

Neutron Powder Diffraction and Magnetic Measurements on CsMnI₃

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Results of neutron powder diffraction and magnetic measurements on single crystals of CsMnI₃ are reported. Three-dimensional ordering takes place at $T_c = 11.1(3)$ K. Above T_c very broad peaks occur in the neutron powder diffraction diagram, indicating one-dimensional correlations along the chain. Below T_c the Mn²⁺ ions are coupled antiferromagnetically along the chain. Interchain exchange leads to a 120° structure, slightly distorted due to anisotropy. One-third of the chains have their magnetic moment parallel to the *c* axis and the rest of the chains have magnetic moments making an angle of 50(2)° with the *c* axis. The magnetic moment as found from neutron diffraction extrapolated to 0 K is 3.7(1) μ_B , indicating a considerable zero-point spin reduction. The intrachain exchange J/k was found to be -9.1(1)K, whereas the ratio of the inter- to intrachain interaction was determined as $J'/J = \times 10^{-3}$. A spin flop occurs at $H = 54$ kOe on application of a magnetic field parallel to the *c* axis. When a field perpendicular to the *c* axis is applied a spin reorientation occurs at 1 kOe.

Introduction

The investigations on CsMnI₃ are part of our research on the crystallographic and magnetic properties of the compounds in the series $AI-BI_2$, *A* representing an alkali metal, In or Tl, and *B* a first-row transition metal, Mg, Zn, Cd, or Hg.

The phase diagram of CsI-MnI₂ was reported by Seifert and Kischka (1) showing CsMnI₃ to melt congruently. CsMnI₃ adopts the BaNiO₃ structure (1, 2). Recent ¹²⁹I Mössbauer measurements (3) have shown that CsMnI₃ undergoes a three-dimensional phase transition at 10(2) K. The Mössbauer data appear to be consistent with an arrangement of the magnetic moment along the *c* axis.

The BaNiO₃ structure is adopted by many ABX_3 compounds, *X* being Cl, Br, or I. The compounds with this structure have

been studied extensively because of their quasi-one-dimensional properties. In this structure the BX_6 octahedra share faces forming infinite chains along the *c* axis. The chains are widely spaced in the basal plane. For CsMnI₃ the Mn²⁺ ions are separated by 8.11 Å in the basal plane and by 3.44 Å along the *c* axis.

Most compounds with this structure have a strong antiferromagnetic exchange along the chain. When the interchain interaction is ferromagnetic one obtains a magnetic structure as found for, e.g., CsCrI₃ (4). With antiferromagnetic interchain interaction not all neighboring chains can be ordered completely antiparallel. When the anisotropy is small, a 120° structure is most favorable, due to the hexagonal symmetry.

Magnetic structures have been reported for several $A MnX_3$ compounds. In CsMnBr₃ (5) the Mn²⁺ ions are coupled antiferro-

magnetically along the chain, whereas the interchain exchange leads to a 120° structure which can be described by a screw spiral along the a axis with a wavelength of $3a/2$. The magnetic moments are situated in the basal plane. RbMnBr_3 (6) has a similar magnetic structure with a screw spiral with wavelength $1.56a$.

Experimental

The sample used for neutron diffraction was prepared by melting a stoichiometric mixture of the binary compounds and annealing for 1 week at 380°C in an evacuated glass tube. MnI_2 was prepared from the elements and was purified by sublimation. Merck's CsI ultrapure was used. Single crystals were grown using the Bridgman method. The single crystals are easily cleaved along the (1 1 0) plane.

Neutron powder diffraction recordings were done at the HFR reactor at Petten (the Netherlands) using $\lambda = 2.5717(2) \text{ \AA}$ with $30'$ collimation in the angular region $4^\circ < 2\theta < 139^\circ$. Diagrams were recorded at 293, 77, 4.2, and 1.2 K. Neutron powder diffraction experiments were done in the angular range $18^\circ < 2\theta < 27^\circ$ at several temperatures between 4.2 and 20.0 K to investigate one-dimensional ordering above T_c .

For the refinements the profile program of Rietveld (7) was used. No absorption correction was applied. The coherent scattering lengths used are $b(\text{Cs}) = 0.55$, $b(\text{Mn}) = -0.37$, and $b(\text{I}) = 0.53$ all in units of 10^{-12} cm (8). The magnetic form factor was taken from Watson and Freeman (9).

Magnetic measurements in the temperature region 2–100 K were carried out on a crystal weighing 152 mg by means of a vibrating sample magnetometer (10), equipped with a superconducting magnet supplying fields up to 56 kOe. Magnetization vs magnetic field measurements at 2.0 K and susceptibility vs temperature mea-

surements in a field of 11.2 kOe were performed parallel and perpendicular to the c axis. In the temperature region 80–300 K the temperature dependence of the susceptibility was measured on a single crystal weighing 52 mg using the Faraday method. Furthermore ac susceptibility measurements at 1.2 and 4.2 K in a magnetic field up to 16 kOe were performed using the mutual inductance technique (11).

Results of Neutron Powder Diffraction

Refinements on the 293- and 77-K Data

In the structure refinements the positional parameters of CsMnI_3 reported by Seifert and Kischka (1) were taken as starting parameters. Full matrix refinement of positional and isotropic thermal parameters of all ions led to convergence at

$$R(\text{total}) = \sum_i |I_i(\text{obs}) - (1/c)I_i(\text{calc})| / \sum_i I_i(\text{obs}) = 0.034$$

and

$$R(\text{profile}) = \left\{ \sum_j w_j \langle y_j(\text{obs}) - (1/c)y_j(\text{calc}) \rangle^2 / \sum_j w_j \langle y_j(\text{obs}) \rangle^2 \right\}^{1/2} = 0.100,$$

where I_i is the integrated intensity of the i th reflection, y_j the intensity of the j th measuring point, w_j a statistical weight factor, and c a scaling factor. Similar refinement of the recording made at 77 K resulted in $R(\text{profile}) = 0.108$ and $R(\text{total}) = 0.050$. The final parameters of both refinements are given in Table I. They are in good agreement with the parameters reported by Seifert and Kischka. The upper portion of Fig. 1 shows the observed and calculated profiles of the recording at 293 K.

TABLE I

CELL DIMENSIONS, POSITIONAL PARAMETERS, ISOTROPIC THERMAL PARAMETERS ($b = 8(\pi U)^2 \text{ \AA}^2$ (20)), AND THE MAGNETIC MOMENT OF CsMnI₃ AT SEVERAL TEMPERATURES

	x/a	y/b	z/c	b
293 K, $a = 8.190(1)$, $c = 6.958(1) \text{ \AA}$				
Cs	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	4.2(3)
Mn	0	0	0	2.9(2)
I	0.1653(3)	-0.1653(3)	$\frac{1}{3}$	2.4(1)
77 K, $a = 8.119(1)$, $c = 6.889(1) \text{ \AA}$				
Cs	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	1.4(3)
Mn	0	0	0	0.9(3)
I	0.1661(4)	-0.1661(4)	$\frac{1}{3}$	0.1(1)
4.2 K, $a = 8.101(1)$, $c = 6.871(1) \text{ \AA}$				
Cs	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	1.2(4)
Mn	0	0	0	0.4(2)
I	0.1665(4)	-0.1665(4)	$\frac{1}{3}$	0.2(3)
Magnetic moment 3.36(4) μ_B				
1.2 K, $a = 8.111(1)$, $c = 6.871(1) \text{ \AA}$				
Cs	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0.7(4)
Mn	0	0	0	0.8(3)
I	0.1653(4)	-0.1653(4)	$\frac{1}{3}$	0.5(3)
Magnetic moment = 3.60(5) μ_B				

Refinements on the 4.2 and 1.2 K Data

The extra reflections in the neutron powder diffraction recordings at 4.2 and 1.2 K could be indexed with a hexagonal unit cell with axes $a_3^{1/2}$, $a_3^{1/2}$, and c ; a and c being the axes of the nuclear unit cell. Since no indication is found in the diffraction pattern of a crystallographic phase transition between 300 and 1.2 K, the nuclear structures at both temperatures are taken to be isostructural. In what follows, the a axis will be the axis of the nuclear unit cell. Four models were introduced in the refinements: two collinear magnetic structures with the magnetic moments parallel to the c axis and parallel to the a axis, respectively, and two 120° structures with the magnetic moments

in the basal plane and the a - c plane, respectively. The best fit was obtained with a model having a 120° structure with the magnetic moments in a plane perpendicular to the basal plane. The final R values with this model are for the 4.2-K refinement $R(\text{profile}) = 0.115$ and $R(\text{total}) = 0.045$, with $R(\text{magnetic}) = 0.093$ and $R(\text{nuclear}) = 0.039$, and for the 1.2-K refinement $R(\text{profile}) = 0.115$ and $R(\text{total}) = 0.053$ with $R(\text{magnetic}) = 0.081$ and $R(\text{nuclear}) = 0.047$. Only the relative direction of the components of the magnetic moments in the basal plane can be determined with neutron powder diffraction. In what follows, the magnetic moments will be supposed to be parallel to the a - c plane for reasons of simplicity.

Due to the anisotropy the magnetic moments which are not parallel to the easy axis will be turned toward this axis. The turning angle, α , will depend on the ratio of the anisotropy and the interchain exchange. Refinement with a model with α as a parameter yielded $\alpha = 11(2)^\circ$ for the 4.2-K recording and $\alpha = 10(2)^\circ$ for the one of 1.2K, both with lower R values. This model is depicted in Fig. 2. With this model the final R values for the profile of 4.2K are $R(\text{profile}) = 0.113$ and $R(\text{total}) = 0.043$ with $R(\text{nuclear}) = 0.038$ and $R(\text{magnetic}) = 0.083$. The R values for the 1.2-K profile refinement are $R(\text{profile}) = 0.113$, $R(\text{total}) = 0.051$, $R(\text{nuclear}) = 0.046$, and $R(\text{magnetic}) = 0.074$. The final parameters of both refinements are listed in Table I and the observed and calculated profiles of the 1.2-K recording are shown in the lower portion of Fig. 1.

Temperature Dependence of the Magnetic $\{1\ 0\ 1\}^*$ Reflection¹

The results of neutron powder diffraction experiments at several temperatures above

¹ $\{h\ k\ l\}^*$ represents the indices of the magnetic unit cell.

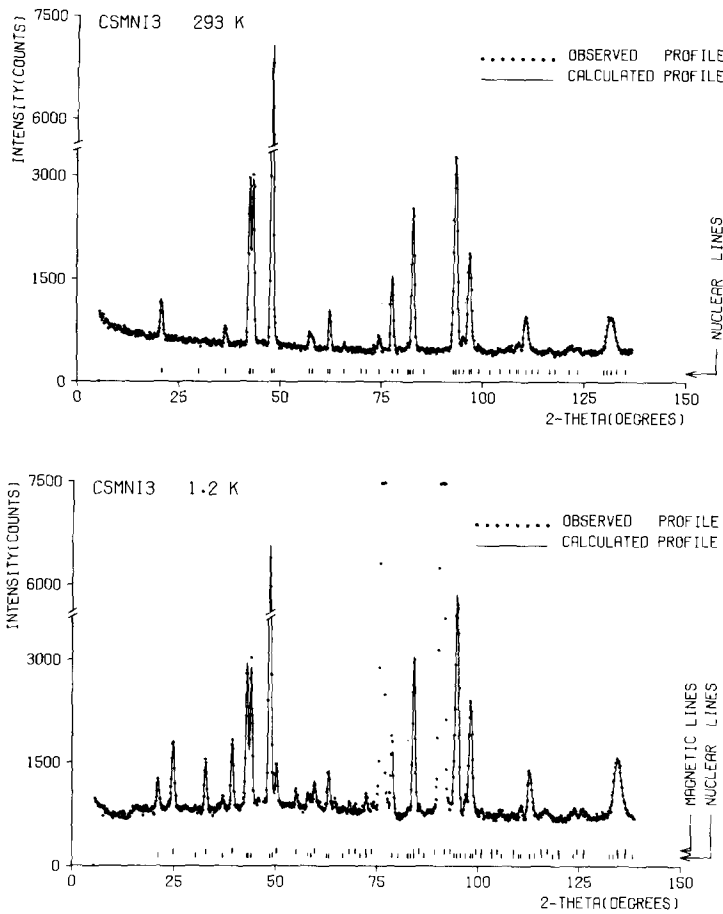


FIG. 1. The calculated and observed profiles of the neutron powder diffraction recordings at 293 K (top) and 1.2 K (bottom).

and below T_c are depicted in Fig. 3. At $T = 1.2$ and 4.2 K a normal Bragg peak of the magnetic $\{101\}^*$ reflection of the $a3^{1/2}$,

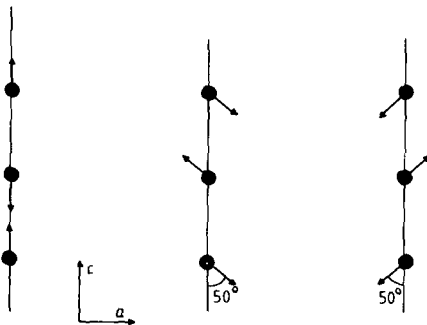


FIG. 2. The magnetic structure of CsMnI_3 .

$a3^{1/2}$, c magnetic unit cell occurs at $2\theta = 24.8^\circ$. At 8.0 K a broad Lorentz peak is found besides the Bragg peak, while the Bragg peak is much smaller, showing the vanishing of the three-dimensional ordering. The Lorentz peak originates in one-dimensional ordering which gives rise to Bragg planes in the reciprocal space. The Lorentz peak remains up to 20.0 K and the Bragg peak vanishes at about $T = 11$ K. The position of the maximum of the Lorentz peak of the 20.0 K recording is found at $2\theta = 24.5^\circ$. The temperature dependence of the magnetic moment is shown in Fig. 4. The magnetic moments at 8.0 and 10.0 K have been determined from the intensity ratio of the $\{110\}^*$ and the $\{101\}^*$

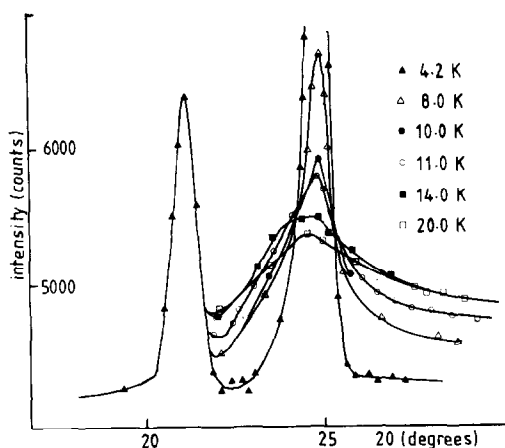


FIG. 3. Neutron powder diffraction diagrams recorded at several temperatures above and below T_c . Only a few measuring points are given to distinguish the profiles. The profiles are scaled on the nuclear $\{110\}^*$ reflection at $2\theta = 20.8^\circ$.

reflections. The uncertainty at 8.0 and 10.0 K is large because at these temperatures a Lorentz peak coincides with the $\{101\}^*$ reflection.

Magnetic Measurements

The magnetic susceptibility, χ , vs temperature curves of CsMnI₃ are shown in Fig. 5. The χ vs T measurements with fields in the basal plane and parallel or perpendicular to the a axis show no significant differences. McPherson *et al.* (12) have reported susceptibility measurements on a powder of CsMnI₃ at five temperatures. The reported values deviate from the values presented in this paper but the reported error

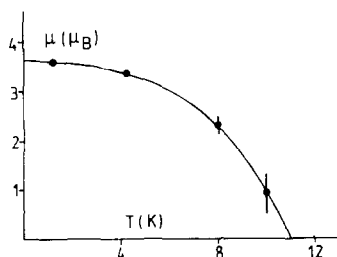


FIG. 4. Temperature dependence of the magnetic moment of CsMnI₃.

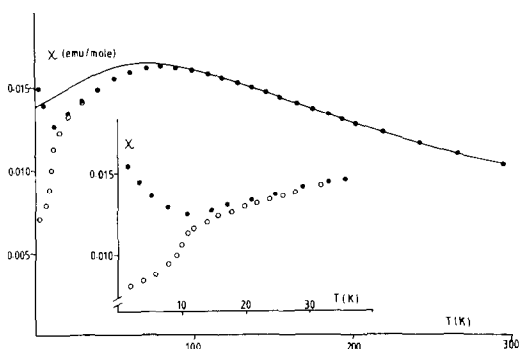


FIG. 5. Molar susceptibility of CsMnI₃ as a function of temperature measured at a field of 11.2 kOe, along the c axis (open circles) and the a axis (full circles). The best fit with Fisher's approximation is given as a full-drawn curve.

(5%) can account for this deviation. The broad maxima near 80 K are characteristic of a linear chain antiferromagnet. The best fit to the experimental data was obtained with Fisher's exact solution (13) for the susceptibility of a classical one-dimensional Heisenberg antiferromagnet with nearest-neighbor interaction. With $g = 2$ and $S = \frac{5}{2}$ the value $J/k = -9.15(10)K$ gives a good fit of the theory to the experimental data down to 80 K. Fitting with the high-temperature series expansion according to Wood and Dalton (14) resulted in $J/K = -9.0(2)K$. χ_{lc} becomes smaller than χ_{lc} below 40 K due to alignment of the magnetic moments along the c -axis by anisotropy. The difference $\chi_{lc} - \chi_{lc}$ increases gradually as T is decreasing. The transition to long-range order between the chains at $T = 11.1(3) K$ is marked by changes in slope of the curves of χ_{lc} and χ_{lc} versus temperature.

Magnetization, M , vs magnetic field measurements at 2 K are shown in Fig. 6. The curve of M vs H with the magnetic field H parallel to the c axis shows a field-dependent slope, with a maximum in dM/dH at $H = 54$ kOe. Our interpretation is that at this field, H_{SF} , the magnetic moments flop from the a - c plane to the basal plane. This spin reorientation is caused by the gain in magnetic energy of $\frac{1}{2}(\chi_{lc} -$

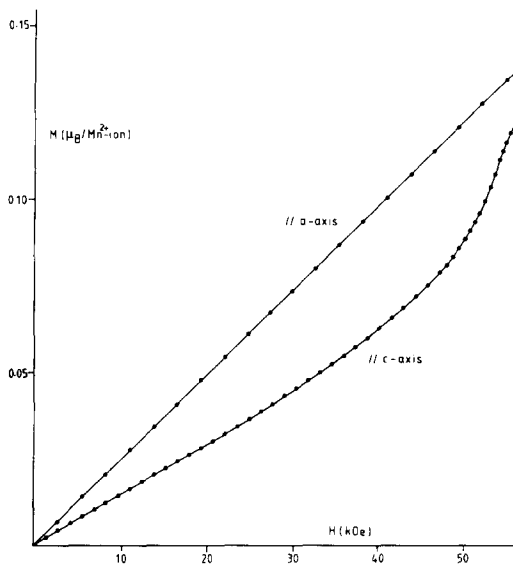


FIG. 6. Magnetization at 2.0 K plotted vs the applied magnetic field.

$\chi_{||c})H^2$ when the magnetic moments change to an orientation that is fully perpendicular to H . It is assumed that for $H > H_{SF}$ the spins are forming a 120° structure in the basal plane.

The measurements of the ac susceptibility, χ' , vs the magnetic field along three orthogonal directions at 1.2 K are depicted in Fig. 7. At low fields both χ' vs H curves with H in the basal plane show a nonlinear field dependence of χ' . On the other hand $\chi'(\parallel c)$ is independent of the magnetic field in this magnetic field region. The difference between $\chi'(\parallel a)$ and $\chi'(\perp a)$ may have been caused by contamination of the single crystal sample when it was reorientated in the open air although it was sealed in Apiezon grease. Because of the large antiferromagnetic exchange the susceptibility is low; the influence of a small paramagnetic contamination will in consequence be very large. Therefore, no conclusions are to be drawn from this difference; the more so because the χ vs T measurements did not show such a difference.

Because of the sixfold axis the compo-

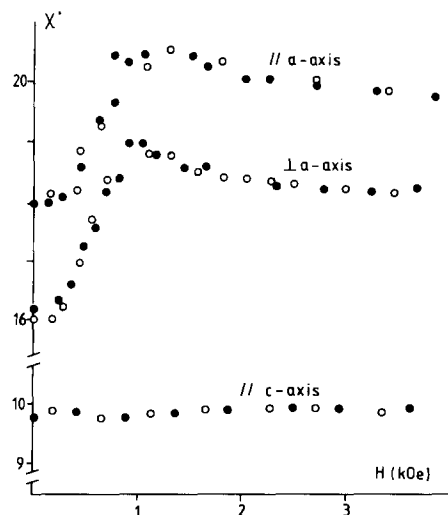


FIG. 7. The ac susceptibility χ' , in relative units, versus the magnetic field. The full and open circles represent measurements with respectively increasing and decreasing magnetic field.

nents of the magnetic moments in the basal plane of CsMnI_3 can be oriented in six equivalent ways. When a crystal is cooled to temperatures below T_c it is expected to contain domains, since ordering will occur at several places in the crystal with six possible orientations (Figs. 8a a'). When a field perpendicular to the c axis is applied, an alignment of the magnetic moments perpendicular to the magnetic field is likely to occur (Figs. 8b b'), yielding a field-dependent behavior of χ' . Since the intrachain interaction is strong, pairs of antiparallel magnetic moments will exist. Consequently no intermediate orientations between the situations depicted in Fig. 8 are expected to occur. Considering also the components of the magnetic moments in the c direction it is evident that with this spin reorientation no single domain is obtained since there exist six possible orientations perpendicular to the magnetic field possible for one Mn^{2+} site. For instance, the Mn^{2+} site with a magnetic moment in the $+c$ direction in one domain can have a magnetic moment in the $-c$ direction in another domain. The

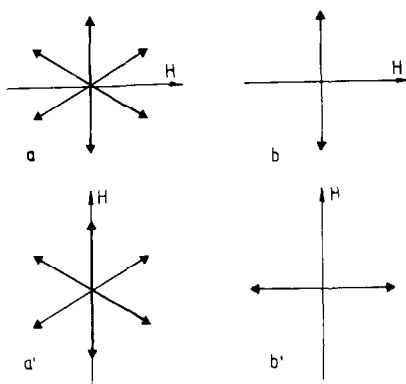


FIG. 8. A (0 0 1) projection of the magnetic moments which will be found in a single crystal due to the forming of domains, contracted to one Mn²⁺ site (*a* and *a'*). When a magnetic field larger than 1 kOe is applied the magnetic moments flop to an orientation fully perpendicular to the applied field (*b* and *b'*).

boundary between these two domains will not be influenced by the spin reorientation at 1 kOe.

Discussion

The results of the magnetic measurements are in agreement with those of the neutron powder diffraction experiments. Both show the *c* axis to be the easy direction and the presence of one-dimensional ordering can be concluded from the χ vs *T* curves and the neutron diffraction experiments above *T_c*. The ¹²⁹I Mössbauer measurements seem to be in conflict with the 120° structure. However, it must be pointed out that the Mössbauer spectra in the ordered phase are poorly resolved.

In spite of the three-dimensional ordering below *T_c* the system still reveals one-dimensional behavior. Below *T_c* one-dimensional spin waves cause a reduction of the magnetic moment (15, 16). For CsMnI₃ the magnetic moment extrapolated to *T* = 0K is found to be 3.7(1) μ_B . A similar reduction has been found for isostructural compounds with an antiferromagnetic intra-chain exchange, e.g., CsMnBr₃: 3.5(3) μ_B

and RbMnBr₃: 3.6(3) μ_B . Sanchez *et al.* (3) have reported that the covalency effect in CsMnI₃ can also cause a reduction of the magnetic moment.

Since CsMnI₃ adopts a 120° structure (see Fig. 2) the magnetic lattice can be divided into six sublattices, each with a sublattice magnetization *M_i* (*i* = 1, 6). The antiparallel pairs of *M_i* are taken to be *M₁* and *M₂*, *M₃* and *M₄*, *M₅* and *M₆*. The axis *M₁* - *M₂* is denoted as Δ_1 ; Δ_2 and Δ_3 denote the other pairs of *M_i*. The measured $\chi_{||c}$ and $\chi_{\perp c}$ are to be regarded as the sum of the susceptibilities of six sublattices. Denoting the susceptibility of each pair of sublattices by $\chi_{||\Delta_i}^s$ and $\chi_{\perp\Delta_i}^s$ and taking $\chi_{||}^s = \chi_{||\Delta_1}^s = \chi_{||\Delta_2}^s = \chi_{||\Delta_3}^s$ and $\chi_{\perp}^s = \chi_{\perp\Delta_1}^s = \chi_{\perp\Delta_2}^s = \chi_{\perp\Delta_3}^s$, the resulting susceptibility is given by

$$\chi = \sum_{i=1}^3 (\chi_{||}^s \cos^2 \psi_i + \chi_{\perp}^s \sin^2 \psi_i)$$

where ψ_i is the angle between Δ_i of the *i*th pair of sublattices and the magnetic field.

From the ac susceptibility measurements it is concluded that the magnetic moments are completely perpendicular to an applied field in the basal plane when the field is higher than about 1 kOe. Since the χ vs *T* measurements are done in a magnetic field of 11.2 kOe the susceptibility perpendicular to the *c* axis will be

$$\chi_{\perp c} = 3\chi_{\perp}^s.$$

With the model for CsMnI₃, where one-third of the magnetic moments are parallel to the *c* axis and two-thirds are at an angle γ with the *c* axis, the parallel susceptibility will be

$$\chi_{||c} = (1 + 2 \cos^2 \gamma)\chi_{||}^s + 2(\sin^2 \gamma)\chi_{\perp}^s.$$

With $\gamma = 50^\circ$ one obtains for the susceptibility parallel to the *c* axis

$$\chi_{||c} = 1.825\chi_{||}^s + 1.175\chi_{\perp}^s.$$

Assuming that χ_{\parallel}^s vanishes at $T = 0$ K, the expected ratio $\chi_{\parallel c}/\chi_{\perp c}$ is 0.4. By extrapolation of the experimental data to $T = 0$ K this ratio is found to be 0.44.

The total free energy of a system with one pair of sublattices as given by Kanamori (17) can be modified to three pairs of sublattices giving

$$F = \sum_{i=1}^3 -0.5(\chi_{\parallel}^s \cos^2 \psi_i + \chi_{\perp}^s \sin^2 \psi_i)H^2 + K \sin^2(\psi_i - \beta),$$

where ψ_i is the angle between Δ_i of the i th pair of sublattices and the magnetic field, β the angle between the easy direction and the magnetic field, and K the anisotropy constant. With $H \parallel c$ axis and $H < H_{SF}$ the free energy becomes for a magnetic structure as found for CsMnI₃ (see Fig. 2):

$$F = -\chi_{\parallel}^s(0.5 + \cos^2 \gamma)H^2 - \chi_{\perp}^s(\sin^2 \gamma)H^2 + 2K \sin^2 \gamma,$$

where γ is the angle between the magnetic moment of two-thirds of the chains and the magnetic field. For $H > H_{SF}$ the free energy is

$$F = -1.5\chi_{\perp}^s H^2 + 3K.$$

When $H = H_{SF}$ both equations yield the same result leading to

$$[\chi_{\perp}^s - \chi_{\parallel}^s(1 + 2 \cos^2 \gamma)/(3 - 2 \sin^2 \gamma)]H_{SF}^2 = 2K.$$

For $\gamma = 50^\circ$, the value found for CsMnI₃ from neutron diffraction the equation becomes

$$(\chi_{\perp}^s - 0.9\chi_{\parallel}^s)H_{SF}^2 = 2K$$

In the limit $T = 0$, χ_{\parallel}^s vanishes, yielding

$$H_{SF}^2 = 2K/\chi_{\perp}^s.$$

This relation can be transformed by using $K = H_A/M$ and $\chi_{\parallel}^s = M/H_E$ (17) to

$$H_A = H_{SF}^2/2H_E,$$

where H_A is the anisotropy field and H_E is the effective exchange field and is equal to $2z|J|s/g\mu_B$ and $M = |\mathbf{M}_i|$. In spite of the 120° structure this formula is identical to the one for a collinear system. The energy gain by the spin flop $\frac{1}{2}(\chi_{\perp c} - \chi_{\parallel c})H^2$ has a similar dependence on γ as the energy loss which is $3K - 2K \sin^2 \gamma$. With $H_{SF} = 54$ kOe and $H_E = 677$ kOe, H_A is calculated to be 2.15 kOe. This derivation is only valid for $H_A \ll H_E$ as is the case for CsMnI₃.

Since the deviation from the 120° structure due to anisotropy is known, it is possible to calculate the interchain exchange field, $H_{E'}$. Taking into account only the magnetic ions in one (0 0 1) plane, the part of the free energy which determines the direction of the magnetizations \mathbf{M}_1 , \mathbf{M}_3 , and \mathbf{M}_5 is

$$F = MH_{E'}(\mathbf{e}_1 \cdot \mathbf{e}_3 + \mathbf{e}_3 \cdot \mathbf{e}_5 + \mathbf{e}_5 \cdot \mathbf{e}_1) + 2MH_A \sin^2 \gamma,$$

where \mathbf{e}_1 , \mathbf{e}_3 , and \mathbf{e}_5 are the unit vectors of the magnetizations \mathbf{M}_1 , \mathbf{M}_3 , and \mathbf{M}_5 , respectively, making an angle of 0, $(\pi - \gamma)$, and $-(\pi - \gamma)$ with the $+c$ axis. With $dF/d\gamma = 0$ the effective interchain exchange field becomes

$$H_{E'} = 2H_A \cos \gamma / (1 - 2 \cos \gamma).$$

With $\gamma = 50(2)^\circ$ one finds $H_{E'} = 10(1)$ kOe and $H_{E'}/H_E = 1.5 \times 10^{-2}$. J'/J is therefore 5×10^{-3} , since $z = 2$ for J and $z = 6$ for J' . This agrees well with an estimation of $J'/J = 3 \times 10^{-3}$ with the aid of the Oguchi relation (18), which holds for a tetragonal structure where $z = 4$ for J' . It must be noted that the value of J' calculated here is the vector sum of competitive interchain exchange interactions.

The neutron powder diffraction patterns recorded at several temperatures above and below T_c reveal little magnetic intensity for the Lorentz peak at the 2θ value of the {0 0 1}* reflection. This absence may be explained by the existence of interchain

ordering which leads to extra intensity around the $\{1\ 0\ 1\}^*$ reciprocal lattice point. A similar short range interchain ordering is found in RbFeCl₃ (19). Alignment of the magnetic moments along the c axis will also lead to a reduction of the intensity around the reciprocal $\{0\ 0\ 1\}^*$ lattice point. However, since $\chi_{lc} - \chi_{lc}$ is small at 20.0 K this alignment will not have a large effect on the profile of the peak.

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