Group theoretical analysis of structural instability, vacancy ordering and magnetic transitions in the system troilite (FeS) – pyrrhotite (Fe1−xS)

Charles Robert Sebastian Haines, Christopher J. Howard, Richard J. Harrison and Michael A. Carpenter
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 Supplementary Material

S1. Tables in full

S1.1. 4C

S1.1.1. 4C U₁ (1/2,0,1/4)

Table S1 Order parameter components and unit cell configurations for subgroups of P6/mmc which can arise from phase transitions in which irrep U₁(1/2,0,1/4) is the active representation. SGN = space group number.

| SGN | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-----|-------------|----------|------------|---------------|--------|
| 12  | C2/m        | P1       | (a,0,0,0,0,0) | (2,1,-4),(0,1,0),(2,1,0) | (0,0,0) |
| 44  | Immm        | P2       | (a,-0.414a,0,0,0,0) | (0,0,4),(0,1,0),(2,-1,0) | (-7/8,1/16,-7/4) |
| 12  | C2/m        | P3       | (a,0,a,0,0,0) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 15  | C2/c        | P4       | (a,0,0,a,0,0) | (2,-2,0),(2,2,0),(-1,1,2) | (0,1/2,0) |
| 42  | Fmmm        | P5       | (a,-0.414a,0.414a,0.414a,0,0) | (0,0,4),(2,2,0),(-2,0) | (-1/8,1/8,1/4) |
| 43  | Fdd2        | P6       | (a,-0.414a,0.414a,0.414a,0,0) | (0,0,4),(2,2,0),(-2,0) | (-7/8,7/8,7/4) |
| 164 | P̅̅̅3m1      | P7       | (a,0,a,0,a) | (2,0,0),(0,2,0),(0,0,4) | (0,0,0) |
| 187 | P̅̅̅6m2      | P8       | (a,-0.414a,a,-0.414a,a,-0.414a) | (0,-2,0),(2,2,0),(0,0,4) | (0,0,1/4) |
| 8   | Cm          | C1       | (a,b,0,0,0,0) | (2,1,-4),(0,1,0),(2,1,0) | (0,0,0) |
| 5   | C2          | C2       | (a,b,a,-b,0,0) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 5   | C2          | C3       | (a,b,0.707a,0.707b,-0.707a,0.707b,0,0) | (2,2,0),(-2,2,0),(1,1,2) | (1/8,15/8,1/4) |
| 2   | P̅1         | C4       | (a,0,b,0,0,0) | (1,1,2),(0,2,0),(-2,0) | (0,0,0) |
| 2   | P̅1         | C5       | (a,0,0,b,0,0) | (1,1,2),(0,2,0),(-2,0) | (0,1/2,0) |
| 8   | Cm          | C6       | (a,-0.414a,b,-0.414b,0,0) | (-2,-2,0),(0,0,4),(-2,0) | (-1/8,-1/8,1/4) |

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S1.1.2. 4C $m\Gamma ^+_{4}$ with $U_1$

Table S2  Magnetic subgroups arising from coupling of irreps $m\Gamma ^+_{4}$ and $U_{1}(1/2,0,1/4)$, with respect to the parent space group $P6_3/mmc$. SGN.M = magnetic space group number.

| SGN.M | Space Group | OPD Name | $U_{1}(1/2,0,1/4)$ | OPD Vector | Vector | Origin |
|-------|-------------|----------|-------------------|------------|--------|--------|
| 12.62 | $C2/m'$    | P1(1)P1(1) | (a,0,0,0,0,0),(b) | (2,1,-4),(0,1,0),(2,1,0) | | |
| Volume   | Space Group | Symbol | Lattice Parameters | Final Coordinates | Final Unit Cell |
|----------|-------------|--------|--------------------|-------------------|----------------|
| 44.232   | Im'm'2      | P2(1)P1(1) | (a,-0.414a,0,0,0,0),(b) | (0,0.4),(0,1.0),(-2,-1,0) | (-7/8,1/16,-7/4) |
| 12.62    | C2'im'     | P3(1)P1(1) | (a,0,a,0,0,0),(b) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 15.89    | C2'ic'     | P4(1)P1(1) | (a,0,0,a,0,0),(b) | (2,-2,0),(2,2,0),(-1,1,2) | (0,1/2,0) |
| 42.222   | Fm'm'2     | P5(1)P1(1) | (a,-0.414a,-0.414a,0,0,0),(b) | (0,0.4),(2,2,0),(-2,2,0) | (-1/8,1/8,1/4) |
| 43.227   | Fd'd'2     | P6(1)P1(1) | (a,-0.414a,0.414a,a,0,0),(b) | (0,0.4),(2,2,0),(-2,2,0) | (-7/8,7/8,7/4) |
| 164.89   | P3m'1      | P7(1)P1(1) | (a,0,a,0,a,0),(b) | (0,-2,0),(2,2,0),(0,0,4) | (0,0,0) |
| 187.211  | P6m'2      | P8(1)P1(1) | (a,-0.414a,a,-0.414a,a,-0.414a),(b) | (2,2,0),(-2,0,0),(0,0,4) | (0,0,1/4) |
| 8.34     | Cm'        | C1(1)P1(1) | (a,b,0,0,0,0),(c) | (2,1,-4),(0,1,0),(2,1,0) | (0,0,0) |
| 5.15     | C2'        | C2(1)P1(1) | (a,b,a,-b,0,0),(c) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 5.13     | C2         | C3(1)P1(1) | (a,b,0.707a-0.707b,-0.707a-0.707b,0,0),(c) | (2,2,0),(-2,2,0),(1,1,2) | (1/8,15/8,1/4) |
| 2.4      | Pı         | C4(1)P1(1) | (a,0,b,0,0,0),(c) | (1,1,2),(0,2,0),(-2,0,0) | (0,0,0) |
| 2.4      | Pı         | C5(1)P1(1) | (a,0,0,b,0,0),(c) | (1,1,2),(0,2,0),(-2,0,0) | (0,1/2,0) |
| 8.34     | Cm'        | C6(1)P1(1) | (a,-0.414a,b,-0.414b,0,0),(c) | (-2,-2,0),(0,0,4),(-2,2,0) | (-1/8,-1/8,1/4) |
| 9.39     | Cc'        | C7(1)P1(1) | (a,-0.414a,b,2.414b,0,0),(c) | (-2,-2,0),(0,0,4),(-2,2,0) | (-5/8,-5/8,5/4) |
| 8.34     | Cm'        | C8(1)P1(1) | (a,b,a,b,0,0),(c) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 9.39     | Cc'        | C9(1)P1(1) | (a,b,b,-a,0,0),(c) | (2,-2,0),(2,2,0),(-1,1,2) | (3/2,0,0) |
| 156.51   | P3m'1      | C10(1)P1(1) | (a,b,a,b,a,b),(c) | (0,-2,0),(2,2,0),(0,0,4) | (0,0,0) |
S1.1.3. 4C mΓ₅⁺ and \( U_1 \)

Table S3  Magnetic subgroups arising from coupling of irreps \( m\Gamma_1^5 \) and \( U_1(1/2,0,1/4) \), with respect to the parent space group \( P6_3/mmc \).

| SGN.M Group | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-------------|-------------|----------|------------|---------------|--------|
|             |             | \( U_1(1/2,0,1/4) \) | \( m\Gamma_1^5 \) | \( U_1(1/2,0,1/4) \) | \( m\Gamma_1^5 \) |

- \( C2'/m' \) C11(1)P1(1) (a,0,b,0,a,0),(c) (-2,-4,0),(2,0,0),(0,0,4) (0,0,0)
- \( C2'/m' \) C12(1)P1(1) (0,a,b,0,-a),(c) (-2,-4,0),(2,0,0),(0,0,4) (1/2,0,0)
- \( Anm'2 \) C13(1)P1(1) (a,-0.414a,b,-0.414b,b,-0.414b),(c) (0,0.4),(0,2,0),(-4,-2,0) (0,0,1/4)
- \( Abm'2 \) C14(1)P1(1) (a,-0.414a,b,2.414b,-2.414b),(c) (0,0.4),(0,2,0),(-4,-2,0) (0,0,1/4)
- \( C2' \) S1(1)P1(1) (a,b,c,0,-a-b),(d) (-2,-4,0),(2,0,0),(0,0,4) (0,0,0)
- \( C2 \) S2(1)P1(1) (a,-0.414a,b,c,0.707b,-0.707c,-0.707c),(d) (0,-2,0),(4,2,0),(0,0,4) (0,0,1/4)
- \( \bar{P} \bar{I} \) S3(1)P1(1) (a,0,b,0,c,0),(d) (0,0.4),(0,2,0),(-4,-2,0) (0,0,0)
- \( \bar{P} \bar{I} \) S4(1)P1(1) (a,0,0,b,0,c),(d) (0,0.4),(0,2,0),(-4,-2,0) (0,1/2,0)
- \( Pm' \) S5(1)P1(1) (a,-0.414a,b,-0.414b,c,-0.414c),(d) (-2,0,0),(0,0.4),(0,2,0) (0,0,1/4)
- \( Pc' \) S6(1)P1(1) (a,-0.414a,b,2.414b,c,2.414c),(d) (-2,0,0),(0,0.4),(0,2,0) (0,0,1/4)
- \( P1 \) 4D1(1)P1(1) (a,b,c,d,0,0),(e) (1,1,2),(0,2,0),(-4,0) (0,0,0)
- \( Cm' \) 4D2(1)P1(1) (a,b,c,d,a,b),(e) (-2,-4,0),(2,0,0),(0,0,4) (0,0,0)
- \( P1 \) 6D1(1)P1(1) (a,b,c,d,e,f),(g) (0,0.4),(0,2,0),(-4,-2,0) (0,0,0)
| No.  | Space Group | Symbol | Transformation  | Basis Parameters  | Symmetry Parameters |
|------|-------------|--------|-----------------|-------------------|---------------------|
| 12.58 | C2/m        | P1(1)P1(1) | (a,0,0,0,0,0),(b,-1.732b) | (2,1,-4),(0,1,0),(2,1,0) | (0,0,0) |
| 44.229 | Imm2      | P2(1)P1(1) | (a,-0.414a,0,0,0,0),(b,-1.732b) | (0,1,0),(0,0,4),(2,1,0) | (0,0,1/4) |
| 12.58 | C2/m        | P3(1)P1(3) | (a,0,a,0,0,0),(b,1.732b) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 15.85 | C2/c        | P4(1)P1(3) | (a,0,0,a,0,0),(b,1.732b) | (2,-2,0),(2,2,0),(-1,1,2) | (0,1/2,0) |
| 42.219 | Fmm2      | P5(1)P1(3) | (a,-0.414a,a,-0.414a,0,0),(b,1.732b) | (2,2,0),(0,0,4),(2,-2,0) | (1/8,-1/8,1/4) |
| 43.224 | Fdd2      | P6(1)P1(3) | (a,-0.414a,0.414a,a,0,0),(b,1.732b) | (2,2,0),(0,0,4),(2,-2,0) | (11/8,-3/8,3/4) |
| 8.32  | Cm          | C1(1)P1(1) | (a,b,0,0,0,0),(c,-1.732c) | (2,1,-4),(0,1,0),(2,1,0) | (0,0,0) |
| 5.13  | C2          | C2(1)P1(3) | (a,b,a,-b,0,0),(c,1.732c) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 5.13  | C2          | C3(1)P1(3) | (a,b,0.707a-0.707b,-0.707a-0.707b,0,0),(c,1.732c) | (2,2,0),(2,2,0),(-1,1,2) | (1/8,15/8,1/4) |
| 8.32  | Cm          | C8(1)P1(3) | (a,b,a,b,0,0),(c,1.732c) | (2,-2,0),(2,2,0),(-1,1,2) | (0,0,0) |
| 9.37  | Cc          | C9(1)P1(3) | (a,b,-a,0,0),(c,1.732c) | (2,-2,0),(2,2,0),(-1,1,2) | (3/2,0,0) |
| 12.58 | C2/m        | C11(1)P1(2) | (a,0,b,0,a,0),(-2c,0) | (-2,-4),(2,0,0),(0,0,4) | (0,0,0) |
| 12.58 | C2/m        | C12(1)P1(2) | (0,a,b,0,-a),(-2c,0) | (-2,-4),(2,0,0),(0,0,4) | (1/2,0,0) |
| 38.187 | Amm2      | C13(1)P1(1) | (a,-0.414a,b,-0.414b,b,-0.414b),(c,-1.732c) | (0,0,4),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 39.195 | Abm2      | C14(1)P1(1) | (a,-0.414a,b,2.414b,-b,2.414b),(c,-1.732c) | (0,0,4),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 5.13  | C2          | S1(1)P1(2) | (a,b,c,0,a,-b),(-2d,0) | (-2,-4),(2,0,0),(0,0,4) | (0,0,0) |
| 5.13  | C2          | S2(1)P1(1) | (a,-0.414a,b,c,0.707b-0.707c,-0.707b-0.707c),(d,-1.732d) | (0,-2),(4,2,0),(0,0,4) | (0,0,1/4) |
| Volume | Space Group | Structure Details |
|--------|-------------|------------------|
| 8.32   | Cm          | 4D2(1)P1(2)      |
|        |             | (a,b,c,d,a,b),(−2c,0) |
|        |             | (−2,−4,0),(2,0,0),(0,0,4) |
| 12.62  | C2'/m'     | P1(1)P2(1)       |
|        |             | (a,0,0,0,0,0),(b,0.577b) |
|        |             | (2,1,−4),(0,1,0),(2,1,0) |
| 44.231 | Im'm2'     | P2(1)P2(1)       |
|        |             | (−a,−0.414a,0,0,0,0),(b,0.577b) |
|        |             | (0,1,0),(0,0,4),(2,1,0) |
| 12.62  | C2'/m'     | P3(1)P2(3)       |
|        |             | (a,0,a,0,0,0),(−b,0.577b) |
|        |             | (−2,−2,0),(2,2,0), (−1,1,2) |
| 15.89  | C2'/c'     | P4(1)P2(3)       |
|        |             | (a,0,a,0,0,0),(−b,0.577b) |
|        |             | (−2,−2,0),(2,2,0), (−1,1,2) |
| 42.221 | Fm'm2'     | P5(1)P2(3)       |
|        |             | (−a,−0.414a,a,−0.414a,0,0,0),(−b,0.577b) |
|        |             | (2,2,0),(0,0,4),(2,−2,0) |
| 43.226 | Fd'd2'     | P6(1)P2(3)       |
|        |             | (−a,−0.414a,0.414a,a,0,0),(−b,0.577b) |
|        |             | (2,2,0),(0,0,4),(2,−2,0) |
| 8.34   | Cm'        | C1(1)P2(1)       |
|        |             | (a,b,0,0,0,0),(c,0.577c) |
|        |             | (2,1,−4),(0,1,0),(2,1,0) |
| 5.15   | C2'        | C2(1)P2(3)       |
|        |             | (a,b,a,−b,0,0),(−c,0.577c) |
|        |             | (2,−2,0),(2,2,0), (−1,1,2) |
| 5.15   | C2'        | C3(1)P2(3)       |
|        |             | (a,b,0.707a−0.707b,−0.707a+0.707b,0,0),(−c,0.577c) |
|        |             | (2,2,0),(−2,2,0),(1,1,2) |
| 8.34   | Cm'        | C8(1)P2(3)       |
|        |             | (a,b,a,b,0,0),(−c,0.577c) |
|        |             | (2,−2,0),(2,2,0), (−1,1,2) |
| 9.39   | Cc'        | C9(1)P2(3)       |
|        |             | (a,b,b,−a,0,0),(−c,0.577c) |
|        |             | (2,−2,0),(2,2,0), (−1,1,2) |
| 12.62  | C2'/m'     | C11(1)P2(2)      |
|        |             | (a,0,b,0,a,0),(−b,0,−1.155c) |
|        |             | (−2,−4,0),(2,0,0),(0,0,4) |
| 12.62  | C2'/m'     | C12(1)P2(2)      |
|        |             | (0,a,b,0,0,−a),(−b,0,−1.155c) |
|        |             | (−2,−4,0),(2,0,0),(0,0,4) |
| 38.19  | Amm'2'     | C13(1)P2(1)      |
|        |             | (a,−0.414a,b−0.414b,b,−0.414b),(c,0.577c) |
|        |             | (0,0,4),(0,2,0),(−4,−2,0) |
| 39.198 | Abm'2'     | C14(1)P2(1)      |
|        |             | (a,−0.414a,b,2.414b,−b,−2.414b),(c,0.577c) |
|        |             | (0,0,4),(0,2,0),(−4,−2,0) |
| 5.15   | C2'        | S1(1)P2(2)       |
|        |             | (a,b,c,0,a,−b),(0,−1.155d) |
|        |             | (−2,−4,0),(2,0,0),(0,0,4) |
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|--------------------------------|-----------------|
| 5.15 C2' S2(1)P2(1) | (a,-0.414a,b,c,0.707b-0.707c,-0.707b-0.707c),(d,0,0,0,0,0) (0,0,0,0,0,0) |
| 8.34 Cm' 4D2(1)P2(2) | (a,b,c,d,a,b),(0,-1.155e) (-2,-4,0),(2,0,0),(0,0,0) |
| 2.4 P1 | P1(1)C1(1) | (a,0,0,0,0,0),(b,c) (1,0,2),(0,1,0),(-2,0,0) |
| 8.32 Cm | P2(1)C1(1) | (a,-0.414a,0,0,0,0),(b,c) (-2,0),(0,0,0,0,0,0) |
| 1.1 P1 | C1(1)C1(1) | (a,b,0,0,0,0),(c,d) (1,0,2),(0,1,0),(-2,0,0) |
| 2.4 P1 | C4(1)C1(1) | (a,0,b,0,0,0),(c,d) (1,1,2),(0,2,0),(-2,0,0) |
| 2.4 P1 | C5(1)C1(1) | (a,0,0,b,0,0),(c,d) (1,1,2),(0,2,0),(-2,0,0) |
| 8.32 Cm | C6(1)C1(1) | (a,-0.414a,b,-0.414b,0,0),(c,d) (-2,-2),(0,0,0,0) (-1/8,1/4) |
| 9.37 Cc | C7(1)C1(1) | (a,-0.414a,b,2.414b,0,0),(c,d) (-2,-2),(0,0,0,0) (-5/8,1/4) |
| 2.4 P1 | S3(1)C1(1) | (a,0,b,0,c,0),(d,e) (0,0,2),(0,0,0) |
| 2.4 P1 | S4(1)C1(1) | (a,0,0,b,0,c),(d,e) (0,0,2),(0,0,0) |
| 6.18 Pm | S5(1)C1(1) | (a,-0.414a,b,-0.414b,c,-0.414c),(d,e) (-2,0),(0,0,0,0) |
| 7.24 Pc | S6(1)C1(1) | (a,-0.414a,b,2.414b,c,2.414c),(d,e) (-2,0),(0,0,0,0) |
| 1.1 P1 | 4D1(1)C1(1) | (a,b,c,d,0,0),(e,f) (1,1,2),(0,2,0),(-2,0,0) |
| 1.1 P1 | 6D1(1)C1(1) | (a,b,c,d,e,f),(g,h) (0,0,4),(0,2,0),(-2,0,0) |

S2. 5C

S2.1. U₁
Table S4  Order parameter components and unit cell configurations for subgroups of \( P6_3/mmc \) which can arise from phase transitions in which irrep \( U_1(1/2,0,1/5) \) is the active representation.

| SGN | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin       |
|-----|-------------|----------|------------|---------------|--------------|
| 58  | \( Pnmm \)  | P1       | (a,0,0,0,0,0) | (0,0,5),(2,1,0),(0,1,0) | (0,0,0)      |
| 59  | \( Pmmm \)  | P2       | (0,a,0,0,0,0) | (0,0,5),(0,-1,0),(2,1,0) | (1/2,1/2,0) |
| 164 | \( P\bar{3}m1 \) | P3       | (a,0,a,0,a,0) | (2,0,0),(0,2,0),(0,0,5) | (0,0,0)      |
| 187 | \( P\bar{6}m2 \) | P4       | (0,a,0,0,0,0) | (0,-2,0),(2,2,0),(0,0,5) | (0,0,1/4)    |
| 64  | \( Cmca \)  | P5       | (a,0,0,a,0) | (2,0,0),(2,4,0),(0,0,5) | (0,0,0)      |
| 63  | \( Cmcm \)  | P6       | (0,a,0,0,-a) | (2,0,0),(2,4,0),(0,0,5) | (1/2,0,0)    |
| 31  | \( Pmn2_1 \) | C1       | (0,b,0,0,0,0) | (0,-1,0),(2,1,0),(0,0,5) | (1/2,1/4,0) |
| 156 | \( P3m1 \)  | C2       | (a,b,a,b,a,b) | (2,0,0),(0,2,0),(0,0,5) | (0,0,0)      |
| 20  | \( C22_1 \)  | C3       | (a,b,0,a,b) | (2,0,0),(2,4,0),(0,0,5) | (1/2,0,0)    |
| 14  | \( P2_{1/c} \) | C4       | (0,a,0,a,b,0) | (-2,0,0),(0,0,5),(2,0,0) | (0,0,0)      |
| 11  | \( P2_{1/m} \) | C5       | (0,0,0,a,0,b) | (-2,0,0),(0,0,5),(0,2,0) | (0,1/2,0)    |
| 14  | \( P2_{1/c} \) | C6       | (a,0,0,0,0,b) | (-2,0,0),(0,0,5),(2,2,0) | (0,1/2,0)    |
| 12  | \( C2/m \)  | C7       | (a,0,b,0,a,0) | (-2,-4,0),(2,0,0),(0,0,5) | (0,0,0)      |
| 12  | \( C2/m \)  | C8       | (0,a,b,0,0,-a) | (-2,-4,0),(2,0,0),(0,0,5) | (1/2,0,0)    |
| 38  | \( Amm_2 \)  | C9       | (a,-0.325a,b,-0.325b,b,-0.325b) | (0,0,5),(0,2,0),(-4,-2,0) | (0,0,1/4)    |
| 39  | \( Abm_2 \)  | C10      | (a,-0.325a,b,3.078b,-b,-3.078b) | (0,0,5),(0,2,0),(-4,-2,0) | (0,0,1/4)    |
| 36  | \( Cmcm_2 \) | C11      | (a,b,0,0,a,b) | (2,0,0),(2,4,0),(0,0,5) | (1/2,-1,0)   |
| 5   | \( C2 \)    | S1       | (a,b,c,0,a,b) | (-2,-4,0),(2,0,0),(0,0,5) | (0,0,0)      |
| 5   | \( C2 \)    | S2       | (a,-0.325a,b,c,0.809b-0.325b,-0.588c,-0.588b-0.809c) | (0,-2,0),(4,2,0),(0,0,5) | (0,0,1/4)    |
| 2   | \( P\bar{T} \) | S3       | (a,0,b,0,c,0) | (0,0,5),(0,2,0),(-2,0,0) | (0,0,0)      |
| 2   | \( P\bar{T} \) | S4       | (a,0,0,b,0,c) | (0,0,5),(0,2,0),(-2,0,0) | (0,1/2,0)    |
| 6   | \( Pm \)    | S5       | (a,-0.325a,b,-0.325b,c,-0.325c) | (-2,0,0),(0,0,5),(0,2,0) | (0,0,1/4)    |
S2.2. $U_1$ and $m\Gamma_4^+$

Table S5  Magnetic subgroups arising from coupling of irreps $m\Gamma_4^+$ and $U_1(1/2,0,1/5)$, with respect to the parent space group $P6_3/mmc$.

| SGN.M | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-------|-------------|----------|------------|---------------|--------|
| 58.398 | $Pm'nm'$ | P1(1)P1(1) | (a,0,0,0,0,0),(b) | (-2,-1,0),(0,0,5),(0,1,0) | (0,0,0) |
| 59.409 | $Pm'm'n$ | P2(1)P1(1) | (0,a,0,0,0,0),(b) | (0,0,5),(0,-1,0),(2,1,0) | (1/2,1/2,0) |
| 164.89 | $P\bar{3}m1$ | P3(1)P1(1) | (a,0,a,0,a,0),(b) | (0,-2,0),(2,2,0),(0,0,5) | (0,0,0) |
| 187.211 | $P\bar{6}m2$ | P4(1)P1(1) | 0.325a,(b) | (2,2,0),(-2,0,0),(0,0,5) | (0,0,1/4) |
| 64.476 | $Cm'ca'$ | P5(1)P1(1) | (a,0,0,a,0,0),(b) | (2,0,0),(2,4,0),(0,0,5) | (0,0,0) |
| 63.464 | $Cm'cm'$ | P6(1)P1(1) | (0,a,0,0,-a),(b) | (2,0,0),(2,4,0),(0,0,5) | (1/2,0,0) |
| 31.125 | $Pm'n2_1$ | C1(1)P1(1) | (a,b,0,0,0,0),(c) | (0,-1,0),(2,1,0),(0,0,5) | (1/2,1/4,0) |
| 156.51 | $P3m1$ | C2(1)P1(1) | (a,b,a,b,a,b),(c) | (0,-2,0),(2,2,0),(0,0,5) | (0,0,0) |
| 20.34 | $C22'2_1$ | C3(1)P1(1) | (a,b,0,0,a,-b),(c) | (2,4,0),(-2,0,0),(0,0,5) | (3/2,2,5/4) |
| 14.79 | $P2_1'/c'$ | C4(1)P1(1) | (0,0,0,a,b,0),(c) | (-2,0,0),(0,0,5),(0,2,0) | (0,0,0) |
| 11.54 | $P2_1'/m'$ | C5(1)P1(1) | (0,0,0,a,0,b),(c) | (-2,0,0),(0,0,5),(0,2,0) | (0,1/2,0) |
| 14.79 | $P2_1'/c'$ | C6(1)P1(1) | (a,0,0,0,0,b),(c) | (-2,0,0),(0,0,5),(2,2,0) | (0,1/2,0) |
### S2.3. $U_1$ and $m\Gamma_5^+$

**Table S6** Magnetic subgroups arising from coupling of irreps $m\Gamma_5^+$ and $U_1(1/2,0,1/5)$, with respect to the parent space group $P6_3/mmc$.

| SGN.M | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-------|-------------|----------|------------|---------------|--------|
|       |             | $U_1(1/2,0,1/5)$ | $m\Gamma_5^+$ |             |        |
| 58.393 | $Pmmm$     | P1(1)P1(1) | (a,0,0,0,0,0),(b,-1.732b) | (-2,-1,0),(0,0,5),(0,1,0) | (0,0,0) |
| 59.405 | $Pmmm$     | P2(1)P1(1) | (0,0,0,0,0,0),(b,-1.732b) | (0,1,0),(0,0,5),(2,1,0) | (1/2,0,0) |
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 64.469 | Cmca | P5(1)P1(2) | (a,0,0,0,a,0),(-2b,0) | (2,0,0),(2,4,0),(0,0,5) | (0,0,0) |
| 63.457 | Cmcm | P6(1)P1(2) | (0,a,0,0,-a),(-2b,0) | (2,0,0),(2,4,0),(0,0,5) | (1/2,0,0) |
| 31.123 | Pmn21 | C1(1)P1(1) | (a,b,0,0,0,0),(c,-1.732c) | (0,-1,0),(2,1,0),(0,0,5) | (1/2,1/4,0) |
| 20.31 | C221 | C3(1)P1(2) | (a,b,0,0,-a,b),(-2c,0) | (2,0,0),(2,4,0),(0,0,5) | (1/2,0,0) |
| 12.58 | C2/m | C7(1)P1(2) | (a,0,b,0,a,0),(-2c,0) | (-2,-4,0),(2,0,0),(0,0,5) | (0,0,0) |
| 12.58 | C2/m | C8(1)P1(2) | (0,a,b,0,0,-a),(-2c,0) | (-2,-4,0),(2,0,0),(0,0,5) | (1/2,0,0) |
| 38.187 | Amm2 | C9(1)P1(1) | (a,-0.325a,b,-0.325b,b,0.325b),(c,-1.732c) | (0,0,5),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 39.195 | Abm2 | C10(1)P1(1) | (a,-0.325a,b,3.078b,-b,3.078b),(c,-1.732c) | (0,0,5),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 36.172 | Cm21 | C11(1)P1(2) | (a,b,0,0,a,0),(-2c,0) | (2,0,0),(2,4,0),(0,0,5) | (1/2,-1,0) |
| 5.13 | C2 | S1(1)P1(2) | (a,b,c,0,-a,b),(-2d,0) | (-2,-4,0),(2,0,0),(0,0,5) | (0,0,0) |
| 5.13 | C2 | S2(1)P1(1) | (a,-0.325a,b,c,0.809b,-0.588c,-0.588b-0.809c),(d,-1.732d) | (0,-2,0),(4,2,0),(0,0,5) | (0,0,1/4) |
| 8.32 | Cm | 4D2(1)P1(2) | (a,b,c,d,a,b),(-2e,0) | (-2,-4,0),(2,0,0),(0,0,5) | (0,0,0) |
| 58.398 | Pmm'n' | P1(1)P2(1) | (a,0,0,0,0,0),(b,0.577b) | (0,0,5),(2,1,0),(0,1,0) | (0,0,0) |
| 59.41 | Pmm'n' | P2(1)P2(1) | (0,a,0,0,0,0),(b,0.577b) | (0,0,5),(0,-1,0),(2,1,0) | (1/2,1/2,0) |
| 64.474 | Cm'c'a | P5(1)P2(2) | (a,0,0,0,a,0),(0,-1.155b) | (2,0,0),(2,4,0),(0,0,5) | (0,0,0) |
| 63.462 | Cm'c'm | P6(1)P2(2) | (0,a,0,0,0,-a),(0,-1.155b) | (2,0,0),(2,4,0),(0,0,5) | (1/2,0,0) |
| 31.127 | Pmn'n'21 | C1(1)P2(1) | (a,b,0,0,0,0),(c,0.577c) | (0,-1,0),(2,1,0),(0,0,5) | (1/2,1/4,0) |
| 20.33 | C2'21 | C3(1)P2(2) | (a,b,0,0,-a,b),(0,-1.155c) | (2,0,0),(2,4,0),(0,0,5) | (1/2,0,0) |
| 12.62 | C2'/m' | C7(1)P2(2) | (a,0,b,0,a,0),(-1.155c) | (-2,-4,0),(2,0,0),(0,0,5) | (0,0,0) |
| 12.62 | C2'/m' | C8(1)P2(2) | (0,a,b,0,0,-a),(0,-1.155c) | (-2,-4,0),(2,0,0),(0,0,5) | (1/2,0,0) |
| 38.19 | Amm2' | C9(1)P2(1) | (a,-0.325a,b,-0.325b,b,0.325b),(c,0.577c) | (0,0,5),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 39.198 | Abm2' | C10(1)P2(1) | (a,-0.325a,b,3.078b,-b,3.078b),(c,0.577c) | (0,0,5),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 36.176 | Cm'c'21 | C11(1)P2(2) | (a,b,0,0,a,0),(0,-1.155c) | (2,0,0),(2,4,0),(0,0,5) | (1/2,-1,0) |
| 5.15 | C2' | S1(1)P2(2) | (a,b,c,0,-a,b),(0,-1.155d) | (-2,-4,0),(2,0,0),(0,0,5) | (0,0,0) |
Table S7  Order parameter components and unit cell configurations for subgroups of \( P6_3/mmc \) which can arise from phase transitions in which irrep \( U_1(1/2,0,1/6) \) is the active representation.

| SGN | Space Group | OPD | OPD Vector | Basis Vectors | Origin |
|-----|-------------|-----|------------|---------------|--------|
| 12  | C2/m        | P1  | (a,0,0,0,0,0) | (2,1,-6),(0,1,0),(2,1,0) | (0,0,0) |
| 44  | Imm2        | P2  | (a,-0.268a,0,0,0,0) | (0,0,6),(0,1,0),(2,-1,0) | (-11/12,1/24,-1/4) |
| 12  | C2/m        | P3  | (a,0,a,0,0,0) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 15  | C2/c        | P4  | (a,0,0,a,0,0) | (2,2,0),(-2,2,0),(1,1,3) | (0,1/2,0) |
| 43  | Fdd2        | P5  | (a,-0.268a,0.268a,a,0,0) | (0,0,6),(-2,2,0),(-1,2,0) | (-43/3,-1/3,1) |
| 42  | Fmm2        | P6  | (a,-0.268a,a,-0.268a,0,0) | (0,0,6),(2,2,0),(-2,2,0) | (-1/12,1/12,1/4) |
| 164 | P₃m₁ | P₇ | (a,0,a,0,a,0) | (2,0,0),(0,2,0),(0,0,6) | (0,0,0) |
| 187 | P₆m₂ | P₈ | (-0.268a,-0.268a,-0.268a,-0.268a,-0.268a) | (0,-2,0),(2,2,0),(0,0,6) | (0,0,1/4) |
| 152 | P₃₁₂₁ | P₉ | (a,1.732a,-2a,0,a,-1.732a) | (2,0,0),(0,2,0),(0,0,6) | (0,0,1) |
| 151 | P₃₁₁₂ | P₁₀ | (a,a,-1.366a,0.366a,0.366a,1.366a) | (0,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 8 | Cm | C₁ | (a,b,0,0,0) | (2,1,-6),(0,1,0),(2,1,0) | (0,0,0) |
| 5 | C₂ | C₂ | (a,a,-b,0,0) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 5 | C₂ | C₃ | (a,b,0.866a,0.500b,-0.500a,0.866b,0,0) | (2,2,0),(-2,2,0),(1,1,3) | (1/12,23/12,1/4) |
| 2 | P₁̅ | C₄ | (a,0,b,0,0) | (1,1,3),(0,2,0),(-2,0,0) | (0,0,0) |
| 2 | P₁̅ | C₅ | (a,0,0,b,0,0) | (1,1,3),(0,2,0),(-2,0,0) | (0,1/2,0) |
| 8 | Cm | C₆ | (-0.268a,b,-0.268b,0,0) | (-2,-2,0),(0,0,6),(-2,0,0) | (-1/2,-1/12,1/4) |
| 9 | Cc | C₇ | (-0.268a,b,3.732b,0,0) | (-2,-2,0),(0,0,6),(-2,0,0) | (-7/12,-7/12,7/4) |
| 8 | Cm | C₈ | (a,b,a,0,0) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 9 | Cc | C₉ | (a,b,0,0,-a) | (2,2,0),(-2,2,0),(1,1,3) | (0,3/2,0) |
| 156 | P₃m₁ | C₁₀ | (a,a,b,a,b) | (2,0,0),(0,2,0),(0,0,6) | (0,0,0) |
| 12 | C₂/m | C₁₁ | (a,0,0,a,0) | (-2,-4,0),(2,0,0),(0,0,6) | (0,0,0) |
| 12 | C₂/m | C₁₂ | (a,b,0,0,-a) | (-2,-4,0),(2,0,0),(0,0,6) | (1/2,0,0) |
| 38 | Amm₂ | C₁₃ | (a,-0.268a,b,-0.268b,b,-0.268b) | (0,0,6),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 39 | Abm₂ | C₁₄ | (a,-0.268a,b,3.732b,-b,3.732b) | (0,0,6),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 144 | P₃₁ | C₁₅ | (a,-0.500a0.866b,0.866a-0.500a+0.866b,-0.866a-0.500b) | (2,2,0),(-2,0,0),(0,0,6) | (0,0,0) |
| 5 | C₂ | S₁ | (a,b,c,0,a,-b) | (-2,-4,0),(2,0,0),(0,0,6) | (0,0,0) |
| 5 | C₂ | S₂ | (a,-0.268a,b,c,0.866b0.500c,-0.500b0.866c) | (0,-2,0),(4,2,0),(0,0,6) | (0,0,1/4) |
| 2 | P₁̅ | S₃ | (a,b,0,a,0) | (0,0,6),(0,2,0),(-2,0,0) | (0,0,0) |
| 2 | P₁̅ | S₄ | (a,0,0,b,c) | (0,0,6),(0,2,0),(-2,0,0) | (0,1/2,0) |
| 6 | Pm | S₅ | (-0.268a,b,-0.268b,c,-0.268c) | (-2,0,0),(0,0,6),(2,0,0) | (0,0,1/4) |
| 7 | Pc | S₆ | (-0.268a,b,3.732b,c,3.732c) | (-2,0,0),(0,0,6),(2,0,0) | (0,0,1/4) |
| 1 | P₁ | 4D₁ | (a,b,c,d,0,0) | (1,1,3),(0,2,0),(-2,0,0) | (0,0,0) |
### S3.1.1. $U_1$ and $m\Gamma_4^+$

**Table S8** Magnetic subgroups arising from coupling of irreps $m\Gamma_4^+$ and $U_1(1/2,0,1/6)$, with respect to the parent space group $P6_3/mmc$.

| SGN.M | Space group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-------|-------------|----------|------------|---------------|--------|
| 12.62 | $C2'/m'$   | P1(1)P1(1) | (a,0,0,0,0,0),(b) | (2,1,-6),(0,1,0),(2,1,0) | (0,0,0) |
| 44.232| $Im'm2'$   | P2(1)P1(1) | (a,-0.268a,0,0,0,0),(b) | (0,0,6),(0,1,0),(-2,-1,0) | (-11/12,1/24,-11/4) |
| 12.62 | $C2'/m'$   | P3(1)P1(1) | (a,0,a,0,0,0),(b) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 15.85 | $C2/c$     | P4(1)P1(1) | (a,0,0,a,0,0),(b) | (2,2,0),(-2,2,0),(1,1,3) | (0,1/2,0) |
| 43.226| $Fd'd2'$   | P5(1)P1(1) | (a,-0.268a,0.268a,a,0,0),(b) | (0,0,6),(-2,2,0),(-2,-2,0) | (-4/3,-1/3,1) |
| 42.222| $Fm'm2'$   | P6(1)P1(1) | (a,-0.268a,a,-0.268a,0,0),(b) | (0,0,6),(2,2,0),(-2,2,0) | (-1/12,1/12,1/4) |
| 164.89| $P\overline{3}m1$ | P7(1)P1(1) | (a,0,a,0,a,0),(b) | (0,-2,0),(2,2,0),(0,0,6) | (0,0,0) |
| 187.211| $P\overline{6}m2$ | P8(1)P1(1) | (a,-0.268a,a,-0.268a,a,-0.268a),(b) | (2,2,0),(-2,2,0),(0,0,6) | (0,0,1/4) |
| 152.35| $P312'$    | P9(1)P1(1) | (a,1.732a,-2a,0,a,-1.732a),(b) | (0,-2,0),(2,2,0),(0,0,6) | (0,0,0) |
| 151.29| $P3112$    | P10(1)P1(1) | (a,a,-1.366a,0.366a,0.366a,-1.366a),(b) | (2,2,0),(-2,2,0),(0,0,6) | (0,0,1/4) |
| 8.34  | $Cm'$      | C1(1)P1(1) | (a,b,0,0,0,0),(c) | (2,1,-6),(0,1,0),(2,1,0) | (0,0,0) |
| 5.15  | $C2'$      | C2(1)P1(1) | (a,b,a,-b,0,0),(c) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 5.13  | $C2$       | C3(1)P1(1) | (a,b,0.866a-0.500b,-0.500a-0.866b,0,0),(c) | (2,2,0),(-2,2,0),(1,1,3) | (1/12,23/12,1/4) |
2.4  $P$  C4(1)P1(1)  \((a,0,b,0,0,0),(c)\)  
\((1,1,3),(0,2,0),(-2,0,0)\)  
\((0,0,0)\)

2.4  $P$  C5(1)P1(1)  \((a,0,0,b,0,0),(c)\)  
\((1,1,3),(0,2,0),(-2,0,0)\)  
\((0,1/2,0)\)

8.34  $Cm'$  C6(1)P1(1)  \((a,-0.268a,b,-0.268b,0,0),(c)\)  
\((-2,-2,0),(0,0,6),(-2,0,0)\)  
\((-1/12,-1/12,1/4)\)

9.39  $Cc'$  C7(1)P1(1)  \((a,-0.268a,b,3.732b,0,0),(c)\)  
\((-2,-2,0),(0,0,6),(-2,0,0)\)  
\((-7/12,-7/12,7/4)\)

8.34  $Cm'$  C8(1)P1(1)  \((a,b,a,b,0,0),(c)\)  
\((2,-2,0),(2,2,0),(-1,1,3)\)  
\((0,0,0)\)

9.37  $Cc$  C9(1)P1(1)  \((a,b,-a,0,0),(c)\)  
\((2,2,0),(2,2,0),(1,1,3)\)  
\((0,3/2,0)\)

156.51  $P3m'$  C10(1)P1(1)  \((a,b,a,b,a,b),(c)\)  
\((0,-2,0),(2,2,0),(0,0,6)\)  
\((0,0,0)\)

12.62  $C2'/m'$  C11(1)P1(1)  \((a,0,b,0,a,0),(c)\)  
\((-2,-4,0),(2,0,0),(0,0,6)\)  
\((0,0,0)\)

12.62  $C2'/m'$  C12(1)P1(1)  \((0,a,b,0,0,-a),(c)\)  
\((-2,-4,0),(2,0,0),(0,0,6)\)  
\((1/2,0,0)\)

\((-4,0),(0,0,6)\)

38.191  $Am'm'2$  C13(1)P1(1)  \((a,-0.268a,b,-0.268b,b,-0.268b),(c)\)  
\((2,0),(0,0,6)\)  
\((0,0,1/4)\)

39.199  $Ab'm'2$  C14(1)P1(1)  \((a,-0.268a,b,3.732b,-b,3.732b),(c)\)  
\((0,0,6),(0,2,0),(-4,-2,0)\)  
\((0,0,1/4)\)

144.4  $P3_1$  C15(1)P1(1)  \((a,b,-0.500a-0.866b,0.866a-0.500b,-0.500a+0.866b,-0.866a+0.500b),(c)\)  
\((2,2,0),(-2,0,0),(0,0,6)\)  
\((0,0,0)\)

5.15  $C2'$  S1(1)P1(1)  \((a,b,c,0,a,-b),(d)\)  
\((-2,-4,0),(2,0,0),(0,0,6)\)  
\((0,0,0)\)

5.13  $C2$  S2(1)P1(1)  \((a,-0.268a,b,c,0.866b-0.500c,-0.500b-0.866c),(d)\)  
\((0,-2,0),(4,2,0),(0,0,6)\)  
\((0,0,1/4)\)

2.4  $P$  S3(1)P1(1)  \((a,0,b,0,c,0),(d)\)  
\((0,0,6),(0,2,0),(-2,0,0)\)  
\((0,0,0)\)
### S3.2. $U_1$ and $\mathbf{mΓ}_5^+$

**Table S9** Magnetic subgroups arising from coupling of irreps $\mathbf{mΓ}_5^+$ and $U_1(1/2,0,1/6)$, with respect to the parent space group $P6_3/mmc$.

| SGN.M | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-------|-------------|----------|------------|---------------|--------|
|       |             |          | $U_1(1/2,0,1/6)$ | $U_1(1/2,0,1/6)$ |        |
| 12.58 | $C2/m$      | P1(1)P1(1) | (a,0,0,0,0,0),(b,-1.732b) | (2,1,-6),(0,1,0),(2,1,0) | (0,0,0) |
| 44.229 | Imm2        | P2(1)P1(1) | (a,-0.268a,0,0,0,0),(b,-1.732b) | (0,1,0),(0,0,6),(2,1,0) | (0,0,1/4) |
| 12.58 | $C2/m$      | P3(1)P1(3) | (a,0,a,0,0,0),(b,1.732b) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 15.85 | $C2/c$      | P4(1)P1(3) | (a,0,0,a,0,0),(b,1.732b) | (2,2,0),(-2,2,0),(1,1,3) | (0,1/2,0) |
| 43.224 | Fdd2        | P5(1)P1(3) | (a,-0.268a,0.268a,a,0,0),(b,1.732b) | (-2,2,0),(0,0,6),(2,2,0) | (5/6,5/6,5/2) |
| 42.219 | Fmm2        | P6(1)P1(3) | (a,-0.268a,a,-0.268a,a,0,0),(b,1.732b) | (2,2,0),(0,0,6),(2,2,0) | (1/12,-1/12,1/4) |
| 8.32  | $Cm$        | C1(1)P1(1) | (a,b,0,0,0,0),(c,-1.732c) | (2,1,-6),(0,1,0),(2,1,0) | (0,0,0) |
| 5.13  | C2          | C2(1)P1(3) | (a,b,a,-b,0,0),(c,1.732c) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| Code  | Space Group | Details                                      | Parameters                   |
|-------|-------------|----------------------------------------------|------------------------------|
| 5.13  | C2          | C3(1)P1(3)                                   | (a,b,0.866a-0.500b,-0.500a-0.866b,0,0),(c,1.732c) | (2,2,0),(-2,2,0),(1,1,3) |
| 6.13  | Cm          | C8(1)P1(3)                                   | (a,b,a,0,0),(c,1.732c)       | (2,-2,0),(2,2,0),(-1,1,3) |
| 9.37  | Cc          | C9(1)P1(3)                                   | (a,b,-a,0,0),(c,1.732c)      | (2,2,0),(-2,2,0),(1,1,3) |
|       |             |                                             |                              | (0,0)                       |
| 12.58 | C2/m        | C11(1)P1(2)                                  | (a,0,b,0,a,0),(-2c,0)       | (-2,-4,0),(2,0,0),(0,0,6)  |
|       |             |                                             |                              | (0,0)                       |
| 12.58 | C2/m        | C12(1)P1(2)                                  | (0,a,b,0,-a,0),(-2c,0)      | (-2,-4,0),(2,0,0),(0,0,6)  |
|       |             |                                             |                              | (1/2,0,0)                   |
| 38.187| Amm2        | C13(1)P1(1)                                  | (a,-0.268a,b,-0.268b,b,-0.268b),(c,-1.732c) | (0,0,6),(0,2,0),(-4,2,0)    |
|       |             |                                             |                              | (0,0,1/4)                   |
| 39.195| Abm2        | C14(1)P1(1)                                  | (a,-0.268a,b,3.732b,b,-3.732b),(c,-1.732c) | (0,0,6),(0,2,0),(-4,2,0)    |
|       |             |                                             |                              | (0,0,1/4)                   |
| 5.13  | C2          | S1(1)P1(2)                                   | (a,b,c,0,a,-b),(-2d,0)      | (-2,-4,0),(2,0,0),(0,0,6)  |
|       |             |                                             |                              | (0,0)                       |
| 5.13  | C2          | S2(1)P1(1)                                   | (a,-0.268a,b,c,0.866b-0.500c,-0.500b-0.866c),(d,-1.732d) | (0,-2,0),(4,2,0),(0,0,6)    |
|       |             |                                             |                              | (0,0,1/4)                   |
| 8.32  | Cm          | 4D2(1)P1(2)                                  | (a,b,c,d,a,b),(-2e,0)       | (-2,-4,0),(2,0,0),(0,0,6)  |
|       |             |                                             |                              | (0,0)                       |
| 12.62 | C2/m'       | P1(1)P2(1)                                   | (a,0,0,0,0,0),(b,0.577b)    | (2,1,-6),(0,1,0),(2,1,0)    |
|       |             |                                             |                              | (0,0)                       |
| 44.231| I4/m2'      | P2(1)P2(1)                                   | (a,-0.268a,0,0,0,0),(b,0.577b) | (0,1,0),(0,0,6),(2,1,0)    |
|       |             |                                             |                              | (0,0,1/4)                   |
| 12.62 | C2/m'       | P3(1)P2(3)                                   | (a,0,a,0,0,0),(-b,0.577b)  | (2,-2,0),(2,2,0),(-1,1,3)  |
|       |             |                                             |                              | (0,0)                       |
| 15.89 | C2/c'       | P4(1)P2(3)                                   | (a,0,0,a,0,0),(-b,0.577b)  | (2,2,0),(-2,2,0),(1,1,3)   |
|       |             |                                             |                              | (0,1/2,0)                   |
| 43.226| Fd3/d2'     | P5(1)P2(3)                                   | (a,-0.268a,0.268a,a,0,0),(-b,0.577b) | (-2,2,0),(0,0,6),(2,2,0) |
|       |             |                                             |                              | (5/6,5/6,5/2)               |
| 42.221| Fm'm2'      | P6(1)P2(3)                                   | (a,-0.268a,a,-0.268a,0,0),(-b,0.577b) | (2,2,0),(0,0,6),(2,-2,0) |
|       |             |                                             |                              | (1/12,-1/12,1/4)            |
| 8.34  | Cm'         | C1(1)P2(1)                                   | (a,b,0,0,0,0),(c,0.577c)    | (2,1,-6),(0,1,0),(2,1,0)    |
|       |             |                                             |                              | (0,0)                       |
| 5.15 | C2' | C2(1)P2(3) | (a,b,a,-b,0,0),(-c,0.577c) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 5.15 | C2' | C3(1)P2(3) | (a,b,0.866a-0.500b,-0.500a-0.866b,0,0),(-c,0.577c) | (2,2,0),(-2,2,0),(1,1,3) | (1/12,23,1/4) |
| 8.34 | Cm' | C8(1)P2(3) | (a,b,a,b,0,0),(-c,0.577c) | (2,-2,0),(2,2,0),(-1,1,3) | (0,0,0) |
| 9.39 | Cc' | C9(1)P2(3) | (a,b,-a,0,0),(-c,0.577c) | (2,2,0),(-2,2,0),(1,1,3) | (0,3/2,0) |
| 12.62 | C2'/m' | C11(1)P2(2) | (a,0,b,0,a,0),(-1.155c) | (-2,-4,0),(2,0,0),(0,0,6) | (0,0,0) |
| 12.62 | C2'/m' | C12(1)P2(2) | (a,b,0,0-a,0,-1.155c) | (-2,-4,0),(2,0,0),(0,0,6) | (1/2,0,0) |
| 38.19 | Amm2' | C13(1)P2(1) | (a,-0.268a,b,-0.268b,-0.268b,(0,0,6),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| 39.198 | Abm2' | C14(1)P2(1) | (a,-0.268a,b,3.732b,-b,-3.732b),(c,0.577c) | (0,0,1/4) |
| 5.15 | C2' | S1(1)P2(2) | (a,b,c,0,a,-b),(0,-1.155d) | (-2,-4,0),(2,0,0),(0,0,6) | (0,0,0) |
| 5.15 | C2' | S2(1)P2(1) | (a,-0.268a,b,c,0.866b-0.500c,-0.500b-0.866b,d,0.577d) | (0,-2,0),(4,2,0),(0,0,6) | (0,0,1/4) |
| 8.34 | Cm' | 4D2(1)P2(2) | (a,b,c,d,a,b),(0,-1.155e) | (-2,-4,0),(2,0,0),(0,0,6) | (0,0,0) |
| 2.4 | P1 | P1(1)C1(1) | (a,0,0,0,0,0),(b,c) | (1,0,3),(0,1,0),(-2,0,0) | (0,0,0) |
| 8.32 | Cm | P2(1)C1(1) | (a,-0.268a,b,0,0,0),(b,c) | (-2,0,0),(0,0,6),(0,1,0) | (-1/12,0,1/4) |
| 1.1 | P1 | C1(1)C1(1) | (a,b,0,0,0,0),(c,d) | (1,0,3),(0,1,0),(-2,0,0) | (0,0,0) |
| 2.4 | P1 | C4(1)C1(1) | (a,0,b,0,0,0),(c,d) | (1,1,3),(0,2,0),(-2,0,0) | (0,0,0) |
| 2.4 | P1 | C5(1)C1(1) | (a,0,b,0,0,0),(c,d) | (1,1,3),(0,2,0),(-2,0,0) | (0,1/2,0) |
| 8.32 | Cm | C6(1)C1(1) | (a,-0.268a,b,-0.268b,0,0),(c,d) | (-2,-2,0),(0,0,6),(-2,0,0) | (-1/12,0,1/12,1/4) |
S3.3. 3C

Table S10  Order parameter components and unit cell configurations for subgroups of $P6_3/mmc$ which can arise from phase transitions in which irrep $U_1(1/2,0,1/3)$ is the active representation.

| SGN | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-----|-------------|----------|------------|---------------|--------|
| 58  | Pnm      | P1       | (a,0,0,0,0,0) | (0,0,3),(2,1,0),(1,0) | (0,0,0) |
| 59  | Pmmn     | P2       | (0,a,0,0,0,0) | (0,0,3),(0,-1,0),(2,1) | (1/2,1/2,0) |
| 164 | P$3\bar{1}$ | P3       | (a,0,a,0,a) | (2,0),(0,2,0),(0,0,3) | (0,0,0) |
| 187 | P$\bar{3}m$ | P4       | (a,-0.577a,a,-0.577a,a,-0.577a) | (0,-2),(2,2,0),(0,0,3) | (0,0,1/4) |
| 64  | Cmca     | P5       | (a,0,0,0,a,0) | (2,0),(2,4,0),(0,0,3) | (0,0,0) |
| 63  | Cmcm     | P6       | (0,a,0,0,0,-a) | (2,0),(2,4,0),(0,0,3) | (1/2,0,0) |
| 152 | P$3_1$21 | P7       | (a,1.732a,-2a,0,a,-1.732a) | (2,0),(0,2,0),(0,0,3) | (0,0,1/2) |
| 151 | P$3_1$12 | P8       | (a,0.577a,-a,0.577a,0,-1.155a) | (0,-2),(2,2,0),(0,0,3) | (0,0,3/4) |
| 31  | P$mnm$_2 | C1       | (a,b,0,0,0,0) | (0,-1),(2,1,0),(0,0,3) | (1/2,1/4,0) |
| 156 | P$3m$_1  | C2       | (a,b,a,b,a,b) | (2,0),(0,2,0),(0,0,3) | (0,0,0) |
| 20  | C$222_1$ | C3       | (a,b,0,0,a,-b) | (2,0),(2,4,0),(0,0,3) | (1/2,0,0) |
Table S11  Magnetic subgroups arising from coupling of irreps $m\Gamma_4^+$ and $U_1(1/2,0,1/3)$, with respect to the parent space group $P6_3/mmc$. 

| SGN.M | Space group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-------|-------------|----------|------------|---------------|--------|
|       |             |          | $(0,0,a,0,b,c)$ | $(-2,0,0),(0,0,3),(0,2,0)$ | $(0,0,0)$ |
| 1     | $P1$        | 6D1      |            | $(-2,0,0),(0,0,3),(0,2,0)$ | $(0,0,0)$ |
| 4     | $P2_1$      | 4D1      |            | $(-2,0,0),(0,0,3),(0,2,0)$ | $(0,1/2,0)$ |
| 8     | $Cm$        | 4D2      |            | $(-4,0),(0,0),(0,3)$ | $(0,0,0)$ |

S3.3.2. $U_1$ and $m\Gamma_4^+$
| Pm'm' | P1(1)P1(1) | (a,0,0,0,0,0),(b) | (-2,-1,0),(0,0,3),(0,1,0) |
|-------|------------|-------------------|--------------------------|
| Pm'm' | P2(1)P1(1) | (0,a,0,0,0,0),(b) | (0,0,3),(0,-1,0),(2,1,0) |
| P3m'2 | P4(1)P1(1) | (0,0,3),(a,-0.577a,a,-0.577a,0,-0.577a),(b) | (2,2,0),(-2,0),(0,0,3) |
| Ca'c'a' | P5(1)P1(1) | (a,0,0,0,0,0),(b) | (2,0),(2,4,0),(0,0,3) |
| Ca'm'c' | P6(1)P1(1) | (0,0,0,-a),(b) | (2,0),(2,4,0),(0,0,3) |
| P312'1 | P7(1)P1(1) | (a,1.732a,-2a,0,a,-1.732a),(b) | (0,-2,0),(2,2,0),(0,0,3) |
| P3112 | P8(1)P1(1) | (0,0,3),(a,0.577a,-a,0.577a,0,-1.155a),(b) | (2,2,0),(-2,0),(0,0,3) |
| Pm'n2'1 | C1(1)P1(1) | (a,b,0,0,0,0),(c) | (-1,0),(2,1,0),(0,0,3) |
| P3m'1 | C2(1)P1(1) | (a,b,a,b,a),(b),(c) | (-2,0),(2,2,0),(0,0,3) |
| C22'2' | C3(1)P1(1) | (a,b,0,0,0,0),(c) | (2,4,0),(-2,0),(0,0,3) |
| P2'/c' | C4(1)P1(1) | (0,0,a,b,0),(b),(c) | (-2,0),(0,0,3),(2,0) |
| P2'/m' | C5(1)P1(1) | (0,0,0,a,b),(c) | (-2,0),(0,0,3),(2,0) |
| P2'/c' | C6(1)P1(1) | (a,0,0,0,0,0),(b),(c) | (-2,0),(0,0,3),(2,0) |
| C2'/m' | C7(1)P1(1) | (a,b,0,0,0,0),(c) | (-2,-4,0),(2,0),(0,0,3) |
| C2'/m' | C8(1)P1(1) | (0,0,0,a),(c) | (-2,-4,0),(2,0),(0,0,3) |
| Am'm'2 | C9(1)P1(1) | (a,-0.577a,b,-0.577b,b,-0.577b),(c) | (0,0,3),(2,0),(-4,-2,0) |
| Ab'm'2 | C10(1)P1(1) | (a,-0.577a,b,1.732b,-b,-1.732b),(c) | (0,0,3),(2,0),(-4,-2,0) |
| Cm'c2'1 | C11(1)P1(1) | (a,b,0,0,a,b),(c) | (2,0),(2,4,0),(0,0,3) |
| P31 | C12(1)P1(1) | (a,b,-0.500a+0.866b,0.866a-0.500b,-0.500a+0.866b,-0.866a-0.500b),(c) | (2,2,0),(-2,0),(0,0,3) |
| C2' | S1(1)P1(1) | (a,b,c,0,a,-b),(d) | (-2,-4,0),(2,0),(0,0,3) |
### Magnetic subgroups arising from coupling of irreps mΓ₅⁺ and U₁(1/2,0,1/3), with respect to the parent space group P6₃/mmc.

| SGN.M | Space Group | OPD Name | OPD Vector | Basis Vectors | Origin |
|-------|-------------|----------|------------|---------------|--------|
| 58.393 | Pnam       | P1(1)P1(1) | (a,0,0,0,0,0),(b,-1.732b) | (-2,-1,0),(0,0,3),(0,1,0) | (0,0,0) |
| 59.405 | Pnamn      | P2(1)P1(1) | (0,a,0,0,0,0),(b,-1.732b) | (0,1,0),(0,0,3),(2,1,0) | (1/2,0,0) |
| 64.469 | Cnca       | P5(1)P1(2) | (a,0,0,0,a,0),(-2b,0) | (2,0,0),(2,4,0),(0,0,3) | (0,0,0) |
| 63.457 | Cnmm       | P6(1)P1(2) | (0,a,0,0,-a),(-2b,0) | (2,0,0),(2,4,0),(0,0,3) | (1/2,0,0) |
| 31.123 | Pmn21      | C1(1)P1(1) | (a,b,0,0,0,0),(-c,-1.732c) | (0,-1,0),(2,1,0),(0,0,3) | (1/2,1/4,0) |
| 20.31  | C222₁      | C3(1)P1(2) | (a,b,0,0,a,-b),(-2c,0) | (2,0,0),(2,4,0),(0,0,3) | (1/2,0,0) |
|        |            |          |            | (-2,-1,0),(0,0,3),(0,1,0) |        |
| 12.58  | C2/m       | C7(1)P1(2) | (a,b,0,a,0),(-c,0) | (2,0,0),(2,4,0),(0,0,3) | (0,0,0) |
| 12.58  | C2/m       | C8(1)P1(2) | (a,b,0,a,-a),(-c,0) | (2,0,0),(2,4,0),(0,0,3) | (1/2,0,0) |
|        |            |          |            | (-2,-1,0),(0,0,3),(0,1,0) |        |
| 38.187 | Amm2       | C9(1)P1(1) | (a,-0.577a,b,-0.577b,c,0.577),(-c,-1.732c) | (0,0,3),(0,2,0),(-4,-2,0) | (0,0,1/4) |
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|---------------------------------|-----------------|
| **39.195 Abm2** C10(1)P1(1)    | (a,-0.577a,b,1.732b,-b,-1.732b),(c,-1.732c) | (0,0,3),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| **36.172 Cmc2₁** C11(1)P1(2)   | (a,b,0,0,a,b),(-2c,0) | (2,0,0),(2,4,0),(0,0,3) | (1/2,-1,0) |
| **5.13 C2** S1(1)P1(2)         | (a,b,c,0,a,-b),(2d,0) | (-2,-4,0),(2,0,0),(0,0,3) | (0,0,0) |
| **5.13 C2** S2(1)P1(1)         | (a,-0.577a,b,c,0.500b-0.866c,-0.866b-0.500c),(d,-1.732d) | (0,-2,0),(4,2,0),(0,0,3) | (0,0,1/4) |
| **8.32 Cm** 4D2(1)P1(2)       | (a,b,c,d,a,b),(-2e,0) | (-2,-4,0),(2,0,0),(0,0,3) | (0,0,0) |
| **58.398 Pnn' m'** P1(1)P2(1)  | (a,0,0,0,0),(b,0.577b) | (0,0,3),(2,1,0),(0,1,0) | (0,0,0) |
| **59.41 Pmm' n'** P2(1)P2(1)  | (0,a,0,0,0),(b,0.577b) | (0,0,3),(0,-1,0),(2,1,0) | (1/2,1/2,0) |
| **64.474 Cm'c'a** P5(1)P2(2)  | (a,0,0,0,a),(0,-1.155b) | (2,0,0),(2,4,0),(0,0,3) | (0,0,0) |
| **63.462 Cm'c'm** P6(1)P2(2)  | (0,a,0,0,-a),(0,-1.155b) | (2,0,0),(2,4,0),(0,0,3) | (1/2,0,0) |
| **31.127 Pm'n'2₁** C1(1)P2(1) | (a,b,0,0,0,0),(c,0.577c) | (0,-1,0),(2,1,0),(0,0,3) | (1/2,1/4,0) |
| **20.33 C2'2₁** C3(1)P2(2)    | (a,b,0,0,a,b),(0,-1.155c) | (2,0,0),(2,4,0),(0,0,3) | (1/2,0,0) |
| **12.62 C2'/m'** C7(1)P2(2)   | (a,b,0,0,a,0),(0,-1.155c) | (-2,-4,0),(2,0,0),(0,0,3) | (0,0,0) |
| **12.62 C2'/m'** C8(1)P2(2)   | (0,a,b,0,0,-a),(0,-1.155c) | (-2,-4,0),(2,0,0),(0,0,3) | (1/2,0,0) |
| **38.19 Amm'2'** C9(1)P2(1)   | (a,-0.577a,b,-0.577b,b,-0.577b),(c,0.577c) | (0,0,3),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| **39.198 Abm'2'** C10(1)P2(1) | (a,-0.577a,b,1.732b,-b,-1.732b),(c,0.577c) | (0,0,3),(0,2,0),(-4,-2,0) | (0,0,1/4) |
| **36.176 Cm'c'2₁** C11(1)P2(2) | (a,b,0,0,a,b),(0,-1.155c) | (2,0,0),(2,4,0),(0,0,3) | (1/2,-1,0) |
| **5.15 C2'** S1(1)P2(2)       | (a,b,c,0,a,-b),(0,-1.155d) | (-2,-4,0),(2,0,0),(0,0,3) | (0,0,0) |
| **5.15 C2'** S2(1)P2(1)       | (a,-0.577a,b,c,0.500b-0.866c,-0.866b-0.500c),(d,0.577d) | (0,-2,0),(4,2,0),(0,0,3) | (0,0,1/4) |
| **8.34 Cm'** 4D2(1)P2(2)     | (a,b,c,d,a,b),(0,-1.155e) | (-2,-4,0),(2,0,0),(0,0,3) | (0,0,0) |
| **14.75 P2₁/c** P1(1)C1(1)    | (a,0,0,0,0),(b,c) | (0,1,0),(0,0,3),(2,0,0) | (0,0,0) |
|      | Space Group | Description | Coordinates | Translation |
|------|-------------|-------------|-------------|------------|
| 11.5 | P21/m       | P2(1)C1(1)  | (0, a, 0, 0, 0, 0), (b, c) | (-2, 0, 0), (0, 0, 3), (0, 1, 0) |
| 4.7  | P21         | C1(1)C1(1)  | (a, b, 0, 0, 0, 0), (c, d) | (-2, 0, 0), (0, 0, 3), (0, 1, 0) |
| 14.75| P21/c       | C4(1)C1(1)  | (0, 0, a, b, 0), (c, d) | (-2, 0, 0), (0, 0, 3), (0, 2, 0) |
| 11.5 | P21/m       | C5(1)C1(1)  | (0, 0, a, 0, b), (c, d) | (-2, 0, 0), (0, 0, 3), (0, 2, 0) |
| 14.75| P21/c       | C6(1)C1(1)  | (a, 0, 0, 0, b), (c, d) | (-2, 0, 0), (0, 0, 3), (2, 2, 0) |
| 2.4  | $\bar{P}$1 | S3(1)C1(1)  | (a, 0, b, 0, c, 0), (d, e) | (0, 0, 3), (0, 2, 0), (-2, 0, 0) |
| 2.4  | $\bar{P}$1 | S4(1)C1(1)  | (a, 0, 0, b, 0, c), (d, e) | (0, 0, 3), (0, 2, 0), (-2, 0, 0) |
| 6.18 | Pm          | S5(1)C1(1)  | (a, -0.577a, b, -0.577b, c, -0.577c), (d, e) | (-2, 0, 0), (0, 0, 3), (0, 2, 0) |
| 7.24 | Pc          | S6(1)C1(1)  | (a, -0.577a, b, 1.732b, c, 1.732c), (d, e) | (-2, 0, 0), (0, 0, 3), (0, 2, 0) |
| 4.7  | P21         | 4D1(1)C1(1) | (0, 0, a, b, c, d), (e, f) | (-2, 0, 0), (0, 0, 3), (0, 2, 0) |
| 1.1  | P1          | 6D1(1)C1(1) | (a, b, c, d, e, f), (g, h) | (0, 0, 3), (0, 2, 0), (-2, 0, 0) |