

Tableau 2. Distances interatomiques (Å) et angles de liaison (°)

Re—O(1)	1,690 (5)	N(2)—N(3)	1,327 (5)
Re—O(2)	1,691 (5)	N(3)—N(4)	1,313 (5)
Re—O(3)	1,707 (4)	N(4)—C(1)	1,340 (6)
Re—O(4)	1,687 (4)	C(1)—C(11)	1,477 (6)
C(1)—N(1)	1,342 (6)	N(2)—C(21)	1,444 (6)
N(1)—N(2)	1,315 (5)	N(3)—C(31)	1,429 (6)
O(1)—Re—O(2)	108,3 (2)	N(4)—C(1)—C(11)	123,6 (4)
O(1)—Re—O(3)	110,4 (2)	C(1)—N(1)—N(2)	103,1 (4)
O(1)—Re—O(4)	111,8 (2)	N(1)—N(2)—N(3)	110,4 (4)
O(2)—Re—O(3)	109,7 (2)	N(1)—N(2)—C(21)	122,7 (4)
O(2)—Re—O(4)	107,2 (2)	N(3)—N(2)—C(21)	126,9 (3)
O(3)—Re—O(4)	109,4 (2)	N(2)—N(3)—N(4)	110,2 (3)
N(4)—C(1)—N(1)	113,1 (4)	N(2)—N(3)—C(31)	126,5 (4)
N(1)—C(1)—C(11)	123,3 (4)	N(4)—N(3)—C(31)	123,3 (4)
		N(3)—N(4)—C(1)	103,4 (4)
Le cycle benzénique 1			
Moyenne C—C	1,382 (8)	C—H	0,96 (5)
Le cycle benzénique 2			
Moyenne C—C	1,372 (7)	C—H	0,91 (5)
Le cycle benzénique 3			
Moyenne C—C	1,377 (7)	C—H	0,94 (5)

est légèrement plus longue que celles de N(1)—N(2) et N(3)—N(4) dont la moyenne est de 1,314 (6) Å. Cette différence s'explique bien par les états d'hybridation différents des atomes N(1), N(4) et N(2), N(3). Les trois cycles aromatiques sont plans avec des

écarts des atomes au plan moyen inférieurs à 0,02 (1) Å. La moyenne des distances C—C des cycles benzéniques est de 1,377 (8) Å; celle des distances C—H est de 0,94 (5) Å. Ces deux valeurs ainsi que la moyenne 120,2 (5)° des angles intracycliques indiquent des cycles aromatiques tout à fait normaux.

Les liaisons de l'atome de rhénium avec les atomes d'oxygène possèdent une symétrie tétraédrique et leur valeurs observées sont en accord avec celles habituellement rencontrées. On remarque que les atomes d'oxygène ont une agitation thermique plus importante que celle des autres atomes. Ceci est attribuable à une grande différence des valeurs de diffusion atomique de l'atome de rhénium et de l'oxygène. Les longueurs et angles de liaison calculés dans le coordiat sont donnés dans le Tableau 2.

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Synthesis and Structure of Ammonium Isoorotate Monohydrate and Bis(isoorotato)manganese(II) Dihydrate

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Abstract. Compound (I): ammonium (1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinecarboxylate) monohydrate, NH₄⁺.C₅H₃N₂O₄⁻.H₂O, *M_r* = 191.14, orthorhombic, *Pbca*, *a* = 6.866 (1), *b* = 12.284 (2), *c* = 18.594 (3) Å, *V* = 1568.4 (5) Å³, *Z* = 8, *D_m* = 1.63, *D_x* = 1.618 Mg m⁻³, λ(Mo *Kα*) = 0.71069 Å, μ = 0.086 mm⁻¹, *F*(000) = 720, *T* = 295 (2) K, final *R* =

0.0432, *wR* = 0.0416 for 1071 observed reflections with *F_o* ≥ 3.0σ(*F_o*). Compound (II): bis(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinecarboxylato)manganese(II) dihydrate, [Mn(C₅H₃N₂O₄)₂].2H₂O, *M_r* = 401.15, monoclinic, *P2₁/n*, *a* = 5.0615 (9), *b* = 10.118 (1), *c* = 13.812 (2) Å, β = 95.67 (1)°, *V* = 703.8 (2) Å³, *Z* = 2, *D_m* = 1.85, *D_x* = 1.892 Mg m⁻³, λ(Mo *Kα*) = 0.71069 Å, μ = 0.913 mm⁻¹, *F*(000) = 366, *T* = 295 (2) K, final *R* = 0.0331, *wR* = 0.0338 for

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1236 reflections (all data). In (II) two isoorotato ligands coordinate to the Mn^{II} ion by chelation through O(4) and the adjacent carboxyl group. The coordination sphere around manganese is octahedral with Mn lying on a center of symmetry. The other two sites of the octahedron are occupied by two water molecules.

Introduction. Isoorotic acid [5-uracil carboxylic acid (see Fig. 1)] is a biologically and medically interesting compound; it exhibits anticancer, antibacterial and antihypertensive properties (Tobiki *et al.*, 1980; Keichi *et al.*, 1986). The complex of isoorotic acid with Cu^{II} shows antibacterial activity (Hueso-Urena, Moreno-Carretero, Salas-Peregrin, Valenzuela-Calahorro & Alvarez de Cienfuegos-Lopez, 1988) and the complex of ethyl isoorotate with *cis*-diaquadiammineplatinum(II) has good antitumor, antibacterial and antiviral activity with low renal toxicity (Rosenberg, Van Camp, Fischer, Kansy, Peresie & Davidson, 1983). Isoorotic acid is an isomer of orotic acid whose metal complexes are involved in the biosynthesis of pyrimidine bases in living organisms.

It is also an interesting potential multidentate ligand, since coordination may occur through the two N atoms of the pyrimidine ring, the two carbonyl O atoms and the carboxyl group.

Hueso-Urena *et al.* (1988) have studied the complexes of isoorotic acid with Cu, Co and Zn and have concluded that these metals coordinate with isoorotic acid through the carboxyl group and the adjacent carbonyl group. There is no information concerning the crystal structure of isoorotic acid or any of its metal complexes. We report here the crystal structures of ammonium isoorotate monohydrate (I) and manganese diisoorotate dihydrate (II).

Experimental. Compound (I) was prepared by saturating a solution of 50% ethanol and 50% 0.8M NH₄OH with isoorotic acid (from Janssen Chimica) at room temperature. After several days colorless crystals of (I) precipitated.

Compound (II) was prepared by mixing aqueous solutions of MnCl₂ and sodium isoorotate in molar ratio 1:2. The microcrystalline powder obtained was recrystallized from hot water.

Crystal dimensions 0.20 × 0.10 × 0.15 mm (I) and 0.10 × 0.10 × 0.35 mm (II). Density measured by flotation. Syntex P₂ diffractometer. Lattice parameters from 15 reflections, 16° < 2θ < 22°. Nb-filtered Mo radiation, θ/2θ scan, 2θ_{max} ≤ 48° (I), 2θ_{max} ≤ 50° (II), range of *hkl*: 0→8, 0→14, 0→21 (I); -6→0, 0→12, -16→16 (II). Scan speed 1.0–20.0 (I), 2.0–20.0 (II) (2θ)° min⁻¹, scan width 1.8°(2θ) (I), 1.7°(2θ) (II) plus α₁–α₂ divergence. Three standard reflections, measured every 67 reflec-

Table 1. *Positional and equivalent thermal parameters (× 10⁴) of the non-H atoms with e.s.d.'s in parentheses*

$$U_{eq} = (U_{11} + U_{22} + U_{33})/3.$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq} (Å ²)
(I)				
N(1)	1261 (4)	3388 (2)	1502 (1)	290
C(2)	899 (5)	4460 (2)	1361 (1)	264
N(3)	435 (4)	5068 (2)	1945 (1)	265
C(4)	440 (4)	4738 (2)	2663 (1)	236
C(5)	908 (4)	3595 (2)	2769 (1)	227
C(6)	1256 (4)	2974 (2)	2183 (2)	255
C(7)	1069 (5)	3097 (2)	3500 (2)	265
O(C2)	967 (4)	4840 (2)	750 (1)	361
O(C4)	7 (4)	5405 (2)	3124 (1)	383
O(C7a)	856 (4)	2081 (2)	3540 (1)	397
O(C7b)	1437 (4)	3690 (2)	4024 (1)	452
O(w)	2135 (4)	1931 (2)	374 (1)	465
N(4)	3141 (4)	859 (2)	4478 (1)	326
(II)				
Mn	5000	-5000	5000	226
N(1)	4399 (3)	106 (2)	3298 (1)	239
C(2)	2588 (4)	138 (2)	3956 (1)	207
N(3)	2390 (3)	-1008 (2)	4467 (1)	203
C(4)	3757 (4)	-2170 (2)	4359 (1)	186
C(5)	5683 (4)	-2129 (2)	3663 (1)	191
C(6)	5882 (4)	-981 (2)	3170 (1)	210
C(7)	7447 (4)	-3252 (2)	3433 (1)	205
O(C2)	1237 (3)	1118 (1)	4098 (1)	302
O(C4)	3208 (3)	-3105 (1)	4887 (1)	261
O(C7a)	9151 (3)	-2999 (1)	2868 (1)	306
O(C7b)	7126 (3)	-4378 (1)	3807 (1)	279
O(w)	1805 (3)	-5879 (1)	3990 (1)	338

tions, showed < 3.0% intensity fluctuations. Lp corrections applied. Data collected/unique/*R*_{int}: 1829/1991/0-0051 (I), 1536/1236/0-011 (II).

The structure of (I) was solved by direct methods using *SHELX76* (Sheldrick, 1976). In the case of (II) the fact that *Z* = 2 indicates that the Mn atom must lie on a special position. We placed it at (0,0,0) and a ΔF calculation revealed all the other non-H atoms. Refinement by full-matrix least squares on *F* in which $\sum w\Delta^2$ was minimized, with *SHELX76* (Sheldrick, 1976). All non-H atoms were refined using anisotropic temperature factors. The positions of H atoms were revealed from ΔF calculations and they were refined isotropically.

Final refinement *R*/*wR*: 0.0613/0.0534 (I), for all data. Unit weights (I), $1/w = \sigma^2(F_o) + 0.0003F_o^2$ (II). *S* = 1.13 (I) and 0.54 (II), $|\Delta/\sigma|_{\max} = 0.039$ (I) and 0.031 (II). $(\Delta\rho)_{\max}/(\Delta\rho)_{\min}$: 0.229/-0.207 (I) and 0.287/-0.317 (II) e Å⁻³. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). The final atomic parameters are given in Table 1.* The number of refined parameters was 154 (I) and 135 (II). The atom-numbering

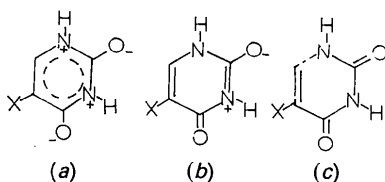
* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53612 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

scheme (same in both compounds) is shown in Fig. 1.

Discussion. Bond lengths and angles of the compounds are given in Table 2. The hydrogen bonds are listed in Table 3. A view of the complex (II) is given in Fig. 1. In the case of (II) the Mn ion is coordinated to two water molecules and two isoorotate ligands through O(7*B*) and O(4). The coordination polyhedron, having a center of symmetry, is a nearly regular octahedron. The bond lengths and angles are in agreement with those of other Mn^{II} complexes (Tranqui, Burlet, Fishol & Thomas, 1977; Lis, 1977; Bats, Kallel & Fues, 1978).

The pyrimidine rings are planar, the largest deviations from the least-squares planes being 0.025 (7) Å [C(2) of (I)] and 0.016 (7) Å [C(4) of (II)].

There are significant differences in the bond lengths of the isoorotate ion between (I) and (II) (Table 2). N(1)—C(2), N(3)—C(4), C(4)—C(5) and C(6)—N(1) are longer in (I) and C(2)—N(3), C(4)—O(4) are longer in (II). We shall discuss these differences with reference to the following resonance structures, where X = COO⁻



The differences are explained if the predominant resonance structure (a) has a significant contribution from (b) in (I) and (c) in (II). These respective contributions of (b) and (c) are in agreement with the crystallographic observations that there are two strong H bonds to O(2), no H bonds to O(4), Table 3, in both structures (I) and (II) and complexation at O(7*B*) and O(4) in structure (II).

Contributions of (b) in (I) and (c) in (II) are expected to cause N(1)—C(2), N(3)—C(4), C(4)—C(5) and C(6)—N(1) to be longer in (I) and C(2)—N(3), C(4)—O(4) and C(5)—C(6) to be longer in (II). This is what is observed, see Table 2.

There is one very large difference in the angles of the isoorotate ion between (I) and (II). The angle

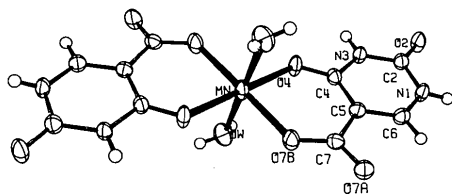


Fig. 1. View of the Mn complex (II), with numbering scheme and thermal ellipsoids enclosing 50% probability.

Table 2. Bond lengths (Å) and angles (°)

	(I)	(II)
N(1)—C(2)	1.366 (4)	1.354 (3)
C(2)—N(3)	1.357 (4)	1.367 (2)
N(3)—C(4)	1.395 (3)	1.380 (2)
C(4)—C(5)	1.454 (4)	1.436 (3)
C(5)—C(6)	1.351 (4)	1.355 (3)
C(6)—N(1)	1.364 (4)	1.355 (2)
C(2)—O(2)	1.230 (3)	1.231 (2)
C(4)—O(4)	1.222 (3)	1.242 (2)
C(5)—C(7)	1.494 (4)	1.499 (3)
C(7)—O(7 <i>a</i>)	1.260 (3)	1.246 (2)
C(7)—O(7 <i>b</i>)	1.242 (3)	1.268 (2)
Mn—O(4)		2.120 (1)
Mn—O(7 <i>b</i>)		2.149 (1)
Mn—O(<i>w</i>)		2.215 (2)
C(6)—N(1)—C(2)	122.5 (2)	121.9 (2)
N(1)—C(2)—N(3)	114.8 (2)	114.5 (2)
C(2)—N(3)—C(4)	127.3 (2)	127.2 (2)
N(3)—C(4)—C(5)	114.2 (2)	115.4 (2)
C(4)—C(5)—C(6)	118.4 (2)	116.8 (2)
C(5)—C(6)—N(1)	122.6 (2)	124.1 (2)
O(2)—C(2)—N(1)	122.5 (2)	123.3 (2)
O(2)—C(2)—N(3)	122.7 (3)	122.1 (2)
N(3)—C(4)—O(4)	118.4 (2)	116.2 (2)
N(3)—C(4)—O(5)	127.3 (2)	128.4 (2)
C(4)—C(5)—C(7)	122.3 (2)	125.3 (2)
C(6)—C(5)—C(7)	119.3 (2)	117.9 (2)
C(5)—C(7)—O(7 <i>a</i>)	116.9 (3)	116.2 (2)
C(5)—C(7)—O(7 <i>b</i>)	119.3 (2)	119.5 (2)
O(7 <i>a</i>)—C(7)—O(7 <i>b</i>)	123.9 (3)	124.4 (2)
O(4)—Mn—O(7 <i>b</i>)		85.5 (0)
O(4)—Mn—O(<i>w</i>)		92.1 (1)
O(7 <i>b</i>)—Mn—O(<i>w</i>)		91.4 (1)

Table 3. Hydrogen-bond distances (Å) and angles (°)

X—H...Y	X...Y	X—H...Y	Symmetry
(I)			
N(1)—H(1)...O(<i>w</i>)	2.822 (3)	171 (3)	<i>x, y, z</i>
N(3)—H(3)...O(7 <i>a</i>)	2.778 (3)	166 (3)	$-x, \frac{1}{2} + y, \frac{1}{2} - z$
O(<i>w</i>)—H(<i>wa</i>)...O(7 <i>b</i>)	2.667 (3)	164 (3)	$x, \frac{1}{2} - y, \frac{1}{2} + z$
O(<i>w</i>)—H(<i>wb</i>)...O(2)	2.963 (3)	146 (2)	$\frac{1}{2} - x, \frac{1}{2} + y, z$
N(4)—H(4 <i>a</i>)...O(7 <i>a</i>)	2.785 (4)	173 (2)	<i>x, y, z</i>
N(4)—H(4 <i>b</i>)...O(2)	2.924 (4)	170 (2)	$x, \frac{1}{2} - y, \frac{1}{2} + z$
N(4)—H(4 <i>c</i>)...O(7 <i>b</i>)	2.810 (3)	158 (2)	$\frac{1}{2} - x, \frac{1}{2} + y, z$
N(4)—H(4 <i>d</i>)...O(<i>w</i>)	3.054 (4)	177 (2)	$\frac{1}{2} + x, y, \frac{1}{2} - z$
(II)			
N(1)—H(1)...O(7 <i>a</i>)	2.653 (2)	165 (1)	$\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$
N(3)—H(3)...O(2)	2.834 (2)	178 (1)	$-x, -y, 1 - z$
O(<i>w</i>)—H(<i>w1</i>)...O(7 <i>b</i>)	2.804 (2)	172 (1)	$-1 + x, y, z$
O(<i>w</i>)—H(<i>w2</i>)...O(2)	3.057 (2)	170 (1)	$x, -1 + y, z$

C(4)—C(5)—C(7) is larger in the complex by 3°. This is probably caused by the 'bite' requirements of Mn^{II}.

The values for the angles C(6)—N(1)—C(2) and C(2)—N(3)—C(4) are in agreement with the two empirical rules that have been established on the basis of previous structural work [Terzis & Mentzafos (1983) and references therein].

We also note that the torsion angle C(4)—C(5)—C(7)—O(7*b*) is 23.5 (2)° in (I) and 6.3 (2)° in (II).

The crystal structure of (II) confirms the structure proposed from solution studies [Doody, Tucci, Scruggs & Li (1966) and references therein].

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Structure of Homochiral Carbonylchloro(3-trifluoroacetylcamphorato)platinum(II)

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Abstract. Carbonylchloro[1,7,7-trimethyl-3-(trifluoroacetyl)bicyclo[2.2.1]heptan-2-onato-*O,O'*]platinum(II), [Pt(Cl)(CO)(C₁₂H₁₄F₃O₂)], $M_r = 505.76$, monoclinic, $P2_1$, $a = 11.035$ (4), $b = 7.216$ (2), $c = 9.824$ (3) Å, $\beta = 99.61$ (3)°, $V = 771.3$ Å³, $Z = 2$, $D_x = 2.177$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 8.929$ mm⁻¹, $F(000) = 474$, $T = 298$ K. Final $R = 0.043$ for 1595 independent reflections [$F_o > 3\sigma(F_o)$]. The unit cell contains two homochiral complex molecules. The Pt atoms form zigzag columns along [010] with coplanar stacking of the Pt coordination plane with a Pt—Pt distance of 4.118 (1) Å.

Introduction. The propensity of many square-planar coordination compounds of Rh^I, Ir^I and Pt^{II} to form linear metal chains in the solid state is well known. Dicarboxyl(3-trifluoroacetylcamphorato)rhodium(I) and dicarboxyl(3-trifluoroacetylcamphorato)iridium(I) form one-dimensional metal chains in the crystalline state in the racemic form but not as pure enantiomers (Schurig, 1981; Pille, 1985). Starting from racemic 3-trifluoroacetylcamphor we have prepared carbonylchloro(3-trifluoroacetylcamphorato)platinum(II) (1), which crystallizes as a conglomerate of enantiomers. The crystal structure of one of the isolated enantiomers is described.

Experimental. The title compound was prepared from K[PtCl₃(C₂H₄)]·H₂O (C₂H₄ = ethene) and the barium salt of racemic 3-trifluoroacetylcamphor (Schurig, 1972) under an N₂ atmosphere in ethanol. After filtration and evaporation of the solvent the residue was redissolved in diethyl ether followed by the bubbling of carbon monoxide through the solution. Crystallization from diethyl ether/*n*-hexane at 253 K yielded short yellow needles (Scheer, 1990).

A single crystal of approximate dimensions 0.3 × 0.15 × 0.15 mm was used for the data collection. Lattice constants were determined from 22 reflections in the θ range $10^\circ \leq 2\theta \leq 23^\circ$ on a Syntex P1 diffractometer. 2010 reflections were measured with the ω -scan technique ($hkl, \bar{h}kl$; $0 \leq h \leq 14$, $0 \leq k \leq 9$, $-12 \leq l \leq 12$; $3^\circ \leq 2\theta \leq 55^\circ$). Three standard reflections measured at constant intervals showed no significant changes in intensities. The data were corrected for Lorentz and polarization effects, empirical absorption correction (ψ scan) with 11 hkl reflections (Sheldrick, 1987), min. and max. transmission factors 0.085 and 0.131, leading to 1595 unique reflections with $F_o > 3\sigma(F_o)$ ($R_{\text{int}} = 0.021$, 235 unobserved). The structure was solved by direct methods (Sheldrick, 1986). Refinement on F with anisotropic parameters and H atoms in geometrically calculated positions (Sheldrick, 1976) converged at $R = 0.0433$, $wR = 0.0345$, $w = k/\sigma(F_o)^2$, k determined by least squares, max. shift/e.s.d. in final cycle < 1, extinction correction as in *SHELX76*: 8.7×10^{-4} ,

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