Hydrogen bonding

Since all six glycine molecules exist as zwitterions, 18 hydrogen bonds involving the terminal N atoms are expected. A hydrogen-bonding scheme* has been proposed based on the interatomic distances in this crystal structure. A tetrahedral environment for the N atom is assumed in the proposal of these hydrogen bonds. In some cases, the model has shown that the H atoms of the NH_3^+ group can exist between two acceptors. In such cases, it is possible that bifurcated hydrogen bonds are present.

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* See deposition footnote.

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The Structure of Dicarbonyl(η^4-cinnamaldehyde)(triphenylphosphine)iron(0)

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Abstract

$C_{29}H_{23}FeO_3P$, M_r = 506·3, monoclinic, $P2_1/c$, a = 9·729 (3), b = 9·277 (3), c = 27·523 (5) Å, β = 105·40 (2)°, Z = 4, D_c = 1·40 Mg m^{-3}, μ(Mo $K\bar{\alpha}$) = 0·669 mm^{-1}. The crystal structure has been determined and refined from diffractometer data to an R of 0·036. The compound is a π complex and can be written as [Fe(CO)$_2$(η^4-PhCH=CHCH=O)PPh$_3$]. It displays a nearly square-pyramidal coordination with the PPh$_3$ group in an apical position and the two outer atoms of the heterodiene group and the two carbonyl groups in basal positions. The differences in bond distances between [Fe(CO)$_2$(η^4-PhCH=CHCH=O)-PPh$_3$] and [Fe(CO)$_3$(η^4-PhCH=CHCH=O)] are interpreted in terms of the different π acidities of PPh$_3$ and CO.

Crystals of [Fe(CO)$_2$(η^4-PhCH=CHCH=O)PPh$_3$] were prepared by reacting triphenylphosphine and [Fe(CO)$_3$(η^4-PhCH=CHCH=O)] in de-aerated benzene as part of a wider study on the mechanism and equilibrium constants of the reaction between (η^4-heterodiene)iron tricarbonyl complexes and Group V ligands such as PPh$_3$ and AsPh$_3$ (Cardaci & Bellachioma, 1977). The molecular structure of the title compound was tentatively established by comparing its IR and NMR spectra with those of other compounds of known molecular structure, namely [Fe(CO)$_3$(η^4-CH$_2$=CHCH=CH$_2$)] (Mills & Robinson, 1963; Davis & Speed, 1970) and [Fe(CO)$_3$(η^4-PhCH=CHCH=O)] (De Cian & Weiss, 1972*a*). Both compounds were shown to have a square-pyramidal structure with the diene ligand and the two CO groups occupying the four basal positions and with the other CO group in the apical position, and by comparison of their spectral

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data with those of the present compound, the latter was assigned a similar molecular structure but the basal or apical position of PPh_3 remained undetermined.

The present structure determination is intended to solve this problem and also to investigate the effect on the molecular parameters of the substitution of CO by the far weaker π acid PPh_3.

Experimental

Intensity data were collected from a crystal of dimensions 0·20 × 0·10 × 0·35 mm by means of an automatic Siemens AED four-circle diffractometer using Zr-filtered Mo $K\alpha$ radiation and the $\omega/2\theta$ scan. Out of 2965 reflections measured ($\theta \leq 26°$), 2368 having $I_o \geq 3\sigma(I_o)$ were used in the subsequent refinement. Irradiated crystals were perfectly stable during the period of data collection. Polarization and Lorentz corrections were applied as usual but no absorption correction was made in view of the small value of $\mu R = 0{\cdot}07$. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974) and computations were mainly carried out by means of the *SHELX* 76 system of crystallographic programs (Sheldrick, 1976).

The structure was solved by Patterson and Fourier methods and refined by blocked-matrix (two blocks) least squares with all the non-hydrogen atoms in the anisotropic mode. H atoms were assigned calculated positions (C—H bond length of 1·08 Å) and isotropic temperature factors equal to the average values of the U_{ii} of the bonded atoms; only the H atoms linked to C(27), C(28) and C(29) were refined isotropically. Weights for the last cycle were calculated as $1/w = \sigma^2(F_o) + 0{\cdot}0015|F_o|^2$. In this cycle R $(=\sum|\Delta|/\sum|F_o|)$ and R_w $[=(\sum w|\Delta|^2/\sum w|F_o|^2)^{1/2}]$ were 0·036 and 0·041 respectively.

The final values of the positional parameters are given in Table 1.*

Table 1. *Positional parameters* (×10⁴) *with e.s.d.'s in parentheses*

	x	*y*	*z*
Fe	5652 (0)	7077 (1)	3363 (0)
P	7385 (1)	6290 (1)	4029 (0)
O(1)	4285 (3)	9391 (3)	3774 (1)
O(2)	7331 (3)	9258 (3)	3041 (1)
O(3)	4225 (3)	5513 (3)	3400 (1)
C(1)	4807 (4)	8434 (5)	3630 (1)
C(2)	6662 (4)	8398 (4)	3171 (1)
C(3)	6946 (3)	6376 (4)	4637 (1)
C(4)	7106 (4)	5208 (4)	4961 (1)
C(5)	6769 (4)	5354 (6)	5420 (1)
C(6)	6302 (5)	6628 (7)	5560 (2)
C(7)	6143 (4)	7783 (6)	5244 (2)
C(8)	6466 (4)	7666 (5)	4781 (1)
C(9)	7906 (3)	4423 (3)	3996 (1)
C(10)	6820 (4)	3396 (4)	3865 (1)
C(11)	7160 (5)	1972 (4)	3837 (1)
C(12)	8575 (4)	1548 (4)	3933 (1)
C(13)	9646 (4)	2557 (4)	4057 (1)
C(14)	9316 (3)	3989 (4)	4090 (1)
C(15)	9082 (3)	7237 (3)	4145 (1)
C(16)	9733 (4)	7342 (4)	3755 (1)
C(17)	11029 (4)	8019 (4)	3827 (1)
C(18)	11666 (4)	8645 (5)	4289 (2)
C(19)	11041 (4)	8540 (5)	4671 (1)
C(20)	9756 (4)	7841 (4)	4608 (1)
C(21)	7103 (4)	5744 (4)	2545 (1)
C(22)	7104 (5)	6824 (4)	2192 (1)
C(23)	8219 (6)	6919 (5)	1961 (2)
C(24)	9317 (6)	5957 (6)	2075 (2)
C(25)	9341 (6)	4889 (5)	2424 (2)
C(26)	8233 (5)	4785 (4)	2649 (1)
C(27)	5977 (4)	5613 (4)	2805 (1)
C(28)	4650 (4)	6308 (4)	2656 (1)
C(29)	3770 (5)	6219 (5)	2972 (2)
H(27)	5943 (31)	4837 (34)	2956 (11)
H(28)	4455 (45)	7138 (44)	2327 (16)
H(29)	2980 (43)	6590 (43)	2893 (15)

Discussion

The structure consists of discrete molecular units without significant intermolecular contacts. An *ORTEP* (Johnson, 1971) view of the molecule is shown in Fig. 1. Bond distances and angles are reported in Tables 2 and 3.

The coordination around the Fe atom can be described with reference to the mean plane through C(1), C(2), C(27) and O(3). These four atoms display a small tetrahedral distortion with alternate shifts of

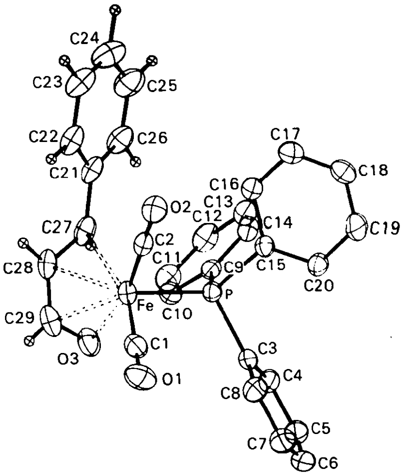

Fig. 1. Molecule of $[Fe(CO)_2(\eta^4\text{-}PhCH{=}CHCH{=}O)PPh_3]$, illustrating the thermal ellipsoids at 40% probability (Johnson, 1971).

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* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35023 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Interatomic distances* (Å) *with e.s.d.'s in parentheses*

Fe–P	2·257 (1)	C(11)–C(12)	1·388 (6)
Fe–O(3)	2·029 (3)	C(12)–C(13)	1·375 (5)
Fe–C(1)	1·767 (4)	C(13)–C(14)	1·375 (5)
Fe–C(2)	1·738 (4)	C(15)–C(16)	1·387 (5)
Fe–C(27)	2·136 (4)	C(15)–C(20)	1·387 (4)
Fe–C(28)	2·059 (4)	C(16)–C(17)	1·375 (5)
Fe–C(29)	2·024 (4)	C(17)–C(18)	1·384 (5)
P–C(3)	1·835 (4)	C(18)–C(19)	1·351 (6)
P–C(9)	1·814 (3)	C(19)–C(20)	1·378 (5)
P–C(15)	1·822 (3)	C(21)–C(22)	1·396 (5)
O(1)–C(1)	1·145 (5)	C(21)–C(26)	1·384 (6)
O(2)–C(2)	1·145 (5)	C(21)–C(27)	1·464 (6)
O(3)–C(29)	1·317 (5)	C(22)–C(23)	1·398 (8)
C(3)–C(4)	1·386 (5)	C(23)–C(24)	1·363 (7)
C(3)–C(8)	1·380 (6)	C(24)–C(25)	1·376 (7)
C(4)–C(5)	1·395 (6)	C(25)–C(26)	1·382 (7)
C(5)–C(6)	1·358 (8)	C(27)–C(28)	1·403 (6)
C(6)–C(7)	1·363 (8)	C(27)–H(27)	0·84 (3)
C(7)–C(8)	1·395 (7)	C(28)–C(29)	1·375 (7)
C(9)–C(10)	1·397 (5)	C(28)–H(28)	1·16 (4)
C(9)–C(14)	1·386 (5)	C(29)–H(29)	0·82 (4)
C(10)–C(11)	1·369 (5)		

Table 3. *Interatomic angles* (°) *with e.s.d.'s in parentheses*

P–Fe–O(3)	95·8 (1)	P–C(9)–C(14)	122·9 (2)
P–Fe–C(1)	102·8 (1)	C(10)–C(9)–C(14)	119·5 (3)
P–Fe–C(2)	96·6 (1)	C(9)–C(10)–C(11)	119·7 (3)
P–Fe–C(27)	99·0 (1)	C(10)–C(11)–C(12)	120·3 (4)
P–Fe–C(28)	136·0 (1)	C(11)–C(12)–C(13)	120·2 (4)
P–Fe–C(29)	132·8 (1)	C(12)–C(13)–C(14)	120·0 (4)
O(3)–Fe–C(1)	95·1 (2)	C(9)–C(14)–C(13)	120·3 (3)
O(3)–Fe–C(2)	165·6 (2)	P–C(15)–C(16)	118·5 (2)
O(3)–Fe–C(27)	79·4 (2)	P–C(15)–C(20)	122·8 (3)
O(3)–Fe–C(28)	69·0 (2)	C(16)–C(15)–C(20)	118·8 (3)
O(3)–Fe–C(29)	37·9 (2)	C(15)–C(16)–C(17)	120·7 (3)
C(1)–Fe–C(2)	89·3 (2)	C(16)–C(17)–C(18)	119·6 (4)
C(1)–Fe–C(27)	157·9 (2)	C(17)–C(18)–C(19)	120·0 (4)
C(1)–Fe–C(28)	119·0 (2)	C(18)–C(19)–C(20)	121·1 (4)
C(1)–Fe–C(29)	92·7 (2)	C(15)–C(20)–C(19)	119·8 (4)
C(2)–Fe–C(27)	91·5 (2)	C(22)–C(21)–C(26)	117·3 (4)
C(2)–Fe–C(28)	96·9 (2)	C(22)–C(21)–C(27)	122·6 (4)
C(2)–Fe–C(29)	128·3 (2)	C(26)–C(21)–C(27)	120·1 (3)
C(27)–Fe–C(28)	39·0 (2)	C(21)–C(22)–C(23)	120·4 (4)
C(27)–Fe–C(29)	69·7 (2)	C(22)–C(23)–C(24)	120·6 (4)
C(28)–Fe–C(29)	39·4 (2)	C(23)–C(24)–C(25)	119·9 (6)
Fe–P–C(3)	115·0 (1)	C(24)–C(25)–C(26)	119·5 (5)
Fe–P–C(9)	115·3 (1)	C(21)–C(26)–C(25)	122·3 (4)
Fe–P–C(15)	115·7 (1)	Fe–C(27)–C(21)	124·9 (3)
C(3)–P–C(9)	102·9 (2)	Fe–C(27)–C(28)	67·5 (3)
C(3)–P–C(15)	103·8 (1)	C(21)–C(27)–C(28)	124·7 (3)
C(9)–P–C(15)	102·5 (1)	C(21)–C(27)–H(27)	116 (2)
Fe–O(3)–C(29)	70·8 (3)	C(28)–C(27)–H(27)	113 (2)
Fe–C(1)–O(1)	174·2 (4)	Fe–C(28)–C(27)	73·4 (3)
Fe–C(2)–O(2)	179·3 (3)	Fe–C(28)–C(29)	69·0 (3)
P–C(3)–C(4)	122·6 (3)	C(27)–C(28)–C(29)	117·8 (4)
P–C(3)–C(8)	118·5 (3)	C(27)–C(28)–H(28)	119 (2)
C(4)–C(3)–C(8)	118·8 (3)	C(29)–C(28)–H(28)	122 (2)
C(3)–C(4)–C(5)	119·6 (4)	Fe–C(29)–O(3)	71·2 (2)
C(4)–C(5)–C(6)	121·2 (5)	Fe–C(29)–C(28)	71·7 (3)
C(5)–C(6)–C(7)	119·5 (5)	O(3)–C(29)–C(28)	118·5 (4)
C(6)–C(7)–C(8)	120·4 (5)	O(3)–C(29)–H(29)	121 (3)
C(3)–C(8)–C(7)	120·3 (4)	C(28)–C(29)–H(29)	120 (3)
P–C(9)–C(10)	117·5 (2)		

±0·08 Å and the Fe atom is displaced from this plane by 0·285 Å towards the PPh$_3$ group. Similar geometries have been found in [Fe(CO)$_3$(η^4-PhCH=CHCH=NPh)] (De Cian & Weiss, 1972*b*), [Fe(CO)$_3$(η^4-PhCH=CHCH=O)] (De Cian & Weiss, 1972*a*), [Fe(CO)$_3$(η^4-PhCH=CHCH=CHPh)] (De Cian, L'Huillier & Weiss, 1973) and [Fe(CO)$_3$(η^4-CH$_2$=CHCH=CH$_2$)] (Mills & Robinson, 1963) with smaller tetrahedral distortions and Fe–plane distances of 0·253, 0·275, 0·239 and 0·18 Å respectively.

The PPh$_3$ ligand is at the apex of the distorted pyramid having C(1), C(2), C(27) and O(3) for its base and the angle formed by the Fe—P vector with the normal to the basal plane is 0·78°. Such an experimental finding is not trivial as the only other compound of similar composition, [Fe(CO)$_2$(η^4-CH$_2$=CHCH=S)PPh$_3$], has been found (Harlow & Pfluger, 1973) to have a similar distorted square-pyramidal coordination around the Fe atom, but with the PPh$_3$ ligand in the basal position. The Fe—P length of 2·257 (1) Å observed in the present compound is in the range of 2·24 ± 0·02 Å given by Einstein & Huang (1978) as an average value for nine different iron–carbonyl–phosphine complexes.

An alternative way of describing the coordination around the Fe atom would be as a deformed octahedron having for the sixth vertex the midpoint of the C(28)—C(29) bond.

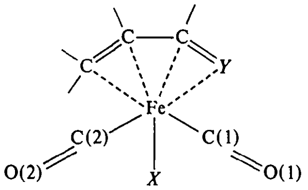
The heterodiene group C(27), C(28), C(29), O(3) displays an *s-cis* conformation and is planar within experimental error, while C(21) is out of plane by 0·16 Å. This plane makes angles of 104·7° with the mean plane of C(1), C(2), C(27), O(3) and 21·0° with the mean plane through the C(21) – C(26) phenyl group. The C(21)—C(27) distance of 1·464 (6) Å, which is slightly smaller than a C(sp^2)—C(sp^2) single-bond distance, and the value of the endocyclic C(22)—C(21)—C(26) angle of 117·3 (4)°, which is significantly smaller than 120°, both indicate a certain degree of conjugation between the π systems of the heterodiene and phenyl groups. The bond distances from Fe to C(27), C(28), C(29) and O(3) agree well with those found in [Fe(CO)$_3$(η^4-PhCH=CHCH=O)] (De Cian & Weiss, 1972*a*).

The relative orientation of the trigonal-pyramidal group Fe(CO)$_2$P with respect to the heterodiene ligand is identical to that found in all similar compounds investigated; that is, two substituents (in this case the two CO groups) are *cis* to the two double bonds and the remaining substituent is *trans* to the single bond of the diene ligand. The Fe(CO)$_2$P group displays approximate C_s symmetry and its mirror plane is nearly perpendicular ($\simeq$ 80°) to the C(28)—C(29) single bond.

The pattern of bond distances [Fe—C(1) = 1·767 (4), Fe—C(2) = 1·738 (4) Å] and angles [C(1)—Fe—C(2) = 89·3 (2), P—Fe—C(2) = 96·6 (1), P—Fe—C(1) = 102·8 (1)°] in the Fe(CO)$_2$P group needs a few

Table 4. *Geometries of the* $Fe(CO)_2X$ *group in different* (η^4*-diene)iron and* (η^4*-heterodiene)iron carbonyl complexes*

The X substituent is *trans* to the C–C single bond of the diene ligand. Distances are in Å and angles in degrees.



Reference	Compound	X	Y	C(1)–Fe–O(2)	X–Fe–C(1)	X–Fe–O(2)	Fe–C(1)	Fe–C(2)	Δ*	Fe–X
(*a*)	$[Fe(CO)_3(\eta^4\text{-}CH_2{=}CHCH{=}CH_2)]$	CO	CH_2	93	102	102	1·77 (3)	1·77 (3)	0	1·74 (4)
(*b*)	$[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}CHPh)]$	CO	CHR	88·6 (5)	100·5 (5)	102·4 (4)	1·774 (6)	1·769 (6)	0·005	1·780 (5)
(*c*)	$[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}NPh)]$	CO	NR	88·9 (3)	101·3 (3)	98·0 (3)	1·794 (7)	1·784 (5)	0·010	1·789 (6)
(*d*)	$[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}O)]$	CO	O	89·7 (3)	103·2 (3)	96·7 (2)	1·802 (5)	1·760 (5)	0·042	1·821 (5)
(*e*)	$[Fe(CO)_2(\eta^4\text{-}PhCH{=}CHCH{=}O)PPh_3]$	PPh_3	O	89·3 (2)	102·8 (1)	96·6 (1)	1·767 (4)	1·738 (4)	0·029	—

References: (*a*) Mills & Robinson (1963); (*b*) De Cian, L'Huillier & Weiss (1973); (*c*) De Cian & Weiss (1972*b*) (monoclinic form); (*d*) De Cian & Weiss (1972*a*); (*e*) present work.

* Δ = difference between Fe–C(1) and Fe–C(2).

comments. C_{3v} symmetry for the $Fe(CO)_3$ group linked to non-cyclic η^4-diene ligands has never been observed, as the ligand causes narrowing of the C–Fe–C angle *cis* to the C–C single bond to a value of 89–93°, while the other two angles remain in the range 100–102° (Table 4). This effect, which reduces the symmetry of the $Fe(CO)_3$ group to C_s, appears to be systematic and has been widely discussed in other papers (see De Cian, L'Huillier & Weiss, 1973, and references therein). Substitution of a C atom by a hetero-atom produces a further distortion in the $Fe(CO)_3$ or $Fe(CO)_2X$ group. With reference to the numbering scheme used in Table 4, this distortion can be described as a small contraction of 0·01–0·04 Å of Fe–C(2) compared with Fe–C(1), and a narrowing of 4–6° of the angle X–Fe–C(2) *trans* to the hetero-atom, the last effect being mainly caused by a change in direction of the vector Fe–X.

It seems to be of particular interest to compare the present structure determination with that of the parent compound $[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}O)]$ (De Cian & Weiss, 1972*a*). The two complexes have similar configurations, differing only in the substitution of a CO for a PPh_3 group; that is of a strong for a far weaker π-acid ligand, and their differences ought to be explainable on this basis. It is to be expected that the decreased competition by PPh_3 as a π acceptor causes a strengthening of the bonding of the iron to the remaining CO groups and the heterodiene moiety. Fe–C bond distances confirm this, as the Fe–C(1) and Fe–C(2) distances of 1·767 (4) and 1·738 (4) Å are significantly shorter than in $[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}O)]$, where they are 1·802 (5) and 1·760 (5) Å respectively. Accordingly, the C–O distances are longer in the present compound, but the differences can hardly be considered significant and a better proof of the weakening of the C–O bond can be obtained from the values of the IR stretching frequencies of the CO groups; these are (Cardaci & Bellachioma, 1977) 2074, 2010 and 1992 cm^{-1} (measured in *n*-hexane) for $[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}O)]$ and 1998 and 1937 cm^{-1} (measured in acetone) for $[Fe(CO)_2(\eta^4\text{-}PhCH{=}CHCH{=}O)PPh_3]$. The increased possibility of back-donation is not reflected in the distance between iron and the heterodiene ligand {average bond distances for Fe–C(27), Fe–C(28), Fe–C(29) and Fe–O(3) of 2·062 Å in the present compound and 2·066 Å in $[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}O)]$}. Nevertheless, it can be inferred from the pattern of bond distances in the ligand itself. The C(27)–C(28), C(28)–C(29) and C(29)–O(3) bond distances are, respectively, 1·403 (6), 1·375 (7) and 1·317 (5) Å in the present compound and 1·412 (7), 1·411 (8) and 1·293 (7) Å in $[Fe(CO)_3(\eta^4\text{-}PhCH{=}CHCH{=}O)]$, which means increased double-bond character for C(28)–C(29) and a decreased one for C(27)–C(28) and C(29)–O(3) for the present compound when compared with the tricarbonyl derivative. It is clear that this shift of the double bond in the central position can only be accounted for by an increased electron transfer from the π to the π^* orbitals of the ligand and therefore by an increased back donation from the central atom to the ligand itself.

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The Structure of Manganese Methylammonium Trichloride Dihydrate, a Member of the $CsMnCl_3.2H_2O$ Family, at Room Temperature

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Abstract

$CH_6N^+.Mn^{2+}.3Cl^-.2H_2O$ is monoclinic, $P2_1/c$, with $a = 7{\cdot}774$ (6), $b = 9{\cdot}122$ (4), $c = 11{\cdot}457$ (8) Å, $\beta = 91{\cdot}41$ (6)°, $Z = 4$. It is isotypic with $CsMnCl_3.2H_2O$, *i.e.*, it forms infinite linear chains of corner-linked $MnCl_4(H_2O)_2$ octahedra. The linkage of adjacent octahedra takes place *via* Cl atoms. The two water molecules are *cis*. The orthorhombic symmetry of the Cs salt is reduced by the non-spherical $CH_3NH_3^+$ cation. The structure was refined to $R = 0{\cdot}039$. All H atoms but one on the methyl group were located. Each water molecule takes part in one interchain and one intrachain O–H$\cdots$Cl hydrogen bond. Only one N–H$\cdots$Cl hydrogen bond is formed. A structural phase transition with a doubling of a takes place at 188·5 K.

Introduction

Different crystalline phases were obtained from aqueous solutions of CH_3NH_3Cl and $MnCl_2$ when we undertook crystal-growth experiments with variable molar ratios of the starting materials. With a 2:1 ratio, the only result was $(CH_3NH_3)_2MnCl_4$, which belongs to the family of perovskite-like layer structures of general formula $(C_nH_{2n+1}NH_3)_2MCl_4$. A 1:2 ratio, however, yielded a sequence of different crystalline phases. It started with $(CH_3NH_3)_2MnCl_4$, followed by faint-pink crystals of long prismatic shape. Last in the sequence were crystals of $MnCl_2.4H_2O$. Observation of the second phase with a polarizing microscope indicated low symmetry. The crystals were only slightly hygroscopic but efflorescent. Chemical analysis revealed the formula $CH_3NH_3MnCl_3.2H_2O$ and X-ray photographs showed a strong relationship with $CsMnCl_3.2H_2O$ (Jensen, Andersen & Rasmussen, 1962), though the symmetry was lower. The Cs compound has recently been of interest, mainly due to its linear-chain antiferromagnetism at low temperatures which made it a kind of guinea-pig in the field of low-dimensional phenomena (Smith & Friedberg, 1968; Skalyo, Shirane, Friedberg & Kobayashi, 1970; Kopinga, 1977). Therefore, it seemed worthwhile to solve the structure of the title compound, which, in contrast to the Cs compound, has the additional possibility of hydrogen bonding between the $CH_3NH_3^+$ cations and the chains.

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