

Table 1. Scattering factors for methane and carbon

sin $\theta$ $\lambda$	Methane				Carbon
	Buckingham Massey & Tibbs (1941)	Bernal (1953)	Mills (1958)	Mills (1961)	International Tables (1962)
0.00	10.003	10.000	9.999	10.000	6.000
0.05	9.273	9.414	9.371	9.369	5.760
0.10	7.527	7.920	7.801	7.789	5.126
0.15	5.613	6.099	5.954	5.932	4.358
0.20	4.069	4.461	4.366	4.339	3.581
0.25	3.020	3.243	3.232	3.205	2.979
0.30	2.382	2.449	2.514	2.493	2.502
0.35	2.022	1.983	2.098	2.084	2.165
0.40	1.826	1.728	1.868	1.861	1.950
0.45	1.715	1.596	1.738	1.737	—
0.50	1.644	1.527	1.655	1.657	1.685
0.55	1.587	1.486	1.591	1.594	—
0.60	1.534	1.454	1.534	1.536	1.536
0.65	1.480	1.422	1.478	1.479	—
0.70	1.425	1.386	1.422	1.423	1.426
0.75	1.371	1.345	1.366	1.366	—
0.80	1.317	1.299	1.311	1.310	1.322
0.85	1.263	1.250	1.257	1.257	—
0.90	1.210	1.199	1.204	1.203	1.218
0.95	1.157	1.146	1.151	1.151	—
1.00	1.104	1.092	1.098	1.098	1.114
1.05	1.052	1.039	1.046	1.046	—
1.10	1.000	0.986	0.996	0.996	1.012
1.15	0.950	0.934	0.946	0.946	—
1.20	0.901	0.884	0.898	0.898	—
1.25	0.854	0.836	0.852	0.851	—
1.30	0.808	0.790	0.807	0.806	0.821
1.35	0.765	0.746	0.764	0.763	—
1.40	0.723	0.703	0.723	0.722	—
1.45	0.683	0.663	0.683	0.683	—
1.50	0.646	0.625	0.646	0.646	0.659
1.55	0.610	0.589	0.611	0.611	—
1.60	0.576	0.555	0.577	0.577	—
1.65	0.544	0.522	0.545	0.545	—
1.70	0.514	0.492	0.515	0.514	0.524
1.75	0.485	0.463	0.486	0.486	—
1.80	0.458	0.436	0.459	0.459	—
1.85	0.433	0.411	0.434	0.434	—
1.90	0.409	0.387	0.410	0.410	0.419

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## Magnetic Symmetry of Vivianite $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$

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Possible magnetic space groups for antiferromagnetic vivianite,  $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ , are derived on the basis of nuclear magnetic resonance measurements. The allowed space groups are  $P_{A2_1}/c$  and  $C_2/c$ . The spin configurations corresponding to these space groups are discussed.

In 1961, possible magnetic space groups for antiferromagnetic vivianite,  $\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$ , were derived by the author on the basis of nuclear magnetic resonance

data of the protons and phosphorus nuclei (van der Lugt & Poulis, 1961). The actual derivation was published in Dutch (van der Lugt, 1961) and is not readily

accessible. Because recent publications (Forstat, Love & McElearney, 1965; S6lyom, 1966) show renewed interest in the rather strange magnetic properties of this material, a brief communication concerning the magnetic symmetry seems to be justified, more particularly because we believe that sometimes not all available information concerning the magnetic structure has been taken into account. The data upon which the discussion that follows below is based can be found in more elaborate form in the paper by van der Lugt & Poulis (1961).

The space group of vivianite, as determined in the paramagnetic state, is  $C2/m$  (Mori & Ito, 1950). We choose the  $b$  axis as the unique axis. There exist two types of iron ion; ions of type I are situated at the intersection of twofold axes and mirror planes; ions of type II occur in pairs situated on the twofold axes between two ions of type I (Fig. 1). The transition from the paramagnetic to the antiferromagnetic state is of rather complicated nature, but at liquid helium temperatures the crystal is certainly antiferromagnetic. It should be noticed that the symmetry of atomic positions in the crystal is not necessarily the same above and below the transition temperature. Many oxides of transition metals and – more recently – the case of azurite (van der Lugt & Poulis, 1959; Riedel & Spence, 1960) form examples where this is most probably not the case. For vivianite there are no indications for such a change of the symmetry.

The magnetic space group must then belong to the 'family' of  $C2/m$ . The definition of the concept of family and a classification of magnetic space groups according to the families to which they belong, is given by Opechowski & Guccione (1965). The ten space groups of the family of  $C2/m$  are:  $C2/m$ ,  $C2'/m$ ,  $C2/m'$ ,  $C2'/m'$ ,  $C_2c/m$  ( $C_{2c}2/m$ ),  $Pc2/m$  ( $C_P2/m$ ),  $C_2/c$  ( $C_{2c}2/m'$ ),  $Pc2_1/m$  ( $C_{P2}2'/m$ ),  $PA2/c$  ( $C_{P2}2'/m'$ ) and  $PA2_1/c$  ( $C_{P2}2'/m'$ ). For each magnetic space group the notation of Belov, Neronova & Smirnova (1957) has been used in the first place and the notation of Opechowski & Guccione is given in parentheses if it differs from the one of Belov *et al.*

We define a 'set' as a collection of internal magnetic field vectors related by the symmetry relations that are characteristic of the magnetic crystal. By this definition a set is almost equivalent to the concept of a form in crystallography. Table 1 of the paper by van der Lugt &

Poulis (1961) shows that there are four sets of fields acting on the different proton positions, each set consisting of four vectors. It should be noted that there also exist four independent proton positions in the X-ray unit cell. The four vectors of each set transform according to the symmetry relations of one of the following Heesch groups:  $2'/m$ ,  $2/m'$ ,  $2/m1'$ ,  $21'$  and  $m1'$ . The transformation properties of these five Heesch groups are equivalent. Of the magnetic space groups belonging to the family of  $C2/m$ , neither  $C2/m$  nor  $C2'/m'$  is compatible with the selected Heesch groups.

Inspection of the remaining eight magnetic space groups shows that arrangements according to  $C2'/m$ ,  $C2/m'$ ,  $Pc2_1/m$  and  $PA2/c$  have only antcentres available for the iron ions of type I and are therefore ruled out. There now remain four possible magnetic space groups:  $C_2c/m$ ,  $Pc2/m$ ,  $C_2/c$  and  $PA2_1/c$ .

Further information can be obtained from the fields at the positions of the phosphorus nuclei. The phosphorus atoms are situated in the mirror planes and the internal magnetic field at a phosphorus nucleus is parallel to the mirror plane. This plane is then necessarily an antimirror plane in the magnetic space group. Antimirror planes are not available in the cases of

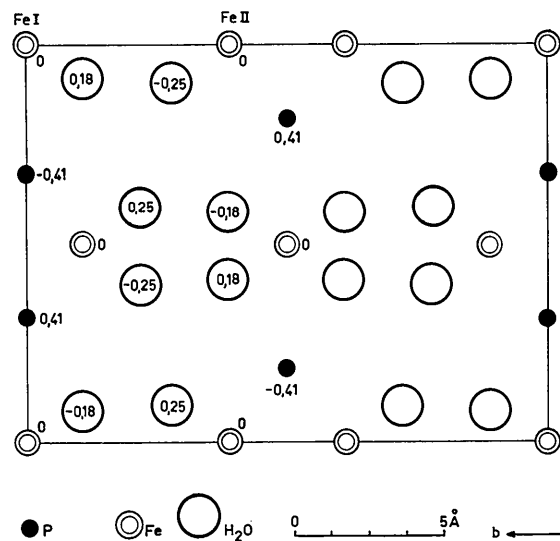


Fig. 1. The positions of the iron and phosphorus ions and of the water molecules projected along the  $c$  axis onto the  $ab$  plane (Mori & Ito, 1950).

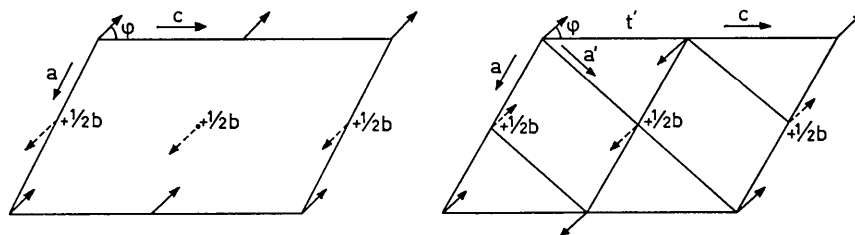


Fig. 2. The magnetic moments of iron ions of type I, corresponding to the groups  $Pc2_1/a$  (left) and  $C_2/c$  (right). The vectors are parallel to the  $ac$  plane;  $\phi$  is unknown.

$P_{C2/m}$  and  $C_{c2/m}$ . It follows that the resulting magnetic space groups allowed by the experimental data are  $P_{A2_1/c}$  and  $C_{c2/c}$ .

It is convenient to write the space group  $P_{A2_1/c}$  as  $P_{C2_1/a}$ , because the latter notation corresponds to the conventional choice of axes for the space group  $C2/m$ . The space group  $P_{C2_1/a}$  requires a magnetic unit cell with the same size as the X-ray unit cell and with an antiferromagnetic centre in the  $ab$  plane (Fig. 2). The unit cell belonging to  $C_{c2/c}$  is twice as large as the X-ray unit cell. Depending on the choice of the  $a$  axis one obtains either a unit cell with a normal centre and an antiferromagnetic translation in the  $c$  direction or a unit cell with an antiferromagnetic centre in the  $ab$  plane and an antiferromagnetic translation in the  $c$  direction.

The following rules apply to the arrangements of magnetic moments, prescribed by either of the two allowed magnetic space groups. The iron ions of type I are situated at the intersection of an antiferromagnetic plane and a twofold anti-axis. Their magnetic moments are therefore parallel to the  $ac$  plane; the direction in the  $ac$  plane cannot be determined on the basis of the experimental data. The iron ions of type II are situated on twofold anti-axes on either side of an antiferromagnetic plane. The magnetic moments of the two members of a pair of these iron ions are then mutually parallel. Their common direction is parallel to the  $ac$  plane. Again, the direction in the  $ac$  plane is not known.

The magnetic structure reported in this paper seems to be confirmed by recent susceptibility measurements (Meijer, van den Handel & Frikkee, 1967).

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## A Modified Theory for the Fourier Transform for a Coiled-Coil

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Published theory for the Fourier transform of a coiled-coil is shown to correspond to a filament with variable line density. A modified expression representing the Fourier transform of a close approximation to a coiled-coil of constant line density is described.

A coiled-coil (super-helix) structure has recently been suggested for nucleohistone (Pardon & Wilkins, 1967) and Fourier transform calculations made to test its feasibility. The theory originally used in the calculations was that previously applied to the coiled-coil model for  $\alpha$ -keratin (Crick, 1953*a, b*; Lang, 1956; Ramachandran, 1960; Fraser, MacRae & Miller, 1964). However, at an early stage in the calculations this theory was found to represent a filament with variable line density and therefore proved unsuitable. A modified theory for the Fourier transform of a coiled-coil,

which represents a close approximation to a filament of constant line density, is outlined in this paper.

The previously published expression representing the Fourier transform of a continuous 'infinitely thin wire of electron density' constrained to form a coiled-coil is:

$$C(R, \psi, l/c) = \sum_p \sum_q \sum_s \sum_d J_p(2\pi Rr_0) \cdot J_q(2\pi R\bar{r}_1) \cdot J_d(2\pi R\Delta) \cdot J_s(2\pi(l/c)r_1 \sin \alpha) \cdot E,$$

where

$$E = \exp[i(p(\psi - \varphi_0 + \frac{1}{2}\pi) + q(-\psi + \varphi_0 + \varphi_1 + \frac{1}{2}\pi) + s(\pi + \varphi_1) + d(\psi + \varphi_1 - \varphi_0 + \frac{1}{2}\pi) + 2\pi z_0 l/c)], \quad (1)$$

subject to

$$N_0 p + (N_1 - N_0) q + (N_1 + N_0) d + N_1 s = l,$$

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