MAGNETIC SYMMETRY AND CRYSTAL LATTICES

BY S. BHAGAVANTAM, F.A.SC. AND P. V. PANTULU

(*Ministry of Defence, South Block, New Delhi-11*)

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ABSTRACT

One-dimensional, two-dimensional and three-dimensional magnetic lattices have been derived making use of methods adopted by the authors in an earlier paper in deriving cystallographic magnetic point groups.

1. INTRODUCTION

IN crystals which possess antiferromagnetic structures, the translational periodicity in certain directions may be accompanied by a reversal of the individual magnetic moments associated with each lattice point out of which the magnetic structure is built. The operation of the reversal of magnetic moment is of order two and may be denoted by $\mathcal{R}$. This can be combined with the elements of a discrete translation group to give rise to a derived group which may be called a variant of the original translation group. The fourteen translation groups corresponding to the 14 Bravais lattices give rise to 22 such variants. The translation groups are also referred to as vector groups in the following. It is customary to refer to these 36 lattices as magnetic lattices.

It is proposed to present here a derivation of the variants of the one-dimensional, two-dimensional and three-dimensional vector groups using methods similar to those given for the derivation of the magnetic variants of crystallographic point groups in an earlier paper by Bhagavantam and Pantulu (1964).

A vector group in one dimension is an infinite group generated from one basic vector by the group operation of vector addition. In two dimensions, such a group is generated from two non-collinear basic vectors. Three non-coplanar basic vectors generate such a group in three dimensions. A vector group may therefore be denoted by its generating elements. Thus, the one-dimensional vector group may be denoted by a single element T_1. All integral multiples—positive or negative or zero—of this basic vector form the group. It is easily seen that there is only one variant of this one-dimensional group and it is generated by a single composite element which is the basic vector T_1 accompanied by the reversal operation $\mathcal{R}$. We shall denote the composite element thus formed by $\underline{T_1}$ and call it a magnetic vector. It is evident that an even multiple of $\underline{T_1}$ is an ordinary vector. This vector group generates a linear chain of equally spaced magnetic moments which are alternately oppositely aligned. If, on the other hand, $\mathcal{R}$ is taken to signify a change of colour of the lattice point, say from black to white and white to black, the group generates a linear chain of equally spaced black and white points. Figure 1 (*a*) shows a one-dimensional lattice of equidistant white dots. Its magnetic variant is shown in Fig. 1 (*b*) and consists of equidistant alternately white and black dots. The distance between two identical lattice points, that is points of the same colour or of the same alignment of magnetic moment, is called the crystallographic cell whereas the distance between the immediate neighbours is called the chemical cell. Similar terminology is adopted in two and three dimensions.

2. Two-Dimensional Vector Groups

Let us denote the two basic vectors which generate a vector group in two dimensions by T_1 and T_2. To obtain the variants of such an infinite group, it is enough if we consider the number of ways in which one or both of the generating vectors may be taken as magnetic. There are evidently 4 ways of doing this. They may be put down as

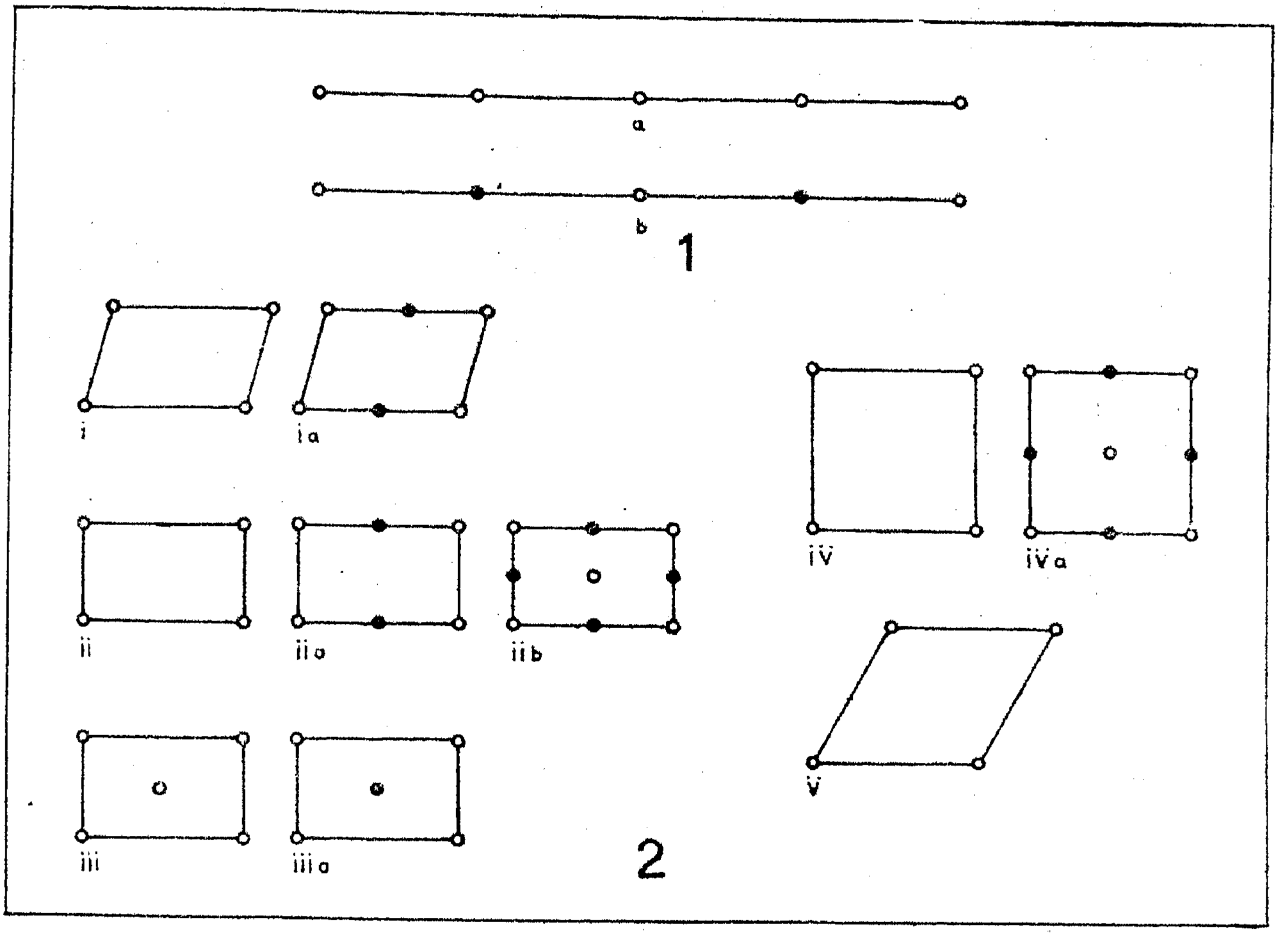
$$(1)\ T_1,\ T_2;\quad (2)\ \underline{T_1},\ T_2;\quad (3)\ T_1,\ \underline{T_2};\quad (4)\ \underline{T_1},\ \underline{T_2}.$$

We shall follow here the alternative notation of denoting an ordinary vector by $+$ and a magnetic vector by $-$ and write the above as

$$(1)\ +\,+\quad;\quad (2)\ -\,+\quad;\quad (3)\ +\,-\quad;\quad (4)\ -\,-.$$

The problem is to consider each of the 5 two-dimensional lattices and pick out such of the above alternatives that are permitted by symmetry in each case. Those that are distinct from amongst such alternatives are the variants. We note that the first alternative gives the conventional lattice and we need consider only (2), (3) and (4) while looking for the variants. Whether a particular variant is distinct or not can be decided in each case by examination with the help of some general principles which emerge during the course of the derivation.

(i) *Monoclinic*.—Alternatives (2) and (3) are not distinct because we can regard either of the two vectors T_1 and T_2 as a magnetic one without



FIGS. 1–2.

any loss of generality. The lattice corresponding to alternative (4) may also be generated by choosing $\underline{T}_1$ and $\underline{T}_1 + \underline{T}_2$ as the basic vectors. $\underline{T}_1 + \underline{T}_2$ is, however, an ordinary vector. This results in (4) not being distinct from (2) and (3). In other words, the lattice which is generated by two unequal basic vectors, both of which are magnetic with no restriction on the angle between them, may equally well be regarded as being generated by another set of two vectors one of which is a magnetic and the other an ordinary vector. There is no restriction on the angle between the vectors nor are they equal in the alternative way of generating the lattice and the lattice therefore is of the same type as (2) or (3). We shall have occasion to use this result in the derivation of the three-dimensional groups. Thus we have only one distinct variant for the monoclinic translation group which may be numbered as (i) *a*.

(ii) *Orthorhombic primitive.*—Alternatives (2) and (3) are not distinct and we can take either of them and number it as (ii) *a*. Alternative (4) is distinct and is numbered as (ii) *b*.

(iii) *Orthorhombic face-centred.*—The vectors T_1 and T_2 that generate the group are equal in length with an arbitrary angle not equal to 90° or 60° between them and they are equivalent by symmetry of the lattice. Thus, alternatives (2) and (3) are not permitted and we have only one variant given by (4) which is numbered (iii) *a*.

(iv) *Tetragonal.*—Symmetry requires that the generating basic vectors T_1 and T_2 which may be taken as the edges of a square are equivalent. The the only possibility is given by (4) which is numbered as (iv) *a*.

(v) *Hexagonal.*—If we take T_1 and T_2 as equal in length and inclined at 60°, we have that both T_1 and T_2 must be magnetic or ordinary and that $\underline{T_2} - \underline{T_1}$ which is non-magnetic is equivalent to $\underline{T_1}$. Thus we arrive at a contradiction and conclude that the sixfold symmetry forbids all alternatives except the conventional one.

The results deduced above in respect of two-dimensional lattices are contained in Table I in a connected form.

TABLE I

Two-dimensional magnetic lattices

Lattice	Basic vectors and angle	Variants	
(i) Monoclinic ..	$T_1 \neq T_2$, $\alpha \neq 90°$	(i) *a*	$+\ -$
(ii) Orthorhombic ..	$T_1 \neq T_2$, $\alpha = 90°$	(ii) *a* (ii) *b*	$+\ -$ $-\ -$
(iii) Orthorhombic face-centred	$T_1 = T_2$, $\alpha \neq \begin{cases} 60° \\ 90° \end{cases}$	(iii) *a*	$-\ -$
(iv) Tetragonal ..	$T_1 = T_2$, $\alpha = 90°$	(iv) *a*.	$-\ -$
(v) Hexagonal ..	$T_1 = T_2$, $\alpha = 60°$	None	

Figure 2 shows the crystallographic unit cells of the five conventional two-dimensional lattices. Against each of the conventional lattices, the appropriate variants are shown. In (i) *a*, (ii) *a*, (ii) *b* and (iv) *a* of Fig. 2, the magnetic vectors are of length half of their corresponding non-magnetic basic vectors of the conventional lattice. There is no loss in generality involved, because it only amounts to altering the scale of the diagram in the direction of the magnetic vector. In the case of the face-centred orthorhombic lattice, this procedure is not followed. It may be noted that if all lattice points in a variant are taken alike—say all as white dots—the variant reduces to its corresponding conventional lattice.

3. Three-Dimensional Vector Groups

The possible alternatives of taking some or all of the three basic vectors as magnetic are 8. They are the following:

(1) $+++$ (2) $-++$ (3) $+-+$ (4) $++-$

(5) $+--$ (6) $-+-$ (7) $--+$ (8) $---$.

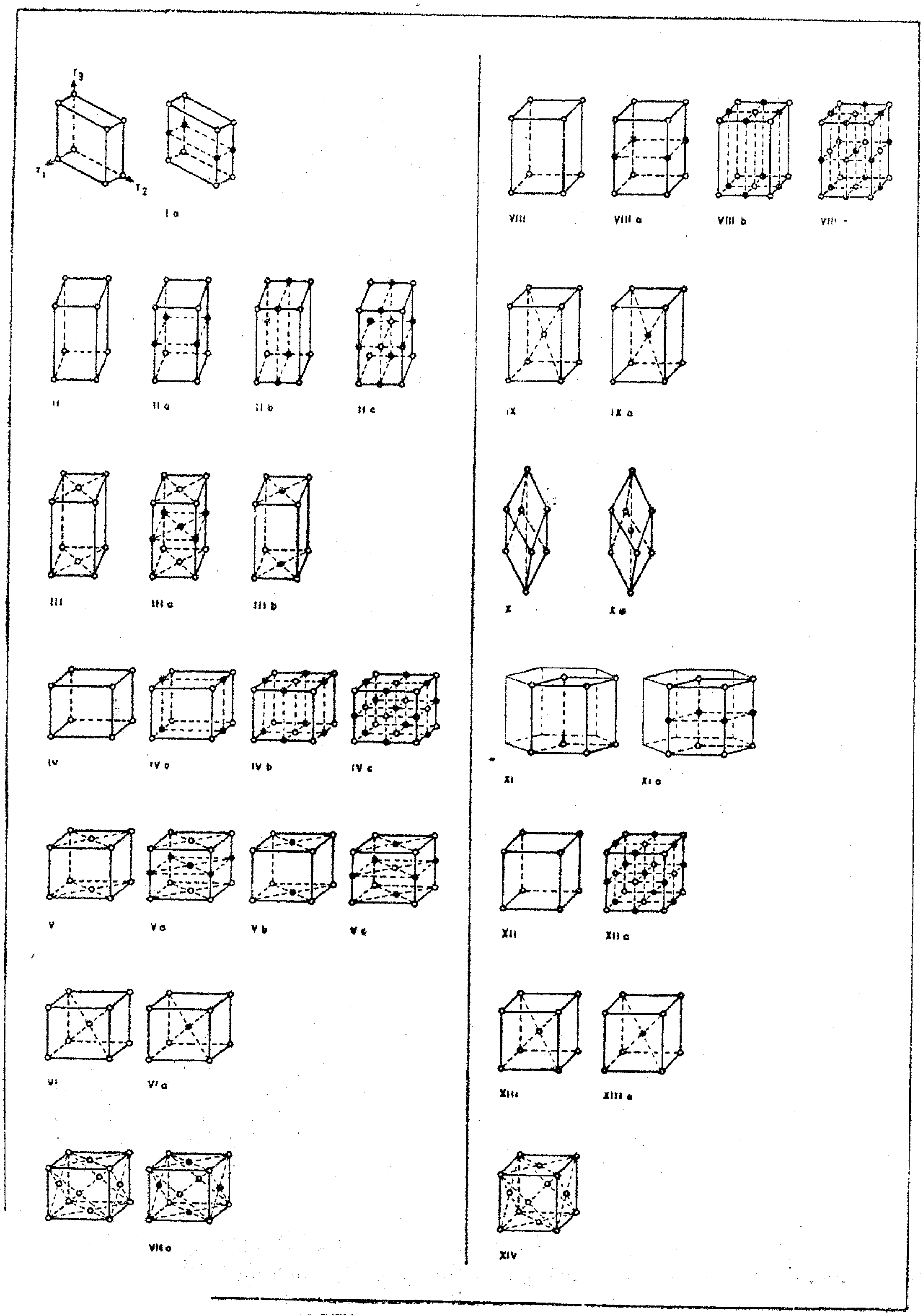
We shall take each of the 14 vector groups and find out the alternatives permitted by symmetry and number the distinct ones among them. Let us denote the basic vectors by T_1, T_2, T_3 and angles between them by α_1, α_2, α_3 such that α_1 is the angle between T_2 and T_3, α_2 is the angle between T_3 and T_1 and α_3 is the angle between T_1 and T_2.

I. *Triclinic.*—From considerations analogous to those given in (i) of the foregoing section, it follows that there is only one distinct alternative. For convenience, we may choose (4) for this purpose and number it as I *a*.

II. *Monoclinic primitive.*—We note that $T_1 \neq T_2 \neq T_3$ with α_2 as arbitrary and $\alpha_1 = \alpha_3 = 90°$ gives the lattice under consideration. T_2 is a twofold axis and T_1 and T_3 are interchangeable. It follows that (2) and (4) are not distinct and we may take (4) and number it II *a*. (3) gives a distinct variant numbered as II *b* and the only remaining distinct one is (5) which is numbered as II *c*.

III. *Monoclinic side-centred.*—We shall take that the side T_1, T_2 of II is centred but in this case denote the vector reaching the lattice point at the centre from the origin as T_1 and the one equivalent to it by T_2. T_2 is obtained from T_1 by the operation of twofold rotation, an element of symmetry for this group. This equivalence rules out (2), (3), (5) and (6). Alternative given by (4) is numbered III *a*. We find from considerations analogous to those given in (i) that (8) is not distinct from this. (7) is distinct and is numbered III *b*.

IV. *Orthorhombic primitive.*—The basic vectors are unequal and mutually perpendicular. We readily see that (2) gives IV *a* and (3) and (4) are not



T_3
T_1
T_2
I a
II
II a
II b
II c
III
III a
III b
IV
IV a
IV b
IV c
V
V a
V b
V c
VI
VI a
VII a
VIII
VIII a
VIII b
IX
IX a
X
X a
XI
XI a
XII
XII a
XIII
XIII a
XIV

FIG. 3.

distinct from it. Similarly (5), (6) and (7) are not distinct and (7) may be numbered IV *b*. (8) is distinct from all the above and is numbered IV *c*.

V. *Orthorhombic side-centred.*—We take basic vectors as in III which rules out (2), (3), (5) and (6). Making use of the considerations given in (iii) of the foregoing section, we have (4) as a distinct alternative and number it V *a*. (7) and (8) are also distinct and are numbered V *b* and V *c* respectively.

VI. *Orthorhombic body-centred.*—We shall take the basic vectors as lines drawn from the body centre of a rectangular parallelepiped to three of its corners not belonging to the same face. Symmetry requires that either all of them be magnetic or all of them be ordinary. Thus we have only (8) as a permissible alternative and this is taken as VI *a*.

VII. *Orthorhombic face-centred.*—We shall take the lines joining a corner to the centres of the three faces meeting at that corner of a rectangular parallelepiped as basic vectors T_1, T_2, T_3. Symmetry requires that either a pair of them or none of them be magnetic. Since we can call any two of them as T_1 and T_2, we have (5), (6) and (7) as not distinct and can take (5) as VII *a*. (2), (3), (4) and (8) are ruled out by symmetry considerations as explained above.

VIII. *Tetragonal primitive.*—We can immediately see that only (4), (7) and (8) are distinct and permissible because T_1 and T_2 being the sides of a square should be equal and both magnetic or ordinary. These are numbered VIII *a*, VIII *b* and VIII *c* respectively.

IX. *Tetragonal body-centred.*—Considerations analogous to those given in VI show that (8) is the only alternative permitted. We number this as IX *a*.

X. *Rhombohedral.*—We take $T_1 = T_2 = T_3$; $\alpha_1 = \alpha_2 = \alpha_3 \neq 90^\circ$ or 60° or $\cos.^{-1} (-\frac{1}{3})$. Symmetry permits only (8) which is numbered X *a*.

XI. *Hexagonal.*—We take $T_1 = T_2$ and $\alpha_3 = 60^\circ$. T_3 is perpendicular to T_1 and T_2. From considerations analogous to those given under (v) of the foregoing section, it follows that only (4) is permitted. This is numbered XI *a*.

XII. *Cubic primitive.*—We take $T_1 = T_2 = T_3$; $\alpha_1 = \alpha_2 = \alpha_3 = 90^\circ$. Again, since all the three basic vectors are symmetrically equivalent, (8) is the only permitted alternative. This is numbered XII *a*.

XIII. *Cubic body-centred.*—From considerations similar to VI and to IX, we get (8) as the only permitted alternative. This is numbered XIII *a*.

TABLE II

Three-dimensional magnetic lattices

Bravais lattice	Basic vectors	Angles	Variants No.	Variants Vectors
I. Triclinic ..	$T_1 \quad T_2 \quad T_3$	$\alpha_1 \neq \alpha_2 \neq \alpha_3$	I *a*	+ + −
II. Monoclinic primitive	$T_1 \quad T_2 \quad T_3$	$\alpha_1 = \alpha_3 = 90°$ $\alpha_2 \neq 90° \neq 120°$	II *a* II *b* II *c*	+ + − + − + + − −
III. Monoclinic side-centred	$T_1 = T_2 \quad T_3$	α_3 is arbitrary $T_1 + T_2$ is at right angles to the plane of $T_1 - T_2$ and T_3	III *a* III *b*	+ + − − − +
IV. Orthorhombic primitive	$T_1 \neq T_2 \neq T_3$	$\alpha_1 = \alpha_2 = \alpha_3 = 90°$	IV *a* IV *b* IV *c*	− + + − − + − − −
V. Orthorhombic side-centred	$T_1 = T_2 \quad T_3$	$T_1 + T_2$, $T_1 - T_2$, T_3 are mutually perpendicular	V *a* V *b* V *c*	+ + − − − + − − −
VI. Orthorhombic body-centred	$T_1 = T_2 = T_3$	$\alpha_1 \neq \alpha_2 \neq \alpha_3$ and $T_1 . T_2 + T_2 . T_3 + T_3 . T_1 = -1$	VI *a*	− − −
VII. Orthorhombic face-centred	$T_1 \neq T_2 \neq T_3$	T_1, T_2, T_3 are the vectors reaching the face centres of a rectangular parallelepiped from one of its corners	VII *a*	+ − −
VIII. Tetragonal primitive	$T_1 = T_2 \neq T_3$	$\alpha_1 = \alpha_2 = \alpha_3 = 90°$	VIII *a* VIII *b* VIII *c*	+ + − − − + − − −
IX. Tetragonal body-centred	$T_1 = T_2 = T_3$	$\alpha_1 = \alpha_3 \neq \alpha_2$ $T_1 . T_2 + T_2 . T_3 + T_3 . T_1 = -1$	IX *a*	− − −
X. Rhombohedral..	$T_1 = T_2 = T_3$	$\alpha_1 = \alpha_2 = \alpha_3 \neq 90°$ or $60°$ or $\cos^{-1}(-\frac{1}{3})$	X *a*	− − −

Table II—(*Contd.*)

Bravais lattice	Basic vectors	Angles	Variants	
			No.	Vectors
XI. Hexagonal ..	$T_1=T_2\neq T_3$	$\alpha_1=\alpha_2=90°$; $\alpha_3=60°$	XI *a*	+ + −
XII. Cubic primitive	$T_1=T_2=T_3$	$\alpha_1=\alpha_2=\alpha_3=90°$	XII *a*	− − −
XIII. Cubic body-centred	$T_1=T_2=T_3$	$\alpha_1=\alpha_2=\alpha_3 = \cos^{-1}(-\frac{1}{3})$	XIII *a*	− − −
XIV. Cubic face-centred	$T_1=T_2=T_3$	$\alpha_1=\alpha_2=\alpha_3=60°$	None	

XIV. *Cubic face-centred.*—Symmetry prohibits all alternatives except (1) which is the conventional lattice.

The variants deduced above in respect of three-dimensional lattices are contained in Table II in a connected form. Results agree with those obtained earlier by Belov, Neronova and Smirnova (1957) and by Zamorzaev (1957). Figure 3 gives the drawings corresponding to the 36 magnetic lattices. Crystallographic unit cells of Bravais lattices are arranged columnwise and against each one are given its magnetic variants. The same procedure as outlined in connection with the drawings of two-dimensional lattices, has been followed. It may be noted that if in a magnetic variant all the lattice points are taken alike—say all of them as white points—it reduces to the conventional Bravais lattice from which it is derived.

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