Z<sub>2</sub>xZ<sub>2</sub> magnetic domains and magnetic moment disproportionation in the spin-orbit Mott insulator Sr<sub>2</sub>IrO<sub>4</sub>

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# Outline

- A short introduction to  $Sr_2IrO_4$
- Z<sub>2</sub>xZ<sub>2</sub> magnetic domain structure



J. W. Kim (APS)



Sunwook Park (POSTECH)

• New magnetic structure from DFT



Alaska Subedi (CNRS)

Representation analysis



Hoon Kim (POSTECH)



#### J<sub>eff</sub>=1/2 Kramers doublet





$$\begin{split} |\tilde{\uparrow}\rangle &= +\sin\theta |0,\uparrow\rangle - \cos\theta |+1,\downarrow\rangle, \\ |\tilde{\downarrow}\rangle &= -\sin\theta |0,\downarrow\rangle + \cos\theta |-1,\uparrow\rangle. \end{split}$$

Heisenberg Kitaev

 $|L_z = 0\rangle = |xy\rangle$  and  $|Lz = \pm 1\rangle = \pm \frac{1}{\sqrt{2}}(|yz\rangle \pm i|zx\rangle)$ ,

#### J<sub>eff</sub>=1/2 Kramers doublet



New feature of pseudospins: a propensity to spontaneously disproportionate possible new instabilities and new magnetic phases!



•A rare realization of spin-1/2 moments on a square lattice

Neel order



- •A rare realization of spin-1/2 moments on a square lattice
- •Neel order
- •Heisenberg AF



- •A rare realization of spin-1/2 moments on a square lattice
  - Neel order
  - •Heisenberg AF
  - •Reproduces a large part of cuprate phenomenology
  - •Superconductivity remains to be seen.



Lattice structure still not fully known

 Long believed to be I4<sub>1</sub>/acd, but recent studies suggest 14<sub>1</sub>/a

 Forbidden peaks in ND



F. Ye et al. PRB 2013

- SHG indicate 4/m point group



D. H. Torchinsky et al. PRL 2015



- Is the magnetic structure correct?
- In hindsight, the currently known magnetic structure is allowed but unlikely to be the ground state in I4<sub>1</sub>/a.
- But is the deviation large enough to detect?

# Magnetic domains



- generated by successive 4<sub>1</sub> screw operations
- •domain 3 & 4 are just A↔ B
   sublattice switching of domain 1 & 2
- different domains have different stacking patterns
- •domain 1: (1 0 4n+2) & (0 1 4n) domain 2: (1 0 4n) & (0 1 4n+2)

#### Magnetic domains



Magnetic domains fully polarized by ~0.1T applied field

- generated by successive 41 screw operations
- •domain 3 & 4 are just A↔B
   sublattice switching of domain 1 & 2
- different domains have different stacking patterns
- domains can be easily imaged by going to different q's

#### Magnetic domains



#### Magnetic Domain Imaging using X-ray Reflection Interference Microscopy (XRIM)



£ 669

644 619

> 380 405 430 455 480 505 Hx (um+1k)



#### ~20 nm Resolution



11.25

15

3.75

7.5

Distance (100 nm)

# **Domain Imaging**



Mostly single domain, but uneven intensity

# **Domain Imaging**



#### Z<sub>2</sub> x Z<sub>2</sub> Domain Structure



### Z<sub>2</sub> x Z<sub>2</sub> Domain Structure



#### two domains within a domain!

#### Known magnetic structure cannot explain the domain structure

Resonant x-ray diffraction measures spin component in the scattering plane

$$I \propto |{f k}_f \!\cdot \! {f S}|^2$$



### Z<sub>2</sub> x Z<sub>2</sub> Domain Structure



Known magnetic structure cannot explain the domain structure

Resonant x-ray diffraction measures spin component in the scattering plane

$$I \propto |\mathbf{k}_f \cdot \mathbf{S}|^2$$





- Unique solution from representation analysis
- Can be stabilized in DFT calculations and has a lower total energy than the previous magnetic solution
- Can be stabilized even in the I4<sub>1</sub>/acd space group (instead of the actual I4<sub>1</sub>/a)



Old



Electronic mechanism of symmetry lowering

#### $I 4_1/a c d$

 $D_{4h}^{2v}$ 

 $I 4_1/a 2/c 2/d$ 

4/*m m m* 

Tetragonal

Patterson symmetry I4/mmm

ORIGIN CHOICE 2

No. 142



- a body-centered cell.
- has inversion symmetry
- 4<sub>1</sub> screw axis, and a glide plane perpendicular to it.
- two additional glides.

**Origin** at  $\overline{1}$  at b(c,a)d, at  $0, -\frac{1}{4}, \frac{1}{8}$  from  $\overline{4}$ 

Asymmetric unit  $0 \le x \le \frac{1}{2}; -\frac{1}{4} \le y \le \frac{1}{4}; 0 \le z \le \frac{1}{8}$ 

#### Symmetry operations

For $(0,0,0)$ + set			
(1) 1	(2) $2(0,0,\frac{1}{2}) = \frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4}) \frac{1}{4},0,z$
(5) 2 $\frac{1}{4}$ , y, 0	(6) $2 = x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{4},\frac{3}{8}$	(8) $2 x,\overline{x}+\frac{1}{4},\frac{1}{8}$
(9) 1 0, 0, 0	(10) $a = x,y,\frac{1}{4}$	(11) $\overline{4}^+ -\frac{1}{2},-\frac{1}{4},z; \frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\overline{4}^{-} 0,\frac{3}{4},z; 0,\frac{3}{4},\frac{1}{8}$
(13) a x, 0, z	(14) $c = 0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) x+\frac{1}{2},\overline{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) x,x,z$
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set			
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2  \theta, \frac{1}{4}, z$	(3) $4^+(0,0,\frac{3}{4})  \frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{4}) = \frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(6) $2(\frac{1}{2}, 0, 0)  x, \frac{1}{4}, 0$	(7) $2(\frac{1}{2},\frac{1}{2},0)  x,x-\frac{1}{4},\frac{1}{8}$	(8) $2 = x, \bar{x} + \frac{3}{4}, \frac{3}{8}$
(9) $\overline{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $b  x, y, 0$	(11) $\overline{4}^+  \frac{1}{2},\frac{1}{4},z;  \frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^{-} = 0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$
(13) $c$ $x,\frac{1}{4},z$	(14) $b  \frac{1}{4}, y, z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})  x+\frac{1}{2},\overline{x},z$	(16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) = x, x, z$

#### $1 4_1 / a c a$

 $D_{4h}^{20}$ 

 $I 4_1/a 2/c 2/d$ 

4/*m m m* 

Tetragonal

Patterson symmetry I4/mmm

ORIGIN CHOICE 2

No. 142



- a body-centered cell.
- has inversion symmetry
- 4<sub>1</sub> screw axis, and a glide plane perpendicular to it.
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**Origin** at  $\overline{1}$  at b(c,a)d, at  $0, -\frac{1}{4}, \frac{1}{8}$  from  $\overline{4}$ 

Asymmetric unit  $0 \le x \le \frac{1}{2}; -\frac{1}{4} \le y \le \frac{1}{4}; 0 \le z \le \frac{1}{8}$ 

#### Symmetry operations

For (0,0,0)+ set

(1) 1 (5) 2 1 0	(2) $2(0,0,\frac{1}{2}) = \frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{3}{4}) = \frac{1}{4},0,z$
$\begin{array}{c} (3) & 2 & 4, 9, 0 \\ (9) & \overline{1} & 0, 0, 0 \end{array}$	(10) $a x, y, \frac{1}{4}$	$\begin{array}{c} (7)  \underline{2(2,2,0)}  \underline{x,x+4,8} \\ (11)  \overline{4^+}  \underline{1}, -\underline{4}, z;  \underline{1}, -\underline{4}, \frac{3}{8} \end{array}$	$\begin{array}{c} (8) & 2 & x, x + 4, \\ (12) & \overline{4}^{-} & 0, \frac{3}{4}, z; & 0, \frac{3}{4}, \frac{1}{8} \end{array}$
(13) a x, 0, z	(14) $c = 0, y, z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) x + \frac{1}{2},\overline{x},z$	$(16) \ d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) \ x,x,z$
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set			
$(1) t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}) (5) 2(0 + 0) 0 y = 1$	$(2) 2^{-}\theta, \frac{1}{4}, z$ $(6) 2(10, 0) r = 10$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccc} (4) & 4^{-}(0,0,\frac{1}{4}) & \frac{3}{4},0,z \\ (8) & 2 & x & \overline{x} + \frac{3}{4} & \frac{3}{4} \end{array}$
(9) $\overline{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	(10) $b x, y, 0$	(11) $\vec{4}^+$ $\frac{1}{2}, \frac{1}{4}, z; \frac{1}{2}, \frac{1}{4}, \frac{1}{8}$	(12) $\overline{4}^{-}$ $0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$
$(13) c x, \frac{1}{4}, z$	$(14) \ b \ 4, y, z$	$-(15)  d(-\frac{1}{4}, \frac{1}{4}, \frac{3}{4})  x + \frac{1}{2}, \overline{x}, z$	$(16) d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) x, x, z$

Removing these symmetry elements will lower the symmetry from  $I4_1/acd$  to  $I4_1/a$ 

$I 4_1/a c d$	$D_{4h}^{20}$	4/ <i>m m m</i>	Tetragonal
No. 142	$I 4_1/a 2/c 2/d$	Patte	rson symmetry I4/mmm
ORIGIN CHOICE 2			·
$ \begin{array}{c} \frac{3}{4} - \underbrace{0}_{4} & \underbrace{1}{4} + \underbrace{0}_{4} & \underbrace{3}{4} + \\ \underbrace{0}_{-} & \underbrace{1}{2} + \underbrace{0}_{-} & \underbrace{0}_{+} & \underbrace{1}{2} - \underbrace{0}_{-} & \underbrace{0}_{-} & \underbrace{1}{2} + \underbrace{0}_{+} & \underbrace{0}_{+} & \underbrace{0}_{+} & \underbrace{1}{2} + \underbrace{0}_{+} & \underbrace{0}_{+} & \underbrace{0}_{+} & \underbrace{1}{2} + \underbrace{0}_{+} & \underbrace{0}_{$	$\frac{1}{4} \xrightarrow{3}{8} \xrightarrow{1}{8} \xrightarrow{3}{8} \xrightarrow{3} \xrightarrow{3}{8} \xrightarrow{3} \xrightarrow{3}{8} \xrightarrow{3} \xrightarrow{3}{8} \xrightarrow{3} \xrightarrow{3} \xrightarrow{3}{8} \xrightarrow{3} \xrightarrow{3} \xrightarrow{3} \xrightarrow{3} \xrightarrow{3} \xrightarrow{3} \xrightarrow{3} 3$	$\begin{bmatrix} & & \\ & $	Ir occupies 8a Wyckoff site, nd in-plane O 16f
$\bigcirc 2 \\ \frac{1}{4} - \bigcirc 3 \\ \frac{3}{4} - \bigcirc 3 \\ \frac{3}{4} + \bigcirc 0 \\ \frac{3}{4} - \bigcirc 0 \\ \frac{1}{2} - \bigcirc 0 \\ \frac{1}{2} - \bigcirc 0 \\ \frac{1}{4} + \bigcirc 0 \\ \frac{3}{4} + \bigcirc 0 \\ \frac{3}{4} - \bigcirc 0 \\ \frac{3}{4} - \bigcirc 0 \\ \frac{1}{4} - \bigcirc 0 \\ \frac{3}{4} - \bigcirc 0 \\ \frac{1}{4} - \bigcirc 0 \\ \frac{3}{4} - \bigcirc 0 \\ \frac{1}{4} - \bigcirc 0 \\ \frac{3}{4} - \bigcirc 0 \\ 0 \\ \frac{3}{4} - \bigcirc 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0$	$ \begin{array}{c} 8 \\ 1 \\ 3 \\ 3 \\ 8 \\ 1 \\ 1 \\ 4 \\ 1 \\ \mathbf$	$ \begin{array}{c} \frac{1}{8} \\ \frac{1}{8} $	Glide plane
$\begin{array}{c} \begin{array}{c} 3 & -3 & -3 & -\frac{1}{4} & -\frac{1}{4} & + & -3 & \frac{3}{4} & + \\ \hline 0 & -\frac{1}{2} & + & 0 & -\frac{1}{4} & -\frac{1}{4} & + & -\frac{3}{4} & + \\ \hline 0 & \frac{1}{2} & -\frac{1}{2} & + & 0 & -\frac{1}{2} & + & -\frac{1}{2} & + & -\frac{1}{2} & + & -\frac{1}{4} & + \\ \hline 1 & \frac{1}{4} & - & 0 & \frac{3}{4} & -\frac{3}{4} & + & 0 & -\frac{1}{4} & + \end{array}$	$\frac{3}{8} + \frac{1}{4} = 0$ $\frac{3}{8} + \frac{1}{4} = 0$ $\frac{3}{8} + \frac{1}{8} + \frac{1}{8$	$\frac{1}{8}$ $\frac{3}{8}$ $\frac{1}{4}$	
<b>Origin</b> at $\overline{1}$ at $b(c, a)d$ , at $0, -\frac{1}{4}, \frac{1}{8}$ from $\overline{4}$		Ç	glide plane
Asymmetric unit $0 \le x \le \frac{1}{2}$ ; $-\frac{1}{4} \le y \le \frac{1}{4}$ ; $0 \le \frac{1}{4}$	$z \leq \frac{1}{8}$		
Symmetry operations For $(0,0,0)$ + set			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c} 4^{-}(0,0,\frac{3}{4}) & \frac{1}{4},0,z \\ \hline 2 & x,\overline{x}+\frac{1}{4},\frac{1}{8} \\ \hline 4^{-} & 0,\frac{3}{4},z; 0,\frac{3}{4},\frac{1}{8} \\ \hline d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) & x,x,z \end{array} $	lo symmetry relations etween octahedra in the A
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2) $2^-\theta, \frac{1}{4}, z$ (5) $2(0, \frac{1}{2}, 0)^-\theta, y, \frac{1}{4}$ (6) $2(\frac{1}{2}, 0, 0)^-x, \frac{1}{4}, 0$ (9) $\overline{1} + \frac{1}{4}, \frac{1}{4}$ (10) $b^-x, y, 0$ (13) $c^-x, \frac{1}{4}, z^-$ (14) $b^-\frac{1}{4}, y, z^-$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 4^{-}(0,0,\frac{1}{4}) & \frac{3}{4},0,z \\ \hline 2 & x,\overline{x}+\frac{3}{4},\frac{3}{4} \\ \hline 4^{-} & 0,\frac{1}{4},z; 0,\frac{1}{4},\frac{3}{4} \\ \hline d(\frac{1}{4},\frac{1}{4},\frac{1}{4}) & x,x,z \end{array}$	nd B sublattices.



almost unchanged

of the moment size!



Requires two order parameters of different symmetries



### Mixing of two IR's gives Z<sub>2</sub>xZ<sub>2</sub>



their interference manifests as deviation of the azimuth angle from zero

# Spontaneous magnetic moment disproportionation

DFT results from I41/acd (Sublattice A and B symmetry-wise equivalent )

Spontanesous disproportionation!

Actual space group 141/a (glide planes c &d removed)

Magnetism drives lattice symmetry lowering!

Modulation of moment size, a new type of instability from pseudospins!

**Origin** at  $\overline{1}$  at b(c,a)d, at  $0, -\frac{1}{4}, \frac{1}{8}$  from  $\overline{4}$ Asymmetric unit  $0 \le x \le \frac{1}{2}$ ;  $-\frac{1}{4} \le y \le \frac{1}{4}$ ;  $0 \le z \le \frac{1}{4}$ Symmetry operations For (0,0,0) + set (4)  $4^{-}(0,0,\frac{3}{4}) = \frac{1}{4},0,z$ (1) 1 (2)  $2(0,0,\frac{1}{2}) = \frac{1}{4},0,z$ (3)  $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$ (7)  $2(\frac{1}{2},\frac{1}{2},0) \quad x,x+\frac{1}{4},\frac{3}{8}$ (11)  $\overline{4}^{+} \quad \frac{1}{2},-\frac{1}{4},z; \ \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ (5) 2  $\frac{1}{4}$ , y, 0 (9)  $\overline{1}$  0, 0, 0 (6) 2  $x, 0, \frac{1}{4}$ (8) 2  $x, \bar{x} + \frac{1}{4}, \frac{1}{4}$ (10)  $a x, y, \frac{1}{4}$ (12)  $\bar{4}^{-}$  0,  $\frac{3}{4}$ , z; 0,  $\frac{3}{4}$ ,  $\frac{1}{4}$ (15)  $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) \quad x+\frac{1}{2},\overline{x},z$ (14) c = 0, y, z(13) a x, 0, z(16)  $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4}) \quad x, x, z$ For  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  + set (3)  $4^+(0,0,\frac{3}{4}) = \frac{1}{4}, \frac{1}{2}, z$ (7)  $2(\frac{1}{2},\frac{1}{2},0) = x, x-\frac{1}{4}, \frac{1}{4}$ (1)  $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (2)  $2^{-}\theta, \frac{1}{4}, z$ (4)  $4^{-}(0,0,\frac{1}{4}) = \frac{3}{4},0,z$ (5)  $\underline{2}(0, \frac{1}{2}, 0) \quad 0, y, \frac{1}{4}$ (6)  $2(\frac{1}{2},0,0) \quad x,\frac{1}{4},0$ (8) 2  $x, \bar{x} + \frac{3}{4}, \frac{3}{8}$ (10) b x, y, 0(11)  $\bar{4}^+$   $\frac{1}{2}, \frac{1}{4}, z; \frac{1}{2}, \frac{1}{4}, \frac{1}{8}$ (12)  $\bar{4}^{-}$  0,  $\frac{1}{4}$ , z; 0,  $\frac{1}{4}$ ,  $\frac{3}{8}$ (9)  $\bar{1}$   $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (14)  $b = \frac{1}{4}, y, z$ (15)  $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4}) x + \frac{1}{2}, \bar{x}, z$ (13)  $c x, \frac{1}{4}, z$ (16)  $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) \quad x, x, z$ 

• 8 distinct Ir sites generated by symmetry operations

- $(1) \{0, 1/4, 3/8\} \\ (2) \{1/2, 3/4, 7/8\} \\ (3) \{0, 3/4, 5/8\} \\ (4) \{1/2, 1/4, 1/8\} \\ (5) \{1/2, 1/4, 5/8\} \\ (6$
- $(5) \quad \{1/2, 1/4, 5/8\}$
- $(6) \quad \{0, 3/4, 1/8\}$
- (7)  $\{1/2, 3/4, 3/8\}$
- $(8) \quad \{0, 1/4, 7/8\}$

<b>Origin</b> at $\overline{1}$ at $b(c,a)d$ , at $0, -\frac{1}{4}, \frac{1}{8}$ from $\overline{4}$							
Asymmetric unit 0	$\leq x \leq \frac{1}{2};  -\frac{1}{4} \leq y \leq \frac{1}{4};  0 \leq z \leq \frac{1}{4}$						
Symmetry operations							
For $(0,0,0)$ + set							
(1) 1 (5) 2 $\frac{1}{4}, y, 0$ (9) 1 0,0,0 (13) $a x, 0, z$	(2) $2(0,0,\frac{1}{2}) = \frac{1}{4},0,z$ (6) $2 = x,0,\frac{1}{4}$ (10) $a = x,y,\frac{1}{4}$ (14) $c = 0,y,z$	(3) $4^{+}(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{4},\frac{3}{8}$ (11) $\overline{4}^{+} -\frac{1}{2},-\frac{1}{4},z; \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ (15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) x+\frac{1}{2},\overline{x},z$	(4) $4^{-}(0,0,\frac{3}{4}) \frac{1}{4},0,z$ (8) $2 x, \overline{x} + \frac{1}{4}, \frac{1}{8}$ (12) $\overline{4}^{-} 0, \frac{3}{4}, z; 0, \frac{3}{4}, \frac{1}{8}$ (16) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4}) x,x,z$				
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ (5) $2(0, \frac{1}{2}, 0)  0, y, \frac{1}{4}$ (9) $\overline{1}  \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (13) $c  x \stackrel{1}{2} z$	(2) $2  \theta, \frac{1}{4}, z$ (6) $2(\frac{1}{2}, 0, 0)  x, \frac{1}{4}, 0$ (10) $b  x, y, 0$ (14) $b  \frac{1}{4}, y, z$	(3) $4^+(0,0,\frac{3}{4}) = \frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) = x,x-\frac{1}{4},\frac{1}{4}$ (11) $4^+ = \frac{1}{2},\frac{1}{4},z; = \frac{1}{2},\frac{1}{4},\frac{1}{4}$ (15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4}) = x+\frac{1}{4},\overline{x},z$	(4) $4^{-}(0,0,\frac{1}{4}) = \frac{3}{4},0,z$ (8) $2 = x, \overline{x} + \frac{3}{4}, \frac{3}{4}$ (12) $\overline{4}^{-} = 0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{4}$ (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) = x, x, z$				

• 8 distinct Ir sites generated by symmetry operations

<ol> <li>(1)</li> <li>(2)</li> <li>(3)</li> <li>(4)</li> <li>(5)</li> <li>(6)</li> <li>(7)</li> </ol>	{0, 1/4, 3/8} {1/2, 3/4, 7/8} {0, 3/4, 5/8} {1/2, 1/4, 1/8} {1/2, 1/4, 5/8} {0, 3/4, 1/8}
(6)	{0, 3/4, 1/8}
(7)	{1/2, 3/4, 3/8}
(8)	{0, 1/4, 7/8}

### • symmetry operations shuffle ir sites

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

<b>Origin</b> at $\overline{1}$ at $b(c,a)d$ , at $0, -\frac{1}{4}, \frac{1}{8}$ from $\overline{4}$					
Asymmetric unit (	$0 \le x \le \frac{1}{2};  -\frac{1}{4} \le y \le \frac{1}{4};  0 \le z \le \frac{1}{2}$				
Symmetry operations For $(0,0,0)$ + set (1) 1 (5) 2 $\frac{1}{4}$ , y, 0 (9) 1 0, 0, 0 (13) a x, 0, z	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (6) $2 x,0,\frac{1}{4}$ (10) $a x,y,\frac{1}{4}$ (14) $c 0,y,z$	(3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{4},\frac{3}{8}$ (11) $\overline{4}^+ -\frac{1}{2},-\frac{1}{4},z; \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ (15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) x+\frac{1}{2},\overline{x},z$	(4) $4^{-}(0,0,\frac{3}{4}) + 0,z$ (8) $2 + x, \overline{x} + \frac{1}{4}, \frac{1}{8}$ (12) $4^{-} + 0, \frac{3}{4}, z; 0, \frac{3}{4}, \frac{1}{8}$ (16) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4}) + x, x, z$		
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (5) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ (9) $\overline{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (13) $c$ $x, \frac{1}{4}, z$	(2) $2  0, \frac{1}{4}, z$ (6) $2(\frac{1}{2}, 0, 0)  x, \frac{1}{4}, 0$ (10) $b  x, y, 0$ (14) $b  \frac{1}{4}, y, z$	(3) $4^+(0,0,\frac{3}{4}) \frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x-\frac{1}{4},\frac{1}{8}$ (11) $\overline{4}^+ \frac{1}{2},\frac{1}{4},z;\frac{1}{2},\frac{1}{4},\frac{1}{8}$ (15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4}) x+\frac{1}{2},\overline{x},z$	(4) $4^{-}(0,0,\frac{1}{4}) \frac{3}{4},0,z$ (8) $2  x,\bar{x}+\frac{3}{4},\frac{3}{4}$ (12) $\bar{4}^{-}  0,\frac{1}{4},z;  0,\frac{1}{4},\frac{3}{4}$ (16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})  x,x,z$		

#### • magnetic moments are rotated under symmetry operations

#### symmetry operations shuffle ir sites

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

<b>Origin</b> at $\overline{1}$ at $b(c,a)d$ , at $0, -\frac{1}{4}, \frac{1}{8}$ from $\overline{4}$						
Asymmetric unit 0	$\leq x \leq \frac{1}{2};  -\frac{1}{4} \leq y \leq \frac{1}{4};  0 \leq z \leq \frac{1}{4}$					
Symmetry operations						
For $(0,0,0)$ + set						
(1) 1 (5) 2 $\frac{1}{4}$ , y, 0 (9) $\overline{1}$ 0, 0, 0 (13) $a$ x, 0, z	(2) $2(0,0,\frac{1}{2}) = \frac{1}{4},0,z$ (6) $2 = x,0,\frac{1}{4}$ (10) $a = x,y,\frac{1}{4}$ (14) $c = 0,y,z$	(3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{4},\frac{3}{8}$ (11) $\overline{4}^+ -\frac{1}{2},-\frac{1}{4},z; \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ (15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) x+\frac{1}{2},\overline{x},z$	$(4) \ 4^{-}(0,0,\frac{3}{4}) \ \frac{1}{4},0,z$ $(8) \ 2 \ x,\overline{x}+\frac{1}{4},\frac{1}{8}$ $(12) \ \overline{4}^{-} \ 0,\frac{3}{4},z; \ 0,\frac{3}{4},\frac{1}{8}$ $(16) \ d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) \ x,x,z$			
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ (5) $2(0, \frac{1}{2}, 0)  0, y, \frac{1}{4}$ (9) $\overline{1}  \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (13) $c  x, \frac{1}{4}, z$	(2) $2  0, \frac{1}{4}, z$ (6) $2(\frac{1}{2}, 0, 0)  x, \frac{1}{4}, 0$ (10) $b  x, y, 0$ (14) $b  \frac{1}{4}, y, z$	(3) $4^+(0,0,\frac{3}{4}) \frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x-\frac{1}{4},\frac{1}{8}$ (11) $\overline{4}^+ \frac{1}{2},\frac{1}{4},z; \frac{1}{2},\frac{1}{4},\frac{1}{8}$ (15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4}) x+\frac{1}{2},\overline{x},z$	(4) $4^{-}(0,0,\frac{1}{4}) = \frac{3}{4},0,z$ (8) $2 = x, \bar{x} + \frac{3}{4}, \frac{3}{8}$ (12) $\bar{4}^{-} = 0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$ (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) = x, x, z$			

magnetic moments are rotated under symmetry operations
 (M<sub>x</sub>,M<sub>y</sub>,M<sub>z</sub>) -> (-M<sub>y</sub>,M<sub>x</sub>,M<sub>z</sub>)

 symmetry operations shuffle ir sites

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

<b>Origin</b> at $\overline{1}$ at $b(c,a)d$ , at $0, -\frac{1}{4}, \frac{1}{8}$ from $\overline{4}$						
Asymmetric unit 0 ≤	$\leq x \leq \frac{1}{2};  -\frac{1}{4} \leq y \leq \frac{1}{4};  0 \leq z \leq \frac{1}{4}$					
Symmetry operations						
For $(0,0,0)$ + set						
(1) 1 (5) 2 $\frac{1}{4}$ , y, 0 (9) $\overline{1}$ 0, 0, 0 (13) $a$ x, 0, z	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (6) $2 x,0,\frac{1}{4}$ (10) $a x,y,\frac{1}{4}$ (14) $c 0,y,z$	(3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{4},\frac{3}{8}$ (11) $\overline{4}^+ -\frac{1}{2},-\frac{1}{4},z; \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ (15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) x+\frac{1}{2},\overline{x},z$	$(4) \ 4^{-}(0,0,\frac{3}{4}) \ \frac{1}{4},0,z$ $(8) \ 2 \ x,\overline{x}+\frac{1}{4},\frac{1}{8}$ $(12) \ \overline{4}^{-} \ 0,\frac{3}{4},z; \ 0,\frac{3}{4},\frac{1}{8}$ $(16) \ d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) \ x,x,z$			
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ (5) $2(0, \frac{1}{2}, 0)  0, y, \frac{1}{4}$ (9) $\overline{1}  \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (13) $c  x, \frac{1}{4}, z$	(2) $2 \stackrel{0}{\rightarrow} 0, \frac{1}{4}, z$ (6) $2(\frac{1}{2}, 0, 0)  x, \frac{1}{4}, 0$ (10) $b  x, y, 0$ (14) $b  \frac{1}{4}, y, z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{4}$ (11) $\overline{4}^+$ $\frac{1}{2},\frac{1}{4},z;$ $\frac{1}{2},\frac{1}{4},\frac{1}{4}$ (15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\overline{x},z$	(4) $4^{-}(0,0,\frac{1}{4}) \frac{3}{4},0,z$ (8) $2 x, \overline{x} + \frac{3}{4}, \frac{3}{4}$ (12) $\overline{4}^{-} 0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$ (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) x, x, z$			

 magnetic moments are rotated under symmetry operations (M<sub>x</sub>,M<sub>y</sub>,M<sub>z</sub>) -> (-M<sub>y</sub>,M<sub>x</sub>,M<sub>z</sub>)

#### • combining site shuffling and moment rotation

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### Assumption: magnetic order does not enlarge the unit cell

1       1       2       3       4       5       6       7       8         2       2       1       4       3       6       5       8       7         3       3       4       2       1       8       7       5       6         4       4       3       1       2       7       8       6       9         5       5       6       7       8       1       2       3       4         7       7       8       6       5       4       3       1       2         6       6       5       8       7       2       1       4       3       1       2         6       6       5       8       7       2       1       4       3       1       2         8       7       5       6       3       4       2       2       3         10       4       3       2       1       8       7       6       8       7       1         11       1       2       4       3       6       5       7       8       1       2       1 </th <th></th>	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7 5 4 3 2 L
3       3       4       2       1       8       7       5       6         4       4       3       1       2       7       8       6       9         5       5       6       7       8       1       2       3       4         6       6       5       8       7       2       1       4       3         7       7       8       6       5       4       3       1       2       3         8       8       7       5       6       3       4       2       3         9       3       4       1       2       7       8       5       6         10       4       3       2       1       8       7       6       5         11       1       2       4       3       6       5       7       8         12       2       1       3       4       5       6       8       7       2       1       3       4       1       2       4       3       1       2       4       3       1       2       4       3       1       2 <td>6 5 4 3 2 1</td>	6 5 4 3 2 1
4       4       3       1       2       7       8       6       9         5       5       6       7       8       1       2       3       4         7       7       8       6       5       4       3       1       2         7       7       8       6       5       4       3       1       2         9       3       4       1       2       7       8       5       6         10       4       3       2       1       8       7       6       5         10       4       3       2       1       8       7       6       5         11       1       2       4       3       6       5       7       8         12       2       1       3       4       5       6       8       7       2       1       3         14       8       7       6       5       4       3       2       2       3         15       5       6       8       7       2       1       3       6       5       8       7       5 <td< td=""><td>5 4 3 2 1</td></td<>	5 4 3 2 1
5       5       6       7       8       1       2       3       4         6       6       5       8       7       2       1       4       3         7       7       8       6       5       4       3       1       2         9       3       4       1       2       7       8       5       6         10       4       3       2       1       8       7       6       5         10       4       3       2       1       8       7       6       5         11       1       2       4       3       6       5       7       8         12       2       1       3       4       5       6       8       7       2         13       7       8       5       6       3       4       1       2         14       8       7       6       5       4       3       2       3         15       5       6       8       7       2       1       3       6       5         18       1       2       3       4	4 3 2 1
6 $6$ $5$ $8$ $7$ $2$ $1$ $4$ $3$ $7$ $7$ $8$ $6$ $5$ $4$ $3$ $1$ $2$ $9$ $3$ $4$ $1$ $2$ $7$ $8$ $5$ $6$ $10$ $4$ $3$ $2$ $1$ $8$ $7$ $6$ $5$ $10$ $4$ $3$ $2$ $1$ $8$ $7$ $6$ $5$ $11$ $1$ $2$ $4$ $3$ $6$ $5$ $7$ $8$ $12$ $2$ $1$ $3$ $4$ $5$ $6$ $8$ $7$ $12$ $2$ $1$ $3$ $4$ $5$ $6$ $8$ $7$ $12$ $2$ $1$ $3$ $4$ $5$ $6$ $8$ $7$ $13$ $7$ $8$ $5$ $6$ $3$ $4$ $1$ $2$ $14$ $8$ $7$ $6$ $5$ $4$ $3$ $2$ $2$ $14$ $8$ $7$ $6$ $5$ $8$ $7$ $2$ $1$ $14$ $8$ $7$ $6$ $5$ $8$ $7$ $2$ $1$ $4$ $16$ $6$ $5$ $7$ $8$ $1$ $2$ $7$ $8$ $6$ $5$ $18$ $1$ $2$ $3$ $4$ $2$ $1$ $8$ $7$ $5$ $6$ $20$ $3$ $4$ $2$ $1$ $8$ $7$ $2$ $1$ $4$ $3$ $19$ $4$ $3$ $1$ $2$ <td< td=""><td>3 2 1</td></td<>	3 2 1
7       7       8       6       5       4       3       1       2         8       8       7       5       6       3       4       2       2         9       3       4       1       2       7       8       5       6         10       4       3       2       1       8       7       6       2         11       1       2       4       3       6       5       7       8         12       2       1       3       4       5       6       8       7         13       7       8       5       6       3       4       1       2         14       8       7       6       5       4       3       2       2         15       5       6       8       7       2       1       3       4       5         16       6       5       7       8       1       2       4       3       6       5         18       1       2       3       4       5       6       7       8         20       3       4       2	2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1
9       3       4       1       2       7       8       5       6         10       4       3       2       1       8       7       6       9         11       1       2       4       3       6       5       7       8         12       2       1       3       4       5       6       8       7         12       2       1       3       4       5       6       8       7         12       2       1       3       4       5       6       8       7         13       7       8       5       6       3       4       1       2         14       8       7       6       5       4       3       2       3         15       5       6       8       7       2       1       3       4       3         16       6       5       7       8       1       2       4       3       6       5       8       7       2       1       4       3       6       5       8       7       5       6       9       9       9 <td< td=""><td>~</td></td<>	~
10       4       3       2       1       8       7       6       8         11       1       2       4       3       6       5       7       8         12       2       1       3       4       5       6       8       7         13       7       8       5       6       3       4       1       2         14       8       7       6       5       4       3       2       2         14       8       7       6       5       4       3       2       2         15       5       6       8       7       2       1       3       4         16       6       5       7       8       1       2       4       3         17       2       1       4       3       6       5       8       7       2         18       1       2       3       4       2       1       8       7       5       6         20       3       4       2       1       8       7       5       6         21       6       5       8	С
11       1       2       4       3       6       5       7       8         12       2       1       3       4       5       6       8       7         13       7       8       5       6       3       4       1       2         14       8       7       6       5       4       3       2       2         14       8       7       6       5       4       3       2       2         15       5       6       8       7       2       1       3       4         16       6       5       7       8       1       2       4       3         17       2       1       4       3       6       5       8       7         18       1       2       3       4       5       6       7       8         19       4       3       1       2       7       8       6       9         20       3       4       2       1       8       7       5       6         21       6       5       8       7       2       1	5
12       2       1       3       4       5       6       8       7         13       7       8       5       6       3       4       1       2         14       8       7       6       5       4       3       2       2         15       5       6       8       7       2       1       3       4         16       6       5       7       8       1       2       4       3         16       6       5       7       8       1       2       4       3         17       2       1       4       3       6       5       8       7       2         18       1       2       3       4       5       6       7       8         19       4       3       1       2       7       8       6       9         20       3       4       2       1       8       7       5       6         21       6       5       8       7       2       1       4       3       3	3
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	7
14       8       7       6       5       4       3       2       1         15       5       6       8       7       2       1       3       4         16       6       5       7       8       1       2       4       3         17       2       1       4       3       6       5       8       7         18       1       2       3       4       5       6       7       8         19       4       3       1       2       7       8       6       5         20       3       4       2       1       8       7       5       6         21       6       5       8       7       2       1       4       3	2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1
16       6       5       7       8       1       2       4       3         17       2       1       4       3       6       5       8       7         18       1       2       3       4       5       6       7       8         19       4       3       1       2       7       8       6       5         20       3       4       2       1       8       7       5       6         21       6       5       8       7       2       1       4       3	4
17       2       1       4       3       6       5       8       7         18       1       2       3       4       5       6       7       8         19       4       3       1       2       7       8       6       5         20       3       4       2       1       8       7       5       6         21       6       5       8       7       2       1       4       3	3
18       1       2       3       4       5       6       7       8         19       4       3       1       2       7       8       6       5         20       3       4       2       1       8       7       5       6         21       6       5       8       7       2       1       4       3	7
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21 6 5 8 7 2 1 4 3	5
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23 8 7 5 6 3 4 2 2	1
24 7 8 6 5 4 3 1 2	2
25 4 3 2 1 8 7 6 5	5
26 3 4 1 2 7 8 5 6	6
27 2 1 3 4 5 6 8	7
28 1 2 4 3 6 5 7 8	3
29 8 7 6 5 4 3 2 2	1
30 7 8 5 6 3 4 1 2	2
31 6 5 7 8 1 2 4 3	3
32   5 6 8 7 2 1 3 4	4

<b>Origin</b> at $\overline{1}$ at $b(c, a)$	) <i>d</i> , at $0, -\frac{1}{4}, \frac{1}{8}$ from $\frac{1}{4}$		
Asymmetric unit 0	$\leq x \leq \frac{1}{2};  -\frac{1}{4} \leq y \leq \frac{1}{4};  0 \leq z \leq \frac{1}{2}$		
Symmetry operations			
For $(0,0,0)$ + set			
(1) 1 (5) 2 $\frac{1}{4}$ , y, 0 (9) 1 0, 0, 0 (13) a x, 0, z	(2) $2(0,0,\frac{1}{2}) = \frac{1}{4},0,z$ (6) $2 = x,0,\frac{1}{4}$ (10) $a = x,y,\frac{1}{4}$ (14) $c = 0,y,z$	(3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x+\frac{1}{4},\frac{3}{8}$ (11) $\overline{4}^+ -\frac{1}{2},-\frac{1}{4},z; \frac{1}{2},-\frac{1}{4},\frac{3}{8}$ (15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4}) x+\frac{1}{2},\overline{x},z$	$(4) \ 4^{-}(0,0,\frac{3}{4}) \ \frac{1}{4},0,z$ $(8) \ 2 \ x,\overline{x}+\frac{1}{4},\frac{1}{8}$ $(12) \ \overline{4}^{-} \ 0,\frac{3}{4},z; \ 0,\frac{3}{4},\frac{1}{8}$ $(16) \ d(\frac{3}{4},\frac{3}{4},\frac{3}{4}) \ x,x,z$
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ set (1) $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})^+$ (5) $2(0, \frac{1}{2}, 0)  0, y, \frac{1}{4}$ (9) $\overline{1}  \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (13) $c  x, \frac{1}{4}, z$	(2) $2 \stackrel{0}{\rightarrow} 0, \frac{1}{4}, z$ (6) $2(\frac{1}{2}, 0, 0)  x, \frac{1}{4}, 0$ (10) $b  x, y, 0$ (14) $b  \frac{1}{4}, y, z$	(3) $4^+(0,0,\frac{3}{4}) \frac{1}{4},\frac{1}{2},z$ (7) $2(\frac{1}{2},\frac{1}{2},0) x,x-\frac{1}{4},\frac{1}{4}$ (11) $\overline{4}^+ \frac{1}{2},\frac{1}{4},z;\frac{1}{2},\frac{1}{4},\frac{1}{4}$ (15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4}) x+\frac{1}{2},\overline{x},z$	(4) $4^{-}(0,0,\frac{1}{4}) \frac{3}{4},0,z$ (8) $2 x, \overline{x} + \frac{3}{4}, \frac{3}{8}$ (12) $\overline{4}^{-} 0, \frac{1}{4}, z; 0, \frac{1}{4}, \frac{3}{8}$ (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}) x, x, z$

 magnetic moments are rotated under symmetry operations (M<sub>x</sub>,M<sub>y</sub>,M<sub>z</sub>) -> (-M<sub>y</sub>,M<sub>x</sub>,M<sub>z</sub>)

- combining site shuffling and moment rotation
- propagation vector k=(0,0,0) or k=(1,0,0)



### Assumption: magnetic order does not enlarge the unit cell

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

<b>Origin</b> at $\overline{1}$ at $b(c, a)$	)d, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\frac{1}{4}$		
Asymmetric unit (	$0 \le x \le \frac{1}{2};  -\frac{1}{4} \le y \le \frac{1}{4};  0 \le z \le \frac{1}{2}$		
Symmetry operations			
For $(0,0,0)$ + set	(2) $2(0,0,\frac{1}{2}) = \frac{1}{4},0,7$	(3) $4^+(0,0,\frac{1}{4}) -\frac{1}{4},\frac{1}{2},7$	$(4) 4^{-}(0,0,\frac{3}{2}) \frac{1}{2},0,7$
$(5)$ 2 $\frac{1}{2}$ $\frac{1}{2}$ , y, 0 (9) $\overline{1}$ 0.0.0	(6) $2^{-} x, 0, \frac{1}{4}$ (10) $a^{-} x, y, \frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$ (11) $4^{+}$ $\frac{1}{2},-\frac{1}{4},7,\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	$(12) \ \overline{4}^{-} \ 0 \ \overline{3} \ 7^{-} \ 0 \ \overline{3} \ \overline{4}^{-} \ 0 \ \overline{3}^{-} \ \overline{4}^{-} \ 0 \ $
(13) $a x, 0, z$	(14) $c$ 0, y, z	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})  x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4}) x, x, z$
For $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ + set	(2) $2 - \frac{1}{2} - \frac{1}{2} - \frac{1}{2}$	(3) $4^+(0,0,\frac{3}{2}) + \frac{1}{2} \frac{1}{2}$	$(4) 4^{-}(0 0 4) 3 0 7$
(1) $2(0, 1, 2)$ (5) $2(0, \frac{1}{2}, 0)$ $0, y, \frac{1}{4}$ (9) $\overline{1}$ $1$ $1$ $1$ $1$	$\begin{array}{c} (2) & 2 & (3,4,2) \\ (6) & 2(\frac{1}{2},0,0) & x,\frac{1}{4},0 \\ (10) & b & x & y,0 \end{array}$	$\begin{array}{c} (3) & 1 & (3,3,4) & 4,2,2 \\ (7) & 2(\frac{1}{2},\frac{1}{2},0) & x,x-\frac{1}{4},\frac{1}{4} \\ (11) & \overline{A}^{+} & 1 & 1 & 7 & 1 & 1 \end{array}$	$(4) = (0, 0, 4) + 4, 0, 2$ $(8) = 2 + x, \bar{x} + \frac{3}{4}, \frac{3}{4}$ $(12) = \bar{4} - 0 + z; 0 + \frac{3}{4}$
(13) $c x, \frac{1}{4}, z$	(14) $b = \frac{1}{4}, y, z$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	(12) $4^{-}$ $0, \overline{4}, \overline{2}, \overline{0}, \overline{4}, \overline{8}$ (16) $d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})  x, x, z$

• magnetic moments are rotated under symmetry operations  $(M_x, M_y, M_z) \rightarrow (-M_y, M_x, M_z)$ 

#### • combining site shuffling and moment rotation

 Find a basis that brings all 32 24x24 matrices to a smallest block-diagonal form

 A second order phase transition involves an order parameter belonging to a single irreducible representation

(	Θ	0	0	Θ	0	0	Θ	1	0	Θ	0	0	Θ	0	0	Θ	0	0	Θ	0	0	0	0	0
	Θ	0	0	Θ	0	0	-1	0	0	Θ	0	0	Θ	0	0	Θ	0	0	Θ	0	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	1	Θ	0	0	Θ	0	0	Θ	0	0	0	0	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	0	1	0	Θ	0	0	0	0	0	0	0	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	-1	0	0	Θ	0	0	Θ	0	0	0	0	0	0	0	0
	Θ	0	Θ	Θ	0	0	0	0	0	0	Θ	1	Θ	0	0	0	0	0	0	0	0	0	0	0
	Θ	Θ	0	Θ	1	0	0	0	0	0	0	0	Θ	0	0	Θ	0	0	0	0	0	0	0	0
	Θ	0	0	-1	0	0	0	0	0	0	0	0	Θ	0	0	Θ	0	0	0	0	0	0	0	0
	Θ	0	0	Θ	0	1	0	0	0	Θ	0	0	Θ	0	0	Θ	0	0	Θ	0	0	0	0	0
	Θ	1	0	Θ	0	0	0	0	0	0	0	0	Θ	0	0	0	0	0	0	0	0	0	0	0
	-1	0	0	Θ	0	0	Θ	0	0	Θ	0	0	Θ	0	0	Θ	0	0	0	0	0	0	0	0
	Θ	0	1	Θ	0	0	0	0	0	0	0	0	Θ	0	0	Θ	0	0	0	0	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	Θ	0	0	Θ	0	0	Θ	0	0	0	0	0	0	1	0
	Θ	0	0	Θ	0	0	0	0	0	0	0	0	Θ	0	0	0	0	0	0	0	0	-1	0	0
r	Θ	0	0	Θ	0	0	0	0	0	0	0	0	Θ	0	0	0	0	0	0	0	0	0	0	1
	Θ	0	0	Θ	0	0	0	0	0	0	0	0	Θ	0	0	0	0	0	0	1	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	0	Θ	0	Θ	0	0	Θ	0	0	-1	0	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	0	0	0	Θ	0	0	0	0	0	0	0	1	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	0	0	0	Θ	1	0	0	0	0	0	0	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	0	0	0	-1	0	0	0	0	0	0	0	0	0	0	0
	Θ	0	0	0	0	0	0	0	0	0	0	0	Θ	0	1	0	0	0	0	0	0	0	0	0
	Θ	0	0	Θ	0	0	0	0	0	0	0	0	Θ	0	0	0	1	0	0	0	0	0	0	0
	Θ	0	0	0	0	0	0	0	0	0	0	0	Θ	0	0	-1	0	0	0	0	0	0	0	0
	Θ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0

# Assumption: magnetic order does not enlarge the unit cell

	1	2	3	4	5	6	7	8
1	1	2	3	4	5	6	7	8
2	2	1	4	3	6	5	8	7
3	3	4	2	1	8	7	5	6
4	4	3	1	2	7	8	6	5
5	5	6	7	8	1	2	3	4
6	6	5	8	7	2	1	4	3
7	7	8	6	5	4	3	1	2
8	8	7	5	6	3	4	2	1
9	3	4	1	2	7	8	5	6
10	4	3	2	1	8	7	6	5
11	1	2	4	3	6	5	7	8
12	2	1	3	4	5	6	8	7
13	7	8	5	6	3	4	1	2
14	8	7	6	5	4	3	2	1
15	5	6	8	7	2	1	3	4
16	6	5	7	8	1	2	4	3
17	2	1	4	3	6	5	8	7
18	1	2	3	4	5	6	7	8
19	4	3	1	2	7	8	6	5
20	3	4	2	1	8	7	5	6
21	6	5	8	7	2	1	4	3
22	5	6	7	8	1	2	3	4
23	8	7	5	6	3	4	2	1
24	7	8	6	5	4	3	1	2
25	4	3	2	1	8	7	6	5
26	3	4	1	2	7	8	5	6
27	2	1	3	4	5	6	8	7
28	1	2	4	3	6	5	7	8
29	8	7	6	5	4	3	2	1
30	7	8	5	6	3	4	1	2
31	6	5	7	8	1	2	4	3
32	5	6	8	7	2	1	3	4

• 24x24 matrices split into:

4 x 2D 4 x 4D

• In general, any physical quantity can be expressed in terms of

8 x 1D 6 x 2D

for the factor group G(k)/T(k) under consideration (32 symmetry operations, 14 classes)

• 24x24 matrices split into:

4 x 2D 4 x 4D

• In general, any physical quantities can be expressed in terms of

8 x 1D 6 x 2D (Gamma1-Gamma6)

for the factor group G(k)/T(k) under consideration (32 symmetry operations, 14 classes)

#### Gamma2

-	lx	1y	1z	2x	2у	2z	3x	Зу	3z	4x	4y	4z	5x	5y	5z	6x	6у	6z	7x	7у	7z	8x	8y	8z
1	-1	0	0	-1	0	0	-1	0	0	-1	0	0	0	1	0	0	1	0	0	1	0	0	1	0
2	Θ	-1	Θ	Θ	-1	Θ	0	-1	0	0	-1	Θ	1	Θ	Θ	1	0	Θ	1	Θ	Θ	1	0	0
3	Θ	1	Θ	Θ	1	Θ	Θ	1	Θ	Θ	1	Θ	1	Θ	Θ	1	Θ	Θ	1	Θ	Θ	1	Θ	0
4	1	Θ	0	1	Θ	Θ	1	Θ	0	1	Θ	0	0	1	Θ	0	1	0	0	1	0	Θ	1	0

#### Gamma3

	lx	1y	1z	2x	2у	2z	3x	Зу	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7у	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	0	0	0	0	0	-1	0	Θ	1	0	Θ	0	0	0	0	0	0
2	Θ	Θ	Θ	Θ	Θ	Θ	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	-1	Θ	Θ	1	0
3	Θ	<b>- 1</b>	Θ	Θ	1	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	Θ	Θ	Θ	0
4	0	0	0	Θ	0	0	1	0	0	-1	0	0	Θ	0	0	0	0	0	1	Θ	0	<b>-1</b>	Θ	0

#### Gamma4

	1x	1y	1z	2x	2у	2z	3x	Зу	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	-1	0	0	1	0	1	0	0	-1	0	0	0	-1	Θ	0	1	0
2	-1	Θ	Θ	1	Θ	Θ	Θ	1	Θ	Θ	-1	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	1	Θ	Θ	-1	0
3	Θ	-1	0	0	1	Θ	-1	Θ	Θ	1	Θ	Θ	Θ	-1	0	0	1	Θ	1	0	0	<b>- 1</b>	Θ	0
4	0	-1	Θ	0	1	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	-1	Θ	Θ	1	Θ	-1	Θ	Θ	1	Θ	Θ

#### Gamma5

	lx	1y	1z	2x	2у	2z	3x	Зу	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7у	7z	8x	8y	8z
1	-1	0	0	-1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	1	Θ	Θ	1	Θ	Θ	-1	Θ	Θ	-1	0
3	Θ	-1	Θ	Θ	-1	Θ	Θ	1	Θ	Θ	1	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ
4	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	1	Θ	Θ	1	Θ	Θ	-1	Θ	Θ	-1	Θ	Θ



	1x	1y	1z	2x	2у	2z	Зx	Зу	3z	4x	4y	4z	5x	5y	5z	6x	6у	6z	7x	7у	7z	8x	8y	8z
1	-1	0	0	-1	O	0	-1	0 <mark>_</mark>	Θ	-1	0	O	0	1	0	0	1	0	0	1	0	0	1	0
2	0	-1	0	Θ	1	0	20	C-IC	70	2P1		/9	h		ro	1	00	0	1	0	0	1	0	0
3	Θ	1	Θ	Θ				212		9		Val	1	$\sim$		<b>y</b> 1			1	Θ	Θ	1	Θ	0
4	1	Θ	Θ	1	Θ	Θ	1	0	0	1	0	Θ	0	1	0	0	1	Θ	0	1	Θ	Θ	1	0

#### Gamma3

	lx	1y	1z	2x	2у	2z	3x	Зу	3z	4x	4y	4z	5x	5y	5z	6x	6y	6z	7x	7у	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	0	0	0	0	0	-1	0	0	1	0	0	0	0	0	0	0	0
2	Θ	Θ	Θ	Θ	Θ	Θ	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	-1	Θ	Θ	1	0
3	Θ	- <b>1</b>	Θ	Θ	1	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	Θ	Θ	Θ	0
4	Θ	0	Θ	Θ	0	Θ	1	Θ	Θ	-1	0	Θ	Θ	Θ	0	0	Θ	0	1	Θ	0	-1	Θ	0

#### Gamma4

	lx	1y	1z	2x	2у	2z	3x	3у	3z	4x	4y	4z	5x	5y	5z	6x	6у	6z	7x	7у	7z	8x	8y	8z
1	-1	0	0	1	0	0	0	-1	0	0	1	0	1	0	0	-1	0	0	0	-1	0	0	1	0
2	-1	Θ	Θ	1	Θ	Θ	Θ	1	Θ	Θ	-1	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	1	Θ	Θ	-1	0
3	0	-1	Θ	Θ	1	0	-1	0	Θ	1	0	Θ	Θ	-1	0	Θ	1	0	1	Θ	Θ	-1	0	0
4	Θ	-1	Θ	Θ	1	Θ	1	Θ	Θ	-1	Θ	Θ	Θ	-1	Θ	Θ	1	Θ	-1	0	Θ	1	Θ	Θ

#### Gamma5

	1x	ly	1z	2x	2у	2z	3x	Зу	3z	4x	4y	4z	5x	5y	5z	6x	6у	6z	7x	7y	7z	8x	8y	8z
1	-1	0	0	-1	0	0	1	Q	0	1	0	0	0	0	0	0	0	0	0	0	Θ	0	0	0
2	Θ	Θ	Θ	Θ	Ð	00	P C	CIC		Ø	0	19+	h		r g	0	<b>ND</b>	6	0	<b>-1</b>	Θ	0	<b>- 1</b>	Θ
3	Θ	-1	Θ	Θ			9	212		0		V I C	6	∕₀		0	<b>U</b> a		0	Θ	Θ	Θ	0	Θ
4	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	1	Θ	Θ	1	Θ	Θ	-1	Θ	Θ	-1	Θ	Θ



Requires two order parameters of different symmetries in 141/acd

# Symmetry of the magnetic order

Gamma3

Gamma4





invariant under

1,2,9,10,21,22,29,30

1,2,5,6,9,10,13,14

# Symmetry of the lattice



invariant under with timer reversal 5,6,13,14,17,18,25,26

17,18,21,22,25,26,29,30

# Symmetry of the lattice

Gamma3

Separately, Gamma3 and Gamma4 both leads to lattice symmetry of lbca, but...

when simultaneously present, the lattice will be I2/a (C2/c)



Gamma4

invariant under invariant under with timer reversal 1,2,9,10 17,18,25,26

# Summary

DFT results from I41/acd (Sublattice A and B symmetrywise equivalent )

Spontanesous disproportionation!

Actual space group 141/a (glide planes c &d removed)



Magnetism drives lattice symmetry lowering!

Modulation of moment size, a new type of instability from pseudospins!