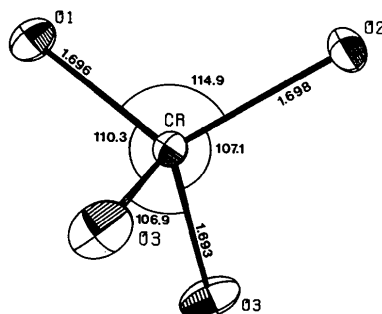


Table 1. Fractional atomic coordinates and equivalent isotropic temperature factors ($\text{\AA}^2 \times 10^4$)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Sr(1)	$\frac{1}{3}$	$\frac{2}{3}$	-0.0007 (1)	169 (1)
Sr(2)	0.0105 (1)	0.2491 (1)	$\frac{1}{3}$	152 (2)
Cr	0.3986 (1)	0.3693 (1)	$\frac{1}{3}$	90 (3)
O(1)	0.3136 (6)	0.4804 (5)	$\frac{1}{3}$	163 (16)
O(2)	0.5956 (5)	0.4700 (5)	$\frac{1}{3}$	158 (14)
O(3)	0.3423 (4)	0.2523 (4)	0.0671 (5)	197 (10)
F	0	0	$\frac{1}{3}$	330 (20)

Fig. 1. Jahn-Teller-distorted (d^1)- CrO_4^{3-} tetrahedron.

structures to Mn_5Si_3 -(D_{8h}) types (Wondratschek, Merker & Schubert, 1964) and even AlB_2 or WC types can be described by the useful tool *non-characteristic orbits* (Engel, Matsumoto, Steinmann & Wondratschek, 1984).

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Structure of the Anti-Cancer Drug Complex Tetrakis(μ -acetato)-bis(1-methyladenosine)dirhodium(II) Monohydrate

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Abstract. $[\text{Rh}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_{11}\text{H}_{16}\text{N}_5\text{O}_4)_2] \cdot \text{H}_2\text{O}$, $M_r = 1024.6$, triclinic, $P1$, $a = 7.808$ (3), $b = 11.469$ (4), $c =$

12.091 (2) \AA , $\alpha = 69.55$ (2), $\beta = 79.46$ (2), $\gamma = 76.61$ (3) $^\circ$, $V = 980.7$ (6) \AA^3 , $Z = 1$, $D_x = 1.735$ g cm^{-3} , $\lambda(\text{Cu } K\alpha) = 1.5418$ \AA , $\mu = 77.6$ cm^{-1} , $F(000) = 522$, room temperature, $R = 0.053$ for 3638 unique reflections. Structure consists of two rhodium(II) ions in a metal-metal bond bridged by

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Table 2. Selected bond distances (\AA) and angles ($^\circ$)

Sr(1)—O(1)	2.567 (3) $3 \times$	Sr(2)—O(1)	2.732 (4)
Sr(1)—O(2)	2.598 (3) $3 \times$	Sr(2)—O(2)	2.514 (3)
Sr(1)—O(3)	2.952 (3) $3 \times$	Sr(2)—O(3)	2.513 (4) $2 \times$
		Sr(2)—O(3)	2.657 (3) $2 \times$
Cr—O(1)	1.696 (4)	Sr(2)—F	2.430 (1)
Cr—O(2)	1.698 (3)		
Cr—O(3)	1.693 (4)		
O(1)—Cr—O(2)	114.9 (2)	O(2)—Cr—O(3)	107.1 (1)
O(1)—Cr—O(3)	110.3 (1)	O(3)—Cr—O(3)	106.9 (2)

I am grateful to Professor Dr H. Wondratschek for his kindness and help.

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Table 1. Positional parameters for all non-H atoms and equivalent isotropic temperature factors

$$B_{eq} = (4/3) \sum_i \beta_i a_i^2$$

	x	y	z	B_{eq} (Å ²)
Rh(1)	0	0	0	2.53 (3)
Rh(2)	0.0835 (1)	-0.2260 (1)	0.0774 (1)	2.62 (4)
O1(Ac1)	0.059 (2)	0.007 (1)	0.157 (1)	2.8 (3)
O2(Ac1)	0.131 (1)	-0.205 (1)	0.232 (1)	2.5 (3)
Cl(Ac1)	0.114 (2)	-0.096 (2)	0.239 (1)	2.6 (4)
C2(Ac1)	0.131 (2)	-0.073 (2)	0.349 (2)	3.8 (5)
O1(Ac2)	-0.248 (2)	-0.017 (1)	0.077 (1)	4.6 (5)
O2(Ac2)	-0.164 (2)	-0.232 (1)	0.146 (1)	4.6 (5)
Cl(Ac2)	-0.265 (3)	-0.132 (2)	0.139 (1)	3.7 (6)
C2(Ac2)	-0.450 (2)	-0.140 (2)	0.204 (2)	4.0 (6)
O1(Ac3)	-0.034 (2)	-0.021 (1)	-0.149 (1)	5.5 (5)
O2(Ac3)	0.033 (2)	-0.229 (1)	-0.078 (1)	6.0 (5)
Cl(Ac3)	0.005 (2)	-0.128 (2)	-0.162 (2)	3.6 (5)
C2(Ac3)	-0.003 (3)	-0.131 (2)	-0.288 (2)	4.3 (5)
O1(Ac4)	0.262 (2)	0.004 (1)	-0.076 (1)	3.3 (3)
O2(Ac4)	0.340 (1)	-0.204 (1)	-0.001 (1)	2.9 (3)
Cl(Ac4)	0.379 (2)	-0.101 (2)	-0.061 (1)	2.8 (4)
C2(Ac4)	0.558 (3)	-0.088 (2)	-0.127 (2)	4.8 (7)
N(1a)	-0.276 (2)	-0.463 (1)	0.056 (1)	3.5 (4)
C(1a)	-0.315 (3)	0.499 (2)	0.167 (2)	4.8 (6)
C(2a)	-0.322 (3)	0.559 (2)	-0.046 (2)	5.1 (6)
N(3a)	-0.295 (2)	0.547 (1)	-0.149 (1)	3.9 (4)
C(4a)	-0.213 (2)	0.426 (1)	-0.155 (1)	2.7 (4)
C(5a)	-0.168 (2)	0.329 (2)	-0.054 (2)	2.9 (4)
C(6a)	-0.177 (3)	0.337 (2)	0.061 (2)	4.0 (6)
N(6a)	-0.136 (3)	0.262 (2)	0.159 (2)	6.3 (7)
N(7a)	-0.097 (2)	0.214 (1)	-0.081 (1)	2.1 (3)
C(8a)	-0.099 (2)	0.250 (1)	-0.198 (2)	3.1 (4)
N(9a)	-0.182 (2)	0.378 (1)	-0.244 (1)	2.9 (3)
Cl(1'a)	-0.220 (2)	0.440 (1)	-0.363 (1)	2.9 (4)
Cl(2'a)	-0.416 (2)	0.495 (1)	-0.379 (1)	3.4 (4)
O(2'a)	-0.506 (2)	0.404 (1)	-0.374 (1)	5.0 (3)
C(3'a)	-0.407 (2)	0.598 (2)	-0.498 (1)	4.7 (5)
O(3'a)	-0.376 (2)	0.541 (1)	-0.590 (1)	5.8 (4)
Cl(4'a)	-0.227 (3)	0.640 (2)	-0.509 (2)	4.7 (6)
O(4'a)	-0.126 (2)	0.543 (1)	-0.418 (1)	4.9 (4)
Cl(5'a)	-0.260 (3)	0.759 (2)	-0.470 (2)	7.2 (8)
O(5'a)	-0.383 (2)	0.758 (1)	-0.359 (1)	7.0 (5)
N(1'b)	0.329 (2)	-0.687 (2)	0.016 (1)	4.0 (4)
Cl(1'b)	0.361 (3)	-0.717 (2)	-0.095 (2)	5.3 (6)
Cl(2'b)	0.382 (4)	-0.772 (2)	0.116 (2)	5.1 (6)
N(3'b)	0.354 (3)	-0.760 (2)	0.222 (2)	5.8 (6)
Cl(4'b)	0.283 (3)	-0.642 (2)	0.214 (2)	3.8 (5)
Cl(5'b)	0.227 (2)	-0.541 (2)	0.124 (1)	2.8 (4)
Cl(6'b)	0.255 (3)	-0.563 (2)	0.010 (1)	3.5 (5)
N(6'b)	0.205 (2)	-0.484 (1)	-0.088 (1)	4.0 (4)
N(7'b)	0.151 (2)	-0.440 (2)	0.165 (1)	3.5 (4)
Cl(8'b)	0.179 (3)	-0.487 (2)	0.280 (1)	4.1 (6)
N(9'b)	0.233 (2)	-0.609 (1)	0.319 (1)	3.5 (4)
Cl(1''b)	0.274 (3)	-0.674 (2)	0.441 (2)	4.5 (6)
Cl(2''b)	0.241 (3)	-0.805 (2)	0.493 (2)	4.5 (5)
O(2''b)	0.060 (2)	-0.802 (1)	0.544 (1)	5.6 (4)
Cl(3''b)	0.367 (3)	-0.869 (2)	0.578 (2)	5.5 (6)
O(3''b)	0.308 (2)	-0.824 (1)	0.685 (1)	7.2 (5)
Cl(4''b)	0.530 (3)	-0.809 (2)	0.519 (2)	5.4 (6)
O(4''b)	0.468 (2)	-0.694 (1)	0.435 (1)	4.5 (4)
Cl(5''b)	0.675 (3)	-0.888 (2)	0.455 (2)	6.2 (6)
O(5''b)	0.833 (2)	-0.820 (2)	0.402 (1)	7.5 (6)
O(w)	-0.820 (2)	0.537 (2)	-0.322 (1)	7.8 (7)

four acetate groups. The remaining axial coordination sites on the rhodium ions are coordinated to the N(7) positions of two 1-methyladenosine molecules.

Experimental. Crystallized as dark-red plates from a 1:1 methanol/water solution. Enraf-Nonius CAD-4 diffractometer, $\omega/2\theta$ scan for data collection, lattice parameters from 23 reflections in range $24 < 2\theta < 85^\circ$. 8290 measured reflections with index range $h - 9$ to 9 , $k - 14$ to 14 , $l - 14$ to 14 up to a $2\theta_{max}$ of 154° . 4146 unique reflections; 3638 reflections with $I/\sigma(I) > 2$ used for refinement. Intensities of 145, $14\bar{5}$, $5\bar{3}\bar{2}$ measured every 2 h; no significant decay

Table 2. Rhodium coordination distances, nucleoside conformation and potential hydrogen bonds in the complex

Rhodium coordination distances (Å)		(distance with e.s.d.)			
Rh...Rh	2.401 (1)	(av. with e.s.d. for 8 bonds)			
Rh...O (acetate)	2.03 (5)	(av. with e.s.d. for 2 bonds)			
Rh...N(7)	2.295 (5)				
Nucleoside conformation (°)					
		Molecule A	Molecule B		
Glycosyl conformation		<i>syn</i>	<i>syn</i>		
C(8)—N(9)—C(1')—O(4')	-119 (2)	-100 (3)			
C(4)—N(9)—C(1')—O(4')	61 (3)	60 (3)			
Ribose pucker		C3'- <i>endo</i>	C3'- <i>endo</i>		
Pseudorotation phase angle P		152 (2)	160 (2)		
Amplitude τ_m		34 (1)	39 (2)		
C(3')—C(4')—C(5')—O(5')		<i>gauche'</i>	<i>trans</i>		
		45 (3)	-179 (3)		
Hydrogen bonds (Å)					
$A-H \cdots B$		Translation for B			
		x	y	z	
N(6a)—H1(N6a)...	O1(Ac1)	2.97 (2)	1	0	1
N(6a)—H2(N6a)...	O(5'B)	2.76 (2)	3.9	0	1
O(3'a)—H(O3'a)...	O(4'B)	3.09 (2)	0	0	0
O(5'a)—H(O5'a)...	N(3A)	2.88 (2)	0	0	0
N(6b)—H1(N6b)...	O2(Ac3)	2.93 (2)	0	1	0
N(6b)—H2(N6b)...	O(w)	2.80 (2)	0	0	-1
O(2'b)—H(O2'b)...	O(5'b)	2.73 (2)	-1	0	0
O(3'b)—H(O3'b)...	O(Ac4)	2.88 (2)	0	0	1
O(w)—H1(w)...	O(2'A)	2.66 (2)	0	0	0
O(w)—H2(w)...	O(4'a)	2.80 (2)	-1	0	0

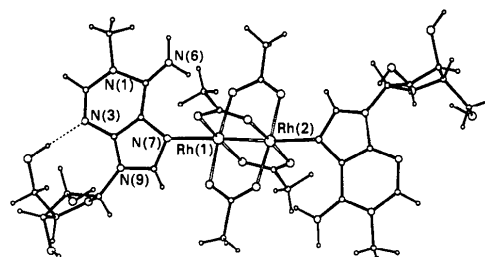


Fig. 1. View of an asymmetric unit of the complex with molecule A on the left side and molecule B on the right side. The coordination bonds are open while the covalent bonds are solid. The intramolecular hydrogen bond is shown as a dashed line.

observed. Empirical absorption correction (φ curve) applied to data; maximum variation of 25%. 4144 reflections measured twice and averaged; discrepancy from the mean is 0.042 defined as $\sum |F_1 - F_2| / \sum (F_1 + F_2)$, where F_1 and F_2 are the two observed structure factor magnitudes for each unique intensity.

Structure solved by multisolution technique and non-H atoms refined by full-matrix least squares (on F) using anisotropic temperature factors. 26 of 46 H atoms in the asymmetric unit were located from difference Fourier maps but not refined. Some proton positions were adjusted slightly (up to 0.1 Å) to improve bonding geometry, especially for the acetate groups. The remaining 20 H atoms, including all water protons and ribose hydroxyl protons, were fixed based on reasonable geometry to maximize hydrogen-bonding interactions in the crystal lattice. $R = 0.053$, $wR = 0.072$, $S = 2.49$, $\Delta/\sigma = 0.1$, $w =$

$1/[\sigma^2(F) + (0.02 F_o)^2]$, residual electron density between -2.0 and $+1.6 \text{ e } \text{Å}^{-3}$ with the largest residuals in the vicinity of the Rh atoms. Scattering factors for non-H atoms from Cromer & Waber (1965) and for H atoms from Stewart, Davidson & Simpson (1965). Table 1* gives the atomic parameters. Fig. 1 shows the molecular complex and Table 2 lists the rhodium coordination, nucleoside conformation, and hydrogen-bonding distances. Calculations performed on a MicroVAX II computer using locally developed programs (Rao, Haromy, McAlister & Merritt, unpublished).

Related literature. Rhodium(II) carboxylates such as the title compound comprise a series of platinum-group metal complexes which are active anti-cancer agents. These compounds are believed to inhibit tumor cell division by reacting covalently with cellular nucleic acids (Rosenberg, 1978). The crystal structure of a dirhodium tetraacetate tRNA^{Phe} complex has also been determined where the dirhodium

tetraacetate forms an intermolecular crosslink between the N(7) atoms of the adenine bases of two symmetry related tRNA molecules (Rubin & Sundaralingam, 1984). The mode of complexation observed in these structures suggests that dirhodium tetraacetate may act by forming interstrand crosslinks to the N(7) positions of two adenine bases in double stranded nucleic acids.

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Structure du Diammine(oxo-5 prolinato)platine(II)

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Abstract. Diammine(5-oxoprolinato)platinum(II), [Pt(C₅H₅NO₃)(NH₃)₂], $M_r = 356.25$, monoclinic, $P2_1$, $a = 8.399$ (2), $b = 7.204$ (2), $c = 14.508$ (3) Å, $\beta = 103.64$ (2)°, $V = 853.1$ (7) Å³, $Z = 4$, $D_x = 2.77 \text{ Mg m}^{-3}$, $\lambda(\text{Mo K}\alpha) = 0.7107$ Å, $\mu = 16.6 \text{ mm}^{-1}$, $F(000) = 656$, $T = 294$ (1) K, $R = 0.021$ for 2037 independent observed reflections. The two independent molecules in the asymmetric unit have similar geometries. In both, the Pt atom displays a square-planar *cis* coordination with two N atoms from the NH₃ groups, one N atom and one O atom from the 5-oxoprolinato ligand. The amide function

exhibits the tautomeric iminoalcohol form and loses the proton of the OH group. Formal local charges on the Pt atom and the 5-oxoprolinato ligand are not compensated and the molecule has a zwitterionic character. One of the two NH₃ ligands is involved in an intramolecular hydrogen bond with the O atom of the iminoalcohol group. This structure was solved in order to establish the relationship between the Pt atom and the 5-oxoprolino ligand.

Partie expérimentale. Cristal approximativement parallélépipédique: $0,06 \times 0,10 \times 0,27 \text{ mm}$. Diffrac-