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Tables of Magnetic Space Groups II. Special Positions

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The table of P4/mmm and related antigroups is presented as an example of the tables of special positions.

Tables of magnetic space groups, for all general positions in all colorless or black-white groups, have been presented at the 1960 International Congress of Crystallography. The present paper deals with the second part of the work, namely the special positions in the above groups. One table, that of P4/mmm and related antigroups, is given as an example. The co-ordinates of the sites of one position are listed vertically under the position symbol, which is the Wyckoff position letter preceded by the multiplicity of the position. Every magnetic moment at a site is given by the trimetric components of the corresponding axial vector. The moment symbols are given, for all the sites of every antiferromagnetic position in P4/mmm or any related antigroup, in the appropriate column, vertically under a symbol that expresses the point-group symmetry or antisymmetry of the first site of the position in the group appearing as column heading. Non-tetragonal symmetries are symbolized in tetragonal form, so as to show the orientation of the symmetry elements of the site. It may be necessary to distinguish the two symmetry directions in the second or third column of the symbol; in such a case we expand the symbol, enclosing the two symmetry directions between parentheses and letting them refer to [100] [010] or to [110] [1$\bar{1}$0] respectively. Examples: $m(2m)1$; $2(m'm')1$. Ferromagnetic positions are marked *FM*; the moment is given only for the first site of the position. Positions that are forbidden to magnetic atoms are called non-magnetic and are designated *NM*.

DISCUSSION

G. E. BACON: Could I make a plea that someone would write a "Child's guide" to magnetic space groups, saying why a knowledge of them is useful and what the main principle to be considered is? Otherwise I fear that although we shall see an excellent set of tables they will not be fully appreciated or used to advantage, except by a very few experts.

J. D. H. DONNAY: An introduction to the tables will give explicit directions as to how to use them.

B. C. FRAZER: I wonder if you could make some comments on some of the strange new magnetic structures which seem to be possible? You included some remarks on spiral structures in your talk, but what can be said of the cases which have recently been observed in which there is a sinusoidal variation in the effective magnitude of the moment? Also, a structure which I do not believe has actually been observed, although it came up at one point in the discussion of chromium at Gatlinburg, is the anisotropic spiral in which the angle between successive spin vectors is not constant.

J. D. H. DONNAY: The sinusoidal variation of the magnetic moment might possibly be the result of a uniform rotation of a vector whose projection is being considered. The generalized space groups in which a rotation matrix is attached to each equivalent point could then be used.

As to the different variation of the angle of rotation from one layer to the next in

Magnetic special positions in $P4/mmm$ and related antigroups

Position symbols and Position sites		339 $P\frac{4}{m}\frac{2}{m}\frac{2}{m}$	341 $P\cdot\frac{4}{m'}\frac{2'}{m}\frac{2'}{m}$	342 $P\frac{4'}{m}\frac{2'}{m'}\frac{2}{m}$	343 $P\frac{4'}{m}\frac{2}{m}\frac{2'}{m'}$	344 $P\cdot\frac{4'}{m'}\frac{2}{m'}\frac{2'}{m}$	345 $P\frac{4}{m}\frac{2'}{m'}\frac{2'}{m'}$	346 $P\cdot\frac{4'}{m'}\frac{2'}{m}\frac{2}{m'}$	347 $P\cdot\frac{4}{m'}\frac{2}{m'}\frac{2}{m'}$
		$P4/mmm$	$P4/m'mm$	$P4'/mm'm$	$P4'/mmm'$	$P4'/m'm'm$	$P4/mm'm'$	$P4'/m'mm'$	$P4/m'm'm'$
$8s$	$8t$	$1(1m)1$	$1(1m)1$	$1(1m')1$	$1(1m)1$	$1(1m')1$	$1(1m')1$	$1(1m)1$	$1(1m')1$
$x0z$	$x\tfrac12 z$	010	010	$u0w$	010	$u0w$	$u0w$	010	$u0w$
$0xz$	$\tfrac12 xz$	$\bar{1}00$	$\bar{1}00$	$0\bar{u}\bar{w}$	100	$0\bar{u}\bar{w}$	$0uw$	100	$0uw$
$\bar{x}0z$	$\bar{x}\tfrac12 z$	$0\bar{1}0$	$0\bar{1}0$	$\bar{u}0w$	$0\bar{1}0$	$\bar{u}0w$	$\bar{u}0w$	$0\bar{1}0$	$\bar{u}0w$
$0\bar{x}z$	$\tfrac12\bar{x}z$	100	100	$0u\bar{w}$	$\bar{1}00$	$0u\bar{w}$	$0\bar{u}w$	$\bar{1}00$	$0\bar{u}w$
$\bar{x}0\bar{z}$	$\bar{x}\tfrac12\bar{z}$	010	$0\bar{1}0$	$u0w$	010	$\bar{u}0\bar{w}$	$u0w$	$0\bar{1}0$	$\bar{u}0\bar{w}$
$0\bar{x}\bar{z}$	$\tfrac12\bar{x}\bar{z}$	$\bar{1}00$	100	$0\bar{u}\bar{w}$	100	$0uw$	$0uw$	$\bar{1}00$	$0\bar{u}\bar{w}$
$x0\bar{z}$	$x\tfrac12\bar{z}$	$0\bar{1}0$	010	$\bar{u}0w$	$0\bar{1}0$	$u0\bar{w}$	$\bar{u}0w$	010	$u0\bar{w}$
$0x\bar{z}$	$\tfrac12 x\bar{z}$	100	$\bar{1}00$	$0u\bar{w}$	$\bar{1}00$	$0\bar{u}w$	$0\bar{u}w$	100	$0u\bar{w}$
	$8r$	$11(1m)$	$11(1m)$	$11(1m)$	$11(1m')$	$11(1m)$	$11(1m')$	$11(1m')$	$11(1m')$
	xxz	$1\bar{1}0$	$1\bar{1}0$	$1\bar{1}0$	uuw	$1\bar{1}0$	uuw	uuw	uuw
	$\bar{x}xz$	110	110	$\bar{1}\bar{1}0$	$u\bar{u}\bar{w}$	$\bar{1}\bar{1}0$	$\bar{u}uw$	$u\bar{u}\bar{w}$	$\bar{u}uw$
	$\bar{x}\bar{x}z$	$\bar{1}10$	$\bar{1}10$	$\bar{1}10$	$\bar{u}\bar{u}w$	$\bar{1}10$	$\bar{u}\bar{u}w$	$\bar{u}\bar{u}w$	$\bar{u}\bar{u}w$
	$x\bar{x}z$	$\bar{1}\bar{1}0$	$\bar{1}\bar{1}0$	110	$\bar{u}u\bar{w}$	110	$u\bar{u}w$	$\bar{u}u\bar{w}$	$u\bar{u}w$
	$\bar{x}\bar{x}\bar{z}$	$1\bar{1}0$	$\bar{1}10$	$1\bar{1}0$	uuw	$\bar{1}10$	uuw	$\bar{u}\bar{u}\bar{w}$	$\bar{u}\bar{u}\bar{w}$
	$x\bar{x}\bar{z}$	110	$\bar{1}\bar{1}0$	$\bar{1}\bar{1}0$	$u\bar{u}\bar{w}$	110	$\bar{u}uw$	$\bar{u}uw$	$u\bar{u}\bar{w}$
	$xx\bar{z}$	$\bar{1}10$	$1\bar{1}0$	$\bar{1}10$	$\bar{u}\bar{u}w$	$1\bar{1}0$	$\bar{u}\bar{u}w$	$uu\bar{w}$	$uu\bar{w}$
	$\bar{x}x\bar{z}$	$\bar{1}\bar{1}0$	110	110	$\bar{u}u\bar{w}$	$\bar{1}\bar{1}0$	$u\bar{u}w$	$u\bar{u}w$	$\bar{u}u\bar{w}$
$8p$	$8q$	$m11$	$m'11$	$m11$	$m11$	$m'11$	$m11$	$m'11$	$m'11$
$xy0$	$xy\tfrac12$	001	$uv0$	001	001	$uv0$	001	$uv0$	$uv0$
$\bar{y}x0$	$\bar{y}x\tfrac12$	001	$\bar{v}u0$	$00\bar{1}$	$00\bar{1}$	$v\bar{u}0$		$v\bar{u}0$	$\bar{v}u0$
$\bar{x}\bar{y}0$	$\bar{x}\bar{y}\tfrac12$	001	$\bar{u}\bar{v}0$	001	001	$\bar{u}\bar{v}0$		$\bar{u}\bar{v}0$	$\bar{u}\bar{v}0$
$y\bar{x}0$	$y\bar{x}\tfrac12$	001	$v\bar{u}0$	$00\bar{1}$	$00\bar{1}$	$\bar{v}u0$		$\bar{v}u0$	$v\bar{u}0$
$yx0$	$yx\tfrac12$	$00\bar{1}$	$\bar{v}\bar{u}0$	$00\bar{1}$	001	$\bar{v}\bar{u}0$	FM	$vu0$	$vu0$
$\bar{x}y0$	$\bar{x}y\tfrac12$	$00\bar{1}$	$u\bar{v}0$	001	$00\bar{1}$	$\bar{u}v0$		$u\bar{v}0$	$\bar{u}v0$
$\bar{y}\bar{x}0$	$\bar{y}\bar{x}\tfrac12$	$00\bar{1}$	$vu0$	$00\bar{1}$	001	$vu0$		$\bar{v}\bar{u}0$	$\bar{v}\bar{u}0$
$x\bar{y}0$	$x\bar{y}\tfrac12$	$00\bar{1}$	$\bar{u}v0$	001	001	$u\bar{v}0$		$\bar{u}v0$	$u\bar{v}0$

$4l$	$4m$	$4n$	$4o$	$m(2m)1$	$m'(2'm)1$	$m(2'm')1$	$m(2m)1$	$m'(2m')1$	$m(2'm')1$	$m'(2'm)1$	$m'(2m')1$
$x00$	$x0\frac{1}{2}$	$x\frac{1}{2}0$	$x\frac{1}{2}\frac{1}{2}$		010	001		100	001	010	100
$0x0$	$0x\frac{1}{2}$	$\frac{1}{2}x0$	$\frac{1}{2}x\frac{1}{2}$		$\bar{1}00$	$00\bar{1}$		$0\bar{1}0$		100	010
$\bar{x}00$	$\bar{x}0\frac{1}{2}$	$\bar{x}\frac{1}{2}0$	$\bar{x}\frac{1}{2}\frac{1}{2}$	*NM*	$0\bar{1}0$	001	*NM*	$\bar{1}00$	*FM*	$0\bar{1}0$	$\bar{1}00$
$0\bar{x}0$	$0\bar{x}\frac{1}{2}$	$\frac{1}{2}\bar{x}0$	$\frac{1}{2}\bar{x}\frac{1}{2}$		100	$00\bar{1}$		010		$\bar{1}00$	$0\bar{1}0$
		$4j$	$4k$	$m1(2m)$	$m'1(2'm)$	$m1(2m)$	$m1(2'm')$	$m'1(2'm)$	$m1(2'm')$	$m'1(2m')$	$m'1(2m')$
		$xx0$	$xx\frac{1}{2}$		$1\bar{1}0$		001	$1\bar{1}0$	001	110	110
		$\bar{x}x0$	$\bar{x}x\frac{1}{2}$		110		$00\bar{1}$	$\bar{1}\bar{1}0$		$1\bar{1}0$	$\bar{1}10$
		$\bar{x}\bar{x}0$	$\bar{x}\bar{x}\frac{1}{2}$	*NM*	$\bar{1}10$	*NM*	001	$\bar{1}10$	*FM*	$\bar{1}\bar{1}0$	$\bar{1}\bar{1}0$
		$x\bar{x}0$	$x\bar{x}\frac{1}{2}$		$\bar{1}\bar{1}0$		$00\bar{1}$	110		$\bar{1}10$	$1\bar{1}0$
			$4i$	$2(mm)1$	$2(mm)1$	$2(m'm')1$	$2(mm)1$	$2(m'm')1$	$2(m'm')1$	$2(mm)1$	$2(m'm')1$
			$0\frac{1}{2}z$			001		001	001		001
			$\frac{1}{2}0z$			$00\bar{1}$		$00\bar{1}$			001
			$0\frac{1}{2}\bar{z}$	*NM*	*NM*	001	*NM*	$00\bar{1}$	*FM*	*NM*	$00\bar{1}$
			$\frac{1}{2}0\bar{z}$			$00\bar{1}$		001			$00\bar{1}$
		$2g$	$2h$	$4mm$	$4m$	$4'm'm$	$4'mm'$	$4'm'm$	$4m'm'$	$4'mm'$	$4m'm'$
		$00z$	$\frac{1}{2}\frac{1}{2}z$						001		001
		$00\bar{z}$	$\frac{1}{2}\frac{1}{2}\bar{z}$	*NM*	*NM*	*NM*	*NM*	*NM*	*FM*	*NM*	$00\bar{1}$
		$2e$	$2f$	$m(mm)1$	$m'(mm)1$	$m(m'm')1$	$m(mm)1$	$m'(m'm')1$	$m(m'm')1$	$m'(mm)1$	$m'(m'm')1$
		$0\frac{1}{2}\frac{1}{2}$	$0\frac{1}{2}0$			001			001		
		$\frac{1}{2}0\frac{1}{2}$	$\frac{1}{2}00$	*NM*	*NM*	$00\bar{1}$	*NM*	*NM*	*FM*	*NM*	*NM*
$1a$	$1b$	$1c$	$1d$	$4/mmm$	$4/m'mm$	$4'/mm'm$	$4'/mmm'$	$4'/m'm'm$	$4/mm'm'$	$4'/m'mm'$	$4/m'm'm'$
000	$00\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	*NM*	*NM*	*NM*	*NM*	*NM*	001	*NM*	*NM*
				339	341	342	343	344	345	346	347

the case of an anisotropic spiral, I can only wonder whether this is a well-established fact. I can see no explanation for it.

On the (helical) spiral it might be of interest to recall that such spirals were the first examples of application of the generalized theory in which a rotation matrix is associated to each site. The concept of rotatory translation (translation rotation), which we introduced at the Gatlinburg conference in 1960, could thus be considered a prediction of the theory; Dr. F.E. Bertaut, starting from the facts of the spiral, in a way rediscovered the theory since he was led to the same new symmetry operation.

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Coherent Bragg Scattering of Resonant Nuclides

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Coherent Bragg scattering studies with neutrons on cadmium, boron and lithium containing compounds have given evidence of anomalous intensity behavior caused by the complex scattering amplitudes associated with neutron resonance. Bragg scattering intensities from (hkl) and $(\bar{h}\bar{k}\bar{l})$ mates in non-centrosymmetric crystals show a non-observance of Friedel's Law for all three elements, characteristic of crystals containing scatterers with complex amplitudes. In the case of cadmium, with its strong low energy resonance, pronounced resonance effects with strongly energy dependent scattering are observed. The Breit-Wigner resonance scattering expression accurately accounts for all of the observed effects.

1. Introduction

Neutron crystallography has recently acquired a new technique, that of Bragg scattering of resonant neutrons[1], which should play a role in neutron diffraction similar to that of anomalous scattering in X-ray diffraction. It is well known that an excited or resonant scatterer introduces a phase shift in the scattered wave which provides a useful tool for identification of the excited scatterer and for determining the phases of the scattered waves[2]. Since the phase determination is absolute, not only crystal structure but absolute configuration of non-centrosymmetric crystals can be determined. In addition the effect of the resonance is to produce large, energy dependent scattering amplitudes which can be utilized in solving specific problems and which must be reckoned with in structural work.

While X-ray resonance scattering is primarily electronic in origin, resonant neutron scattering as well as the recently observed resonant γ-ray scattering[3] involve nuclear interactions. Appropriate theoretical treatments yield the Breit-Wigner dispersion relations[4] which have been very successful in correlating both absorption and total scattering at resonance[5]. Specific applications of the theory to bound nuclei in crystals have been given by Lamb[6] and more recently by Trammell[7] who have considered the effects of Doppler broadening and finite lifetime of the compound nucleus. The single level scattering expression, applicable to free nuclei at rest, for the scattering amplitude may be written in the form $f=\Delta f'+i\Delta f''+f_0$ and is in detail

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