
8 P4/mbm[0,0,0]GM4+(a)[W2:i:rot]A'(a)
```

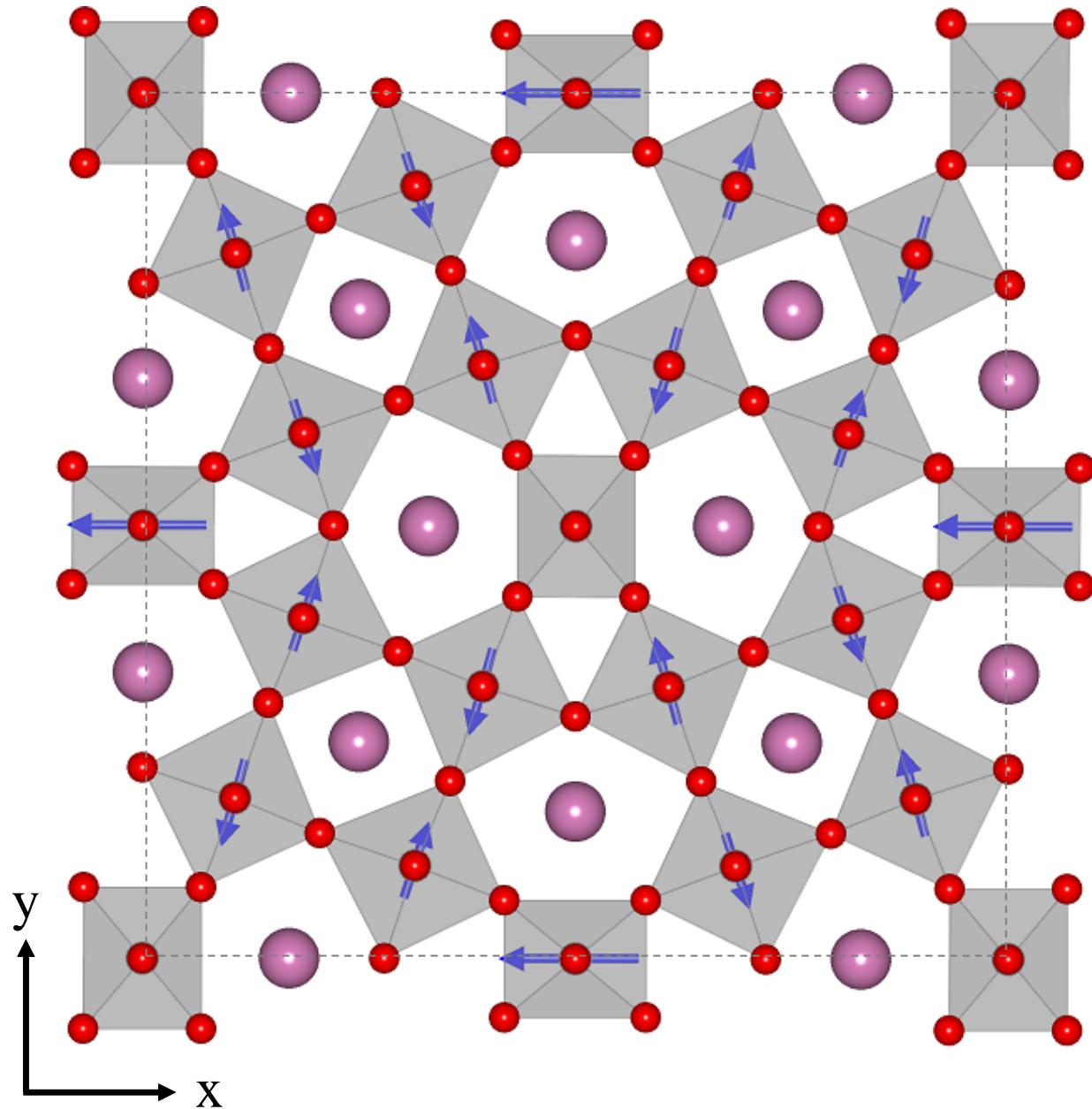
Independent modes:

```
6 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_4(a)
```

Dependent modes:

```
1 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W1:d:rot]B3g(a) a[1] -> 0.027941 a[6]  
2 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W1:d:rot]B2g(a) a[2] -> -0.784723 a[6]  
3 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_1(a) a[3] -> 0.884715 a[6]  
4 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_2(a) a[4] -> 0.326172 a[6]  
5 P4/mbm[1/2,1/2,1/2]A5-(a,a)[W2:i:rot]A''_3(a) a[5] -> -0.379164 a[6]
```

TTB Z5+ P1($a, 0$)



TTB Z5+ P1(a,0)

63 Cmcm, basis={(1,1,0),(-1,1,0),(0,0,2)}, origin=(0,1/2,0), s=2, i=4,
k-active= (0,0,1/2)
Amplitudes = 8, SADPs = 36, Equations = 36 x 2 = 72, Variables = 36 + 8 = 44

All modes:

1 P4/mbm[0,0,1/2]Z5+(a,0)[W1:d:rot]B3g(a)
2 P4/mbm[0,0,1/2]Z5+(a,0)[W1:d:rot]B2g(a)
3 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_1(a)
4 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_2(a)
5 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_3(a)
6 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_4(a)
7 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)
8 P4/mbm[0,0,0]GM4+(a)[W2:i:rot]A'(a)

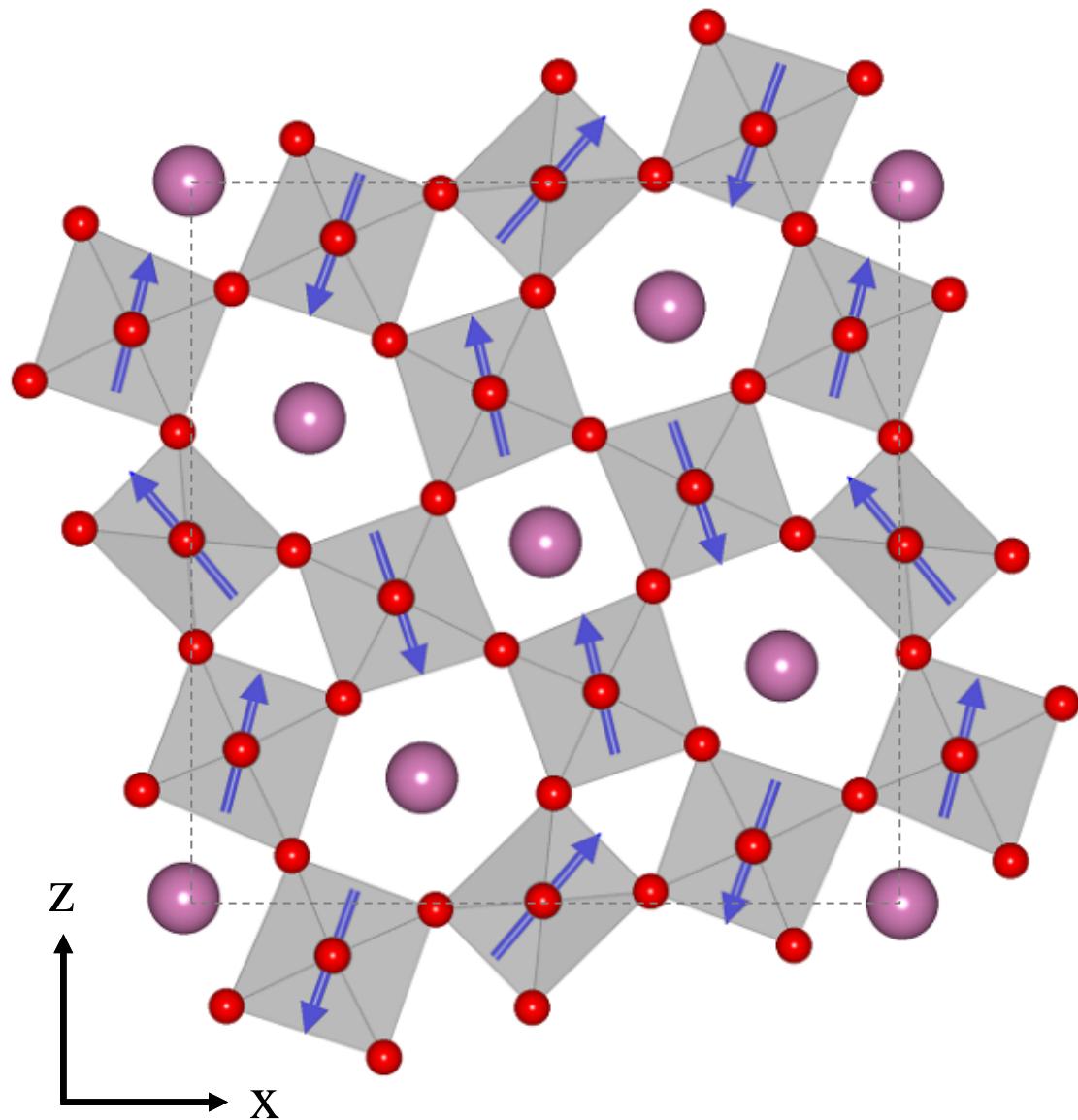
Independent modes:

6 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_4(a)

Dependent modes:

1 P4/mbm[0,0,1/2]Z5+(a,0)[W1:d:rot]B3g(a) a[1] -> 0.155341 a[6]
2 P4/mbm[0,0,1/2]Z5+(a,0)[W1:d:rot]B2g(a) a[2] -> -1.78679 a[6]
3 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_1(a) a[3] -> -1.19833 a[6]
4 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_2(a) a[4] -> 1.95041 a[6]
5 P4/mbm[0,0,1/2]Z5+(a,0)[W2:i:rot]A''_3(a) a[5] -> 2.09759 a[6]

TTB Z5+ P3(a,a)



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TTB Z5+ P3(a,a)
62 Pnma, basis={(1,0,0),(0,0,2),(0,-1,0)}, origin=(0,0,0), s=2, i=4,
k-active= (0,0,1/2)
Amplitudes = 9, SADPs = 30, Equations = 30x2 = 60, Variables = 30+9 = 39

```

All modes:

- 1 P4/mbm[0,0,1/2]Z5+(a,a)[W1:d:rot]B3g(a)
- 2 P4/mbm[0,0,1/2]Z5+(a,a)[W1:d:rot]B2g(a)
- 3 P4/mbm[0,0,0]GM2+(a)[W1:d:rot]B1g(a)
- 4 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_1(a)
- 5 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_2(a)
- 6 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_3(a)
- 7 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_4(a)
- 8 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)
- 9 P4/mbm[0,0,0]GM2+(a)[W2:i:rot]A'(a)

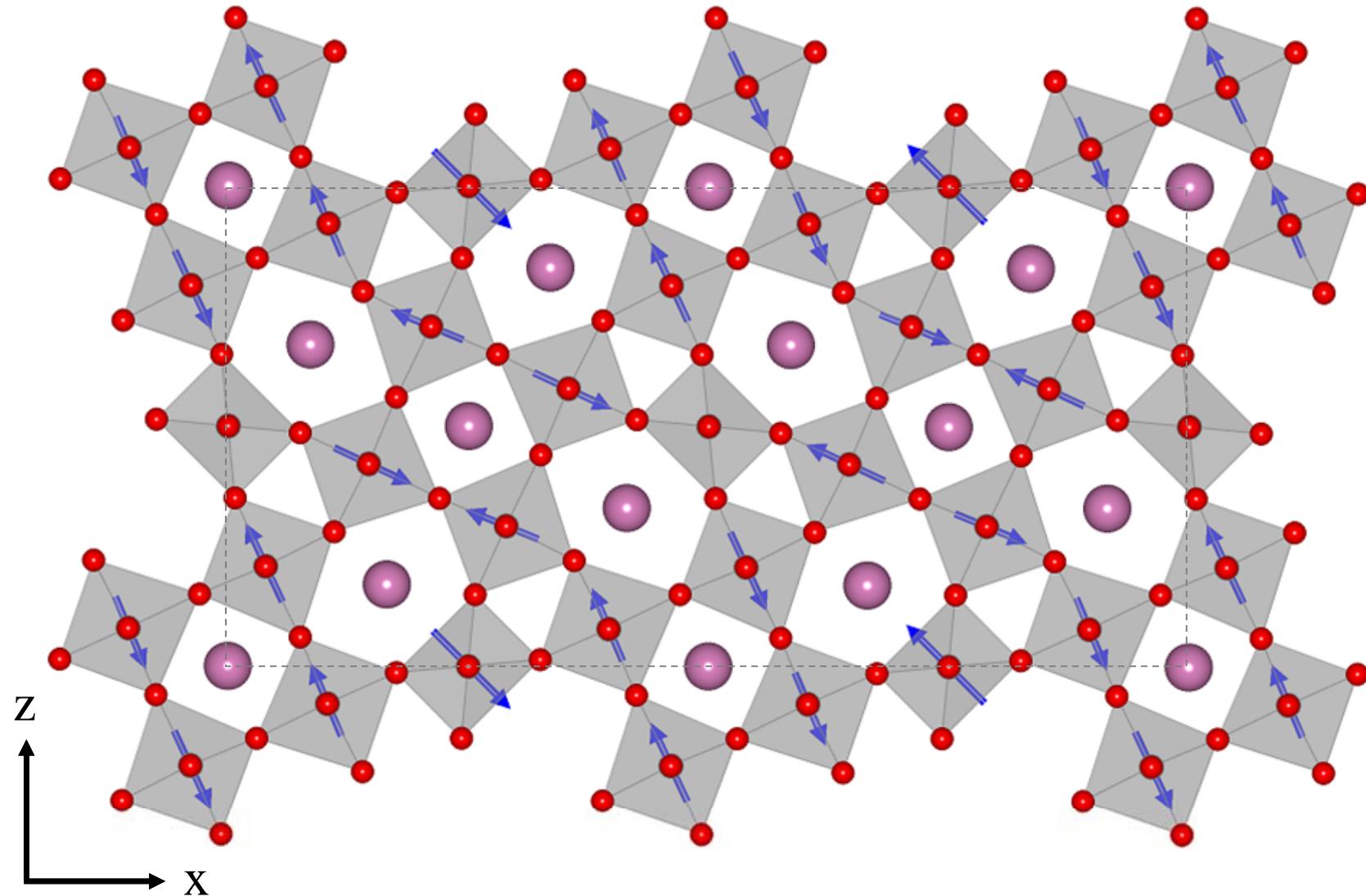
Independent modes:

- 7 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_4(a)

Dependent modes:

- 1 P4/mbm[0,0,1/2]Z5+(a,a)[W1:d:rot]B3g(a)", a[1] -> 0.15536 a[7]
- 2 P4/mbm[0,0,1/2]Z5+(a,a)[W1:d:rot]B2g(a) a[2] -> -1.78699 a[7]
- 4 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_1(a) a[4] -> -1.19833 a[7]
- 5 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_2(a) a[5] -> 1.95041 a[7]
- 6 P4/mbm[0,0,1/2]Z5+(a,a)[W2:i:rot]A''_3(a) a[6] -> 2.09759 a[7]

TTB R1 P1(0,0,a,-a)



TTB R1(0,0,a,-a)

12 C2/m, basis={(2,0,0),(0,0,2),(0,-1,0)}, origin=(1/2,0,1/2), s=2, i=8,
k-active=(1/2,0,1/2)

Amplitudes = 16, SADPs = 63, Equations = 63 X 2 = 126, Variables = 63 + 16 = 79

All modes:

1 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W1:d:rot]B3g(a)
2 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W1:d:rot]B2g(a)
3 P4/mbm[0,0,0]GM2+(a)[W1:d:rot]B1g(a)
4 P4/mbm[0,0,0]GM3+(a)[W1:d:rot]B1g(a)
5 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_1(a)
6 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_2(a)
7 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_3(a)
8 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_4(a)
9 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_5(a)
10 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_6(a)
11 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_7(a)
12 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_8(a)
13 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)
14 P4/mbm[0,0,0]GM2+(a)[W2:i:rot]A'(a)
15 P4/mbm[0,0,0]GM3+(a)[W2:i:rot]A'(a)
16 P4/mbm[0,0,0]GM4+(a)[W2:i:rot]A'(a)

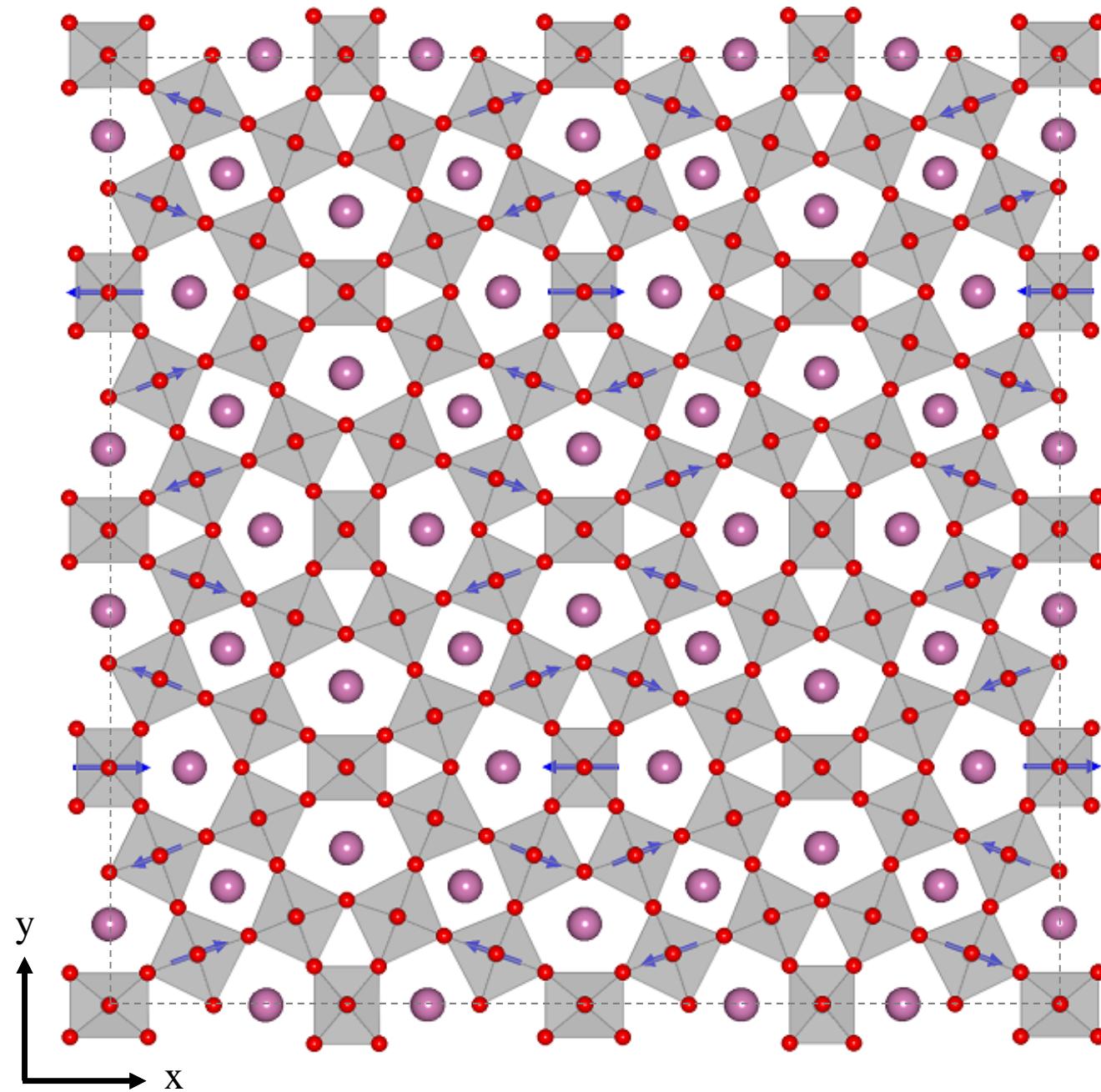
Independent modes:

12 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_8(a)

Dependent modes:

1 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W1:d:rot]B3g(a) a[1] -> 2.20926 a[12]
2 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W1:d:rot]B2g(a) a[2] -> 0.00297 a[12]
5 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_1(a) a[5] -> -0.75065 a[12]
6 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_2(a) a[6] -> 2.25714 a[12]
7 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_3(a) a[7] -> 0.75592 a[12]
8 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_4(a) a[8] -> -2.26092 a[12]
9 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_5(a) a[9] -> -2.25007 a[12]
10 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_6(a) a[10] -> -0.97886 a[12]
11 P4/mbm[0,1/2,1/2]R1(0,0,a,-a)[W2:i:rot]A''_7(a) a[11] -> 2.23344 a[12]

TTB R1 P3($a, -a, -a, a$)



TTB R1 P3(a,-a,-a,a)

69 Fmmm, basis={(2,2,0),(-2,2,0),(0,0,2)}, origin=(1/2,0,1/2), s=4, i=8,
k-active= (0,1/2,1/2),(1/2,0,1/2)
Amplitudes = 14, SADPs = 75, Equations = 75 X 2 = 150, Variables = 75 + 14 = 89

All modes:

1 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W1:d:rot]B3g(a)
2 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W1:d:rot]B2g(a)
3 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_1(a)
4 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_2(a)
5 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_3(a)
6 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_4(a)
7 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_5(a)
8 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_6(a)
9 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_7(a)
10 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_8(a)
11 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)
12 P4/mbm[0,0,0]GM4+(a)[W2:i:rot]A'(a)
13 P4/mbm[1/2,1/2,0]M2-M3-(a,b)[W2:i:rot]A'(a)
14 P4/mbm[1/2,1/2,0]M2-M3-(a,b)[W2:i:rot]A'(b)

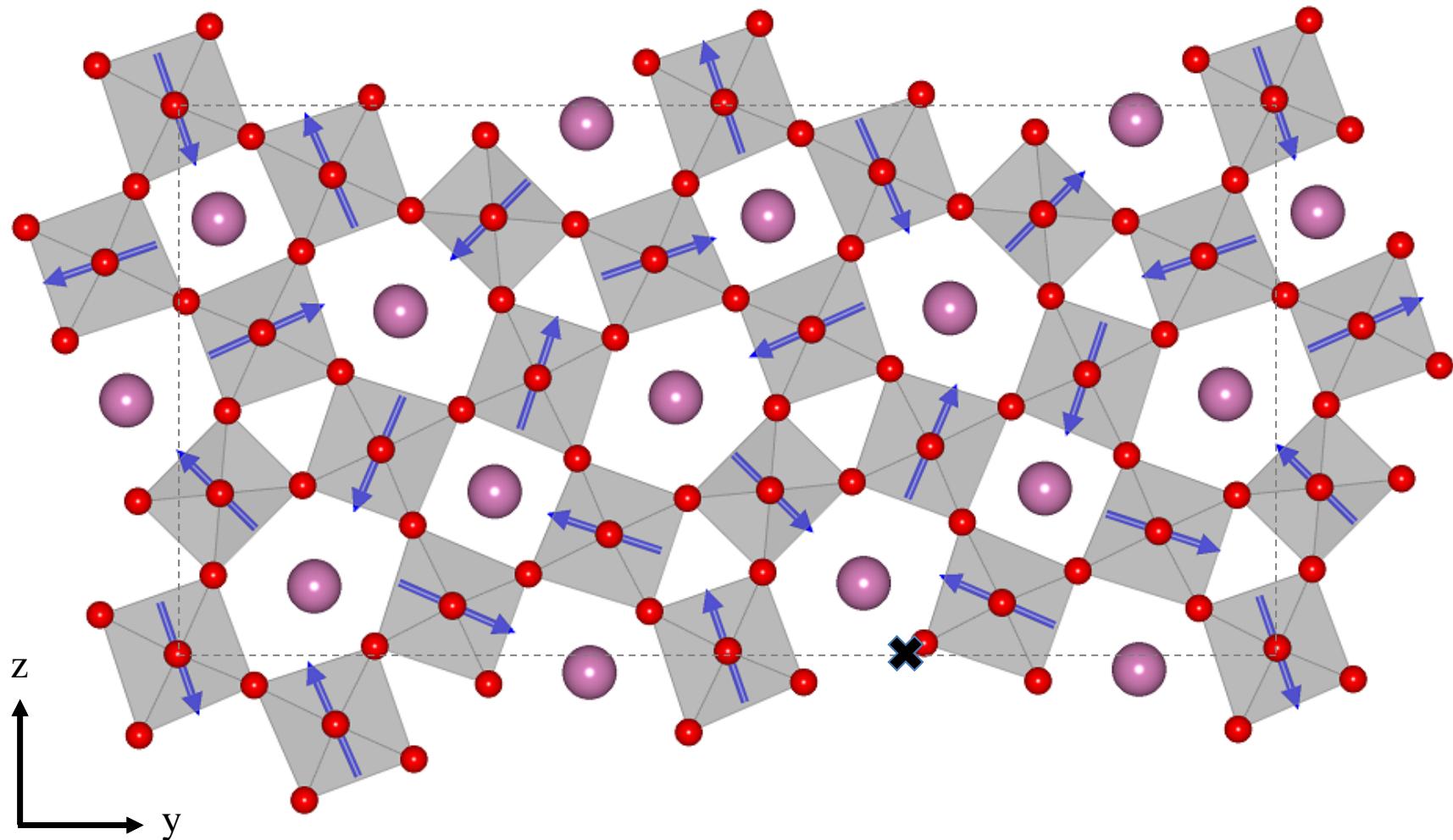
Independent modes:

10 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_8(a)

Dependent modes:

1 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W1:d:rot]B3g(a) a[1] -> 2.21973 a[10]
2 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W1:d:rot]B2g(a) a[2] -> 0.00282 a[10]
3 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_1(a) a[3] -> -0.75406 a[10]
4 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_2(a) a[4] -> 2.27257 a[10]
5 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_3(a) a[5] -> 0.75645 a[10]
6 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_4(a) a[6] -> -2.27257 a[10]
7 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_5(a) a[7] -> -2.25738 a[10]
8 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_6(a) a[8] -> -0.98730 a[10]
9 P4/mbm[0,1/2,1/2]R1(a,-a,-a,a)[W2:i:rot]A''_7(a) a[9] -> 2.24798 a[10]

TTB R1 P4(0,0,a,0)



Dashed box is shifted in plane relative to standard cell origin (indicated by black "x").

TTB R1 P4(0,0,a,0)

36 Cmc2_1, basis={(0,0,2),(2,0,0),(0,1,0)}, origin=(3/4,0,1/2), s=2, i=8,
k-active= (1/2,0,1/2)
Amplitudes = 15, SADPs = 60, Equations = 60 X 2 = 120, Variables = 60 + 15 = 75

All modes:

1 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W1:d:rot]B3g(a)
2 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W1:d:rot]B2g(a)
3 P4/mbm[0,0,0]GM2+(a)[W1:d:rot]B1g(a)
4 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_1(a)
5 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_2(a)
6 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_3(a)
7 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_4(a)
8 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_5(a)
9 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_6(a)
10 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_7(a)
11 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_8(a)
12 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)
13 P4/mbm[0,0,0]GM2+(a)[W2:i:rot]A'(a)
14 P4/mbm[0,0,0]GM5-(0,a)[W2:i:rot]A'_1(a)
15 P4/mbm[0,0,0]GM5-(0,a)[W2:i:rot]A'_2(a)

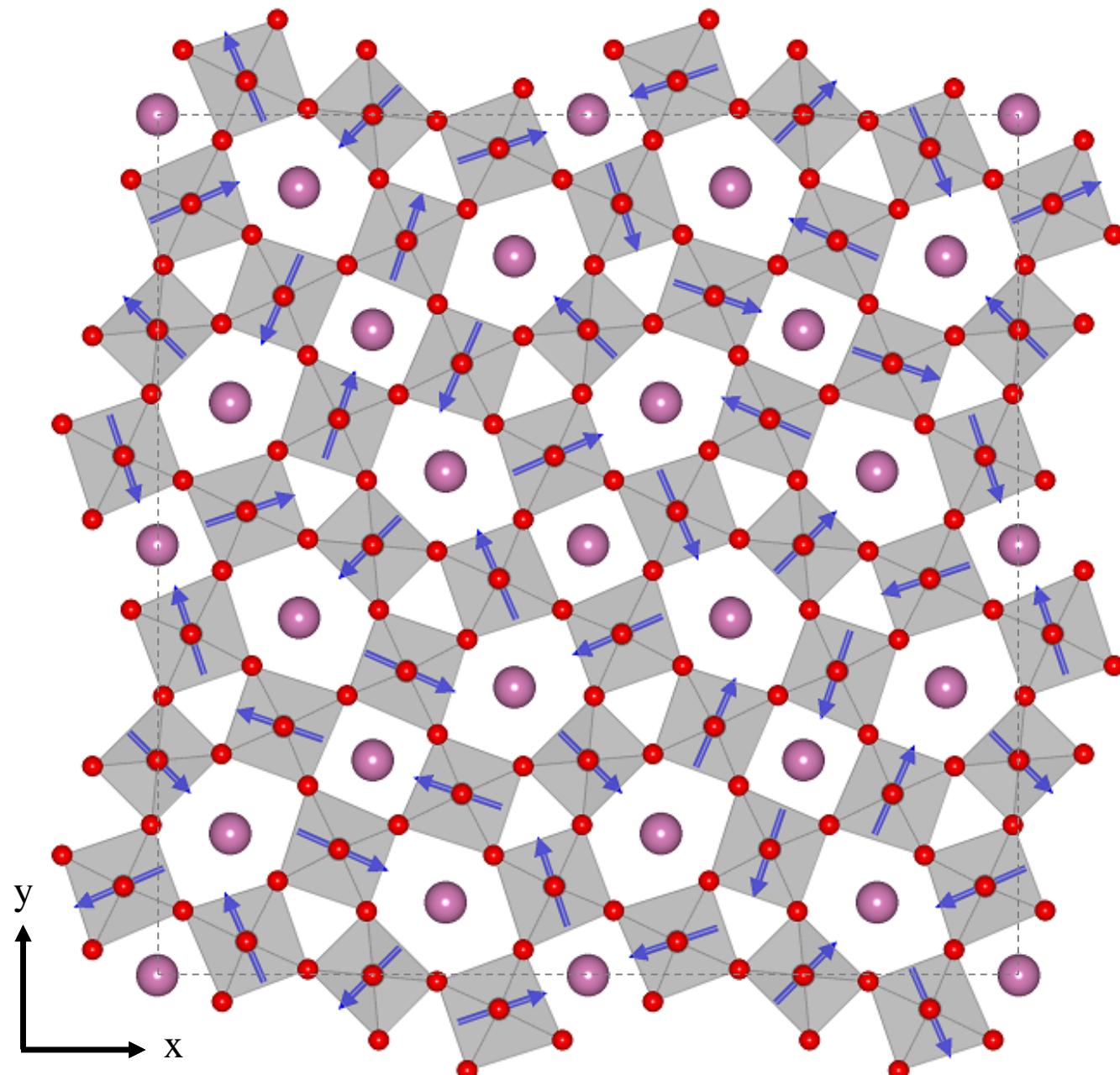
Independent modes:

11 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_8(a)

Dependent modes:

1 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W1:d:rot]B3g(a) a[1] -> 2.21003 a[11]
2 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W1:d:rot]B2g(a) a[2] -> 0.00297 a[11]
4 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_1(a) a[4] -> -0.75065 a[11]
5 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_2(a) a[5] -> 2.25714 a[11]
6 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_3(a) a[6] -> 0.75610 a[11]
7 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_4(a) a[7] -> -2.26147 a[11]
8 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_5(a) a[8] -> -2.25061 a[11]
9 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_6(a) a[9] -> -0.97909 a[11]
10 P4/mbm[0,1/2,1/2]R1(0,0,a,0)[W2:i:rot]A''_7(a) a[10] -> 2.23344 a[11]

TTB R1 P5($a, a, -a, a$)



```

TTB R1 P5(a,a,-a,a)
87 I4/m, basis={(2,0,0),(0,2,0),(0,0,2)}, origin=(1/2,3/2,1/2), s=4, i=8,
k-active= (0,1/2,1/2),(1/2,0,1/2)
Amplitudes = 15, SADPs = 60, Equations = 60 X 2 = 120, Variables = 60 + 15 = 75

```

All modes:

```

1 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W1:d:rot]B3g(a)
2 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W1:d:rot]B2g(a)
3 P4/mbm[0,0,0]GM3+(a)[W1:d:rot]B1g(a)
4 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_1(a)
5 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_2(a)
6 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_3(a)
7 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_4(a)
8 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_5(a)
9 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_6(a)
10 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_7(a)
11 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_8(a)
12 P4/mbm[0,0,0]GM1+(a)[W2:i:rot]A'(a)
13 P4/mbm[0,0,0]GM3+(a)[W2:i:rot]A'(a)
14 P4/mbm[1/2,1/2,0]M5+(a,0)[W2:i:rot]A'_1(a)
15 P4/mbm[1/2,1/2,0]M5+(a,0)[W2:i:rot]A'_2(a)

```

Independent modes:

```
11 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_8(a)
```

Dependent modes:

1 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W1:d:rot]B3g(a)	a[1] -> 2.21023 a[11]
2 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W1:d:rot]B2g(a)	a[2] -> 0.00297 a[11]
4 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_1(a)	a[4] -> -0.75065 a[11]
5 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_2(a)	a[5] -> 2.25714 a[11]
6 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_3(a)	a[6] -> 0.75592 a[11]
7 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_4(a)	a[7] -> -2.26092 a[11]
8 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_5(a)	a[8] -> -2.25007 a[11]
9 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_6(a)	a[9] -> -0.97886 a[11]
10 P4/mbm[0,1/2,1/2]R1(a,a,-a,a)[W2:i:rot]A''_7(a)	a[10] -> 2.23344 a[11]