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Crystal and Molecular Structure of Bis(μ -(1-methyluracilato- N^3, O^4))-bis(*cis*-diammineplatinum(II)) Dinitrate Trihydrate, [(NH₃)₂Pt(C₅H₅N₂O₂)₂Pt(NH₃)₂](NO₃)₂·3H₂O

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Crystals obtained by the reaction of (NH₃)₂Pt(OH)₂Pt(NH₃)₂²⁺ with 1-methyluracil have been shown to be bis(μ -(1-methyluracilato- N^3, O^4))-bis(*cis*-diammineplatinum(II)) dinitrate trihydrate, [(NH₃)₂Pt(C₅H₅N₂O₂)₂Pt(NH₃)₂](NO₃)₂·3H₂O. The crystal structure has been determined by X-ray diffraction. The monoclinic space group *P2₁/c* has cell dimensions $a = 14.293(5) \text{ \AA}$, $b = 16.485(5) \text{ \AA}$, $c = 15.634(4) \text{ \AA}$, and $\beta = 140.88(3)^\circ$ and has four formula units in the unit cell. Data were collected by using Mo $K\alpha$ radiation and a Syntex P₂₁ diffractometer. The crystal structure was determined by standard methods and refined to $R_1 = 0.058$ and $R_2 = 0.049$ on the basis of 3056 independent reflections. The cation is a dimer in which two square-planar arrays about each platinum lie above each other, and these are bridged in *cis* positions by the 1-methyluracilate ligands through N3 and O4. The bridging ligands are arranged head to tail. The Pt-Pt distance is 2.954(2) Å. Pt-N distances (range 2.03(2)-2.08(2) Å) and Pt-O distances (2.03(2), 2.07(2) Å) are normal.

Introduction

There is considerable interest in the nature of the platinum-pyrimidine blues.² Studies of the platinum-pyrimidine blues have revealed variations in composition and properties from experiment to experiment, but it is clear they are unstable, amorphous paramagnetic polymers.³⁻⁶ Barton et al.⁷ managed to isolate crystals of a synthetic α -pyridone blue and showed it contained a four-platinum chain bridged by the α -pyridone groups with a platinum average oxidation state of 2.25. Other studies⁸ suggested a similarity to the platinum-pyrimidine blues which have been shown⁹ to contain Pt-Pt distances comparable to those in the α -pyridone blue.

We have obtained blue crystals by the interaction of 1-methyluracil and "*cis*-Pt(NH₃)₂(OH)₂²⁺" prepared by treating *cis*-Pt(NH₃)₂Cl₂ with aqueous silver nitrate solution.¹⁰ We have examined one crystal by single-crystal X-ray diffraction, and the structure is very similar to that of a dimeric platinum-1-methylthymine complex we have reported previously.¹¹ Since the 1-methylthymine complex was not a "blue", it seemed unlikely that the 1-methyluracil complex was a true platinum-pyrimidine blue. As we shall show below, further work revealed this was the case.

Experimental Section

Preparation of Bis(μ -(1-methyluracilato- N^3, O^4))-bis(*cis*-diammineplatinum(II)) Dinitrate Trihydrate, [(NH₃)₂Pt(C₅H₅N₂O₂)₂·

Table I

compd	C ₁₀ H ₂₈ N ₁₀ O ₁₃ Pt ₂
fw	886.57
cryst size, mm	cylinder, $r = 0.0625$, $l = 0.25$
systematic abs	$0k0$, $k = 2n + 1$; $h0l$, $l = 2n + 1$
space group	<i>P2₁/c</i>
unit cell parameters	
a , Å	14.293(5)
b , Å	16.485(5)
c , Å	15.634(4)
β , deg	140.88(3)
V , Å ³	2324
Z	4
ρ_{calcd} , g cm ⁻³	2.53
ρ_{obsd} , g cm ⁻³	2.49(2)
linear abs coeff, cm ⁻¹	127.31
transmission coeff limits	3.03-3.16
max 2θ , deg; quadrant	55; $h, k, \pm l$
std reflectns	104, $2\bar{2}4$
overall esd, %	2.26, 1.90
temp, °C	22
no. of independent reflectns	3056
no. with $I > 3\sigma(I)$	2295
$3\sigma(I) > I > \sigma(I)$ where $F_c > F_o$	294
$3\sigma(I) > I > \sigma(I)$ where $F_c < F_o$	467
$I < \sigma(I)$ rejected	0
final R_1^a	0.058
final R_2^a	0.049
final shift in esd	
max.	0.011
av	0.0007
g (secondary extinction)	2.258×10^{-8}
final difference map	
highest peak, e/Å ³ ; location	1.5; 0.25, 0.70, 0.65
lowest valley, e/Å ³ ; location	-1.1; 0.35, 0.15, 0.55
weighting	$1/w = 80.53 - 0.548 F_o + 0.00137F_o^2$

$$^a R_1 = \sum \|F_o| - |F_c|\| / \sum |F_o|; R_2 = [\sum w(|F_o| - |F_c|)^2 / \sum w F_o^2]^{1/2}.$$

Pt(NH₃)₂](NO₃)₂·3H₂O. *cis*-Pt(NH₃)₂Cl₂ was aquated by reaction with 99.5% of the stoichiometric amount of AgNO₃ in the dark, overnight on a 0.1 M scale. An equimolar amount of 1-methyluracil in H₂O was added. The pH was adjusted to 7.0 with NaOH. The solution slowly turned blue (several days), and after treatment with 200 mL of absolute ethanol the mixture was filtered. A powdery blue precipitate was removed, leaving a blue solution. The solution was allowed to crystallize in a refrigerator over several weeks. Blue crystals formed which were used for the crystallographic study. The yield was very low (<2%), and no analysis was performed on this sample.

For the powder diffraction experiments a fresh sample was made by using a modification of the above procedure. After the treatment

- (1) (a) McMaster University. (b) Michigan State University.
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- (10) This solution is much more complex than indicated by the formula and certainly contains hydroxide-bridged polymeric species: (a) Faggiani, R.; Lippert, B.; Lock, C. J. L.; Rosenberg, B. *J. Am. Chem. Soc.* **1977**, *99*, 777; *Inorg. Chem.* **1977**, *16*, 1192; **1978**, *17*, 1941. (b) Lippert, B.; Lock, C. J. L.; Rosenberg, B.; Zvagulis, M. *Inorg. Chem.* **1977**, *16*, 1525; **1978**, *17*, 2971.
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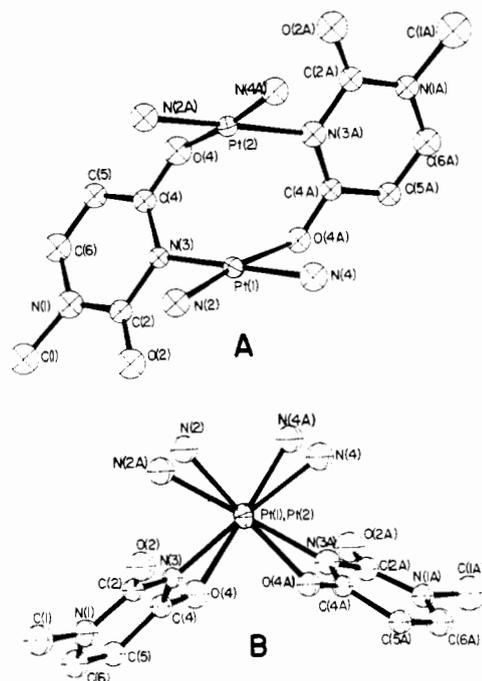


Figure 1. (A) Diagram of the cation $[(\text{NH}_3)_2\text{Pt}(\text{C}_5\text{H}_5\text{N}_2\text{O}_2)_2\text{Pt}(\text{NH}_3)_2]^{2+}$ showing the numbering of the atoms. The platinum atoms are in the plane of the paper (view distance ∞). (B) Same cation viewed along the Pt-Pt axis showing the twist of the two square planes.

with alcohol, the solution was filtered through a very fine sintered-glass frit. (Experiment showed that most of the blue precipitate stayed in suspension when filtered through a medium glass frit, giving apparently a blue solution.) The reaction was very slow, and the addition of extra alcohol (50 mL) followed by filtration was repeated 5 times, at 12-h intervals, before the blue color was removed. Crystallization of the resultant solution gave predominantly a pale green powder, but microscopic examination showed some color variation in the product from pale blue to pale yellow. No single crystals could be obtained. The X-ray powder diffraction pattern and an analysis were performed on the pale green-yellow fraction. Anal. Calcd for $\text{C}_{10}\text{H}_{28}\text{N}_{10}\text{O}_{13}\text{Pt}_2$: C, 13.55; H, 3.18. Found: C, 13.9; H, 3.3.

Powder diffraction photographs were obtained with use of a 360 mm circumference Debye-Scherrer camera and exposure to nickel-filtered $\text{Cu K}\alpha$ radiation (22° , 1.5418 \AA). Electron microscopic pictures of the surface of the crystals were obtained with use of a Cambridge Stereoscan Mk 2A scanning electron microscope operating at 20 kV (pictures were kindly obtained by Mr. Fred Pearson) at magnifications of 430, 950, and 1930.

Collection of the X-ray Data. A crystal was selected after examination under a polarizing microscope. Precession photographs showed the systematic absences of the monoclinic space group $P2_1/c$. Unit cell parameters were obtained from a least-squares fit of χ , ϕ , and 2θ for 15 reflections in the range $20^\circ < 2\theta < 35^\circ$ recorded on a Syntex $P2_1$ diffractometer using graphite-monochromated $\text{Mo K}\alpha$ radiation (0.71069 \AA). Crystal data and other numbers related to data collection are summarized in Table I. The density was obtained by flotation in a carbon tetrachloride-diiodomethane mixture. Intensity data were also recorded on the Syntex $P2_1$ diffractometer using a coupled $\theta(\text{crystal})-2\theta(\text{counter})$ scan. The methods of selection of scan rates and initial data treatment have been described.^{10,12} Corrections were made for Lorentz-polarization effects and absorption.

Solution of the Structure. The coordinates of the platinum atoms were found from a three-dimensional Patterson synthesis and a series of full-matrix least-squares refinements followed by three-dimensional electron density difference syntheses revealed all the nonhydrogen atoms. At this stage, the temperature factors of the platinum atoms, which were previously isotropic, were made anisotropic. Tests were made to show the use of increased parameters was significant.¹³ Further refinement, using full-matrix least-squares minimizing $\sum w(|F_o| - |F_c|)^2$, was terminated when the maximum shift/error was about

Table II. Positional Parameters and Temperature Factors (A^2) ($\times 10^3$)

	x	y	z	U
Pt(1)	236.14 (8)	214.24 (4)	586.81 (6)	a
Pt(2)	178.68 (7)	209.43 (5)	360.14 (6)	a
N(1)	-135 (2)	73 (1)	406 (1)	34 (4)
C(1)	-223 (2)	69 (1)	424 (2)	44 (5)
C(2)	-14 (2)	126 (1)	490 (2)	24 (4)
O(2)	27 (2)	158 (1)	585 (1)	41 (3)
N(3)	57 (2)	137.9 (8)	463 (1)	19 (3)
C(4)	6 (2)	100 (1)	355 (2)	24 (4)
O(4)	66 (2)	111.6 (8)	325 (2)	38 (3)
C(5)	-114 (2)	41 (1)	275 (2)	28 (4)
C(6)	-184 (2)	33 (1)	300 (2)	36 (5)
N(1A)	576 (2)	93.8 (8)	562 (2)	26 (3)
C(1A)	663 (3)	92 (1)	541 (2)	57 (6)
C(2A)	443 (2)	131 (1)	467 (2)	27 (4)
O(2A)	384 (2)	158.8 (8)	360 (1)	44 (4)
N(3A)	373 (2)	144.8 (9)	497 (1)	30 (4)
C(4A)	430 (2)	114 (1)	608 (2)	22 (4)
O(4A)	370 (1)	120.9 (7)	639 (1)	28 (3)
C(5A)	563 (2)	65 (1)	700 (2)	26 (4)
C(6A)	634 (2)	61 (1)	674 (2)	35 (5)
N(2)	116 (2)	306 (1)	557 (1)	35 (4)
N(4)	424 (2)	287 (1)	717 (1)	36 (4)
N(2A)	-16 (2)	273 (1)	225 (1)	36 (4)
N(4A)	280 (2)	306 (1)	375 (1)	35 (4)
N(5)	34 (2)	511 (1)	404 (2)	50 (5)
O(51)	155 (2)	544 (1)	485 (2)	72 (5)
O(52)	-73 (2)	548 (1)	359 (2)	69 (5)
O(53)	15 (2)	442 (1)	363 (2)	76 (5)
N(6)	308 (2)	724 (1)	327 (2)	60 (5)
O(61)	196 (2)	763 (1)	226 (2)	67 (5)
O(62)	396 (2)	703 (1)	333 (2)	88 (6)
O(63)	328 (3)	705 (1)	417 (2)	82 (5)
OH(1)	251 (2)	788 (1)	70 (2)	73 (5)
OH(2)	495 (2)	426 (1)	393 (2)	59 (4)
OH(3)	349 (2)	432 (9)	551 (1)	52 (4)

^a Anisotropic temperature factors U_{ij} were obtained from $\beta_{ij} = 2\pi^2 b_i b_j U_{ij}$, where β_{ij} 's appear as a temperature effect of the form $\exp[-(\beta_{11}h^2 + \dots + 2\beta_{12}hk + \dots)]$ and b_i and b_j are the reciprocal lattice vectors. Pt(1): $U_{11} = 0.0219$ (4), $U_{22} = 0.0294$ (3), $U_{33} = 0.0221$ (3), $U_{12} = -0.0035$ (3), $U_{13} = 0.0178$ (3), $U_{23} = -0.0036$ (3). Pt(2): $U_{11} = 0.0202$ (4), $U_{22} = 0.0328$ (4), $U_{33} = 0.0195$ (3), $U_{12} = 0.0005$ (3), $U_{13} = 0.0154$ (3), $U_{23} = 0.0012$ (2).

0.01. A Cruickshank weighting scheme was used, and corrections were made for secondary extinction with use of the method of Larson.¹⁴ Throughout the refinement, the scattering curves were taken from ref 15, and anomalous dispersion corrections from ref 16 were applied to the curve for platinum. The atom parameters for nonhydrogen atoms are listed in Table II.¹⁷

Results and Discussion

The molecular cation is shown in Figure 1A, and selected interatomic distances and angles are given in Table III. As can be seen from the errors, the structure is not a particularly accurate one, but it does answer a chemical question, and even though we have been unable to prepare good crystals in order to obtain better data, it is possible to draw some conclusions about detailed structural features.

The cation is dimeric, being bridged by 1-methyluracilato ligands through N3 and O4.¹⁸ These atoms and the two cis

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 (17) All calculations were carried out on a CDC-6400 computer. The programs DATCO3, ABSORB, and DATRDN from the X-RAY 76 package were used for preliminary data treatment. The full-matrix least-squares program CUDLS, Fourier program, SYMFOU, and least-squares planes program, PALS, were written locally by J. S. Stephens, J. S. Rutherford, and P. G. Ashmore, respectively. Diagrams were prepared by using the program ORTEP-II: Johnson, C. K. U.S. Atomic Energy Commission Report ORNL-5138; Oak Ridge National Laboratory: Oak Ridge, TN, 1976.

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Table III. Selected Interatomic Distances (Å) and Angles (Deg) (Except Rings; See Supplementary Material)^a

atoms	dist	atoms	dist	atoms	dist
Nonhydrogen Bonds					
Pt(1)-Pt(2)	2.954 (2)	Pt(1)-N(2)	2.05 (2)	Pt(1)-N(4)	2.08 (2)
Pt(1)-N(3)	2.05 (1)	Pt(1)-O(4A)	2.07 (2)	Pt(2)-N(2A)	2.05 (2)
Pt(2)-N(4A)	2.03 (2)	Pt(2)-N(3A)	2.05 (2)	Pt(2)-O(4)	2.03 (2)
N(5)-O(51)	1.22 (3)	N(5)-O(52)	1.23 (4)	N(5)-O(53)	1.24 (3)
N(6)-O(61)	1.25 (2)	N(6)-O(62)	1.24 (6)	N(6)-O(63)	1.23 (5)
Possible Hydrogen Bonds					
O(2)-N(4A) ⁱ	2.92 (2)	O(2)-N(2)	2.94 (3)	O(2)-N(2A) ^j	2.92 (3)
O(2A)-N(4A)	2.95 (3)	O(2A)-N(4) ⁱⁱ	2.85 (5)	O(2A)-N(2) ⁱⁱⁱ	3.05 (2)
O(4A)-OH(2) ⁱ	2.93 (3)	N(2)-O(53)	3.08 (3)	N(2)-O(61) ⁱⁱⁱ	3.06 (2)
N(2)-O(52) ^{iv}	3.03 (4)	N(2A)-O(53)	3.33 (3)	N(2A)-OH(1) ^v	3.08 (2)
N(2A)-O(61) ⁱⁱⁱ	3.27 (4)	N(4)-O(62) ^{vi}	3.21 (5)	N(4)-OH(3)	3.05 (3)
N(4)-OH(1) ^{vi}	3.20 (3)	N(4A)-OH(3)	2.95 (3)	N(4A)-O(62) ^{vi}	3.08 (2)
O(51)-OH(1) ^{vii}	2.91 (3)	O(51)-OH(3)	2.78 (3)	O(53)-OH(3)	3.11 (3)
O(61)-OH(1)	3.10 (5)	O(62)-OH(1)	3.15 (4)	O(63)-OH(1) ^{vii}	3.33 (5)
O(63)-OH(2) ^{vi}	2.86 (3)	OH(2)-OH(3)	2.86 (3)		
atoms	angle	atoms	angle	atoms	angle
Pt(2)-Pt(1)-N(2)	110.0 (7)	Pt(2)-Pt(1)-N(4)	97.7 (8)	Pt(2)-Pt(1)-N(3)	82.3 (7)
Pt(1)-Pt(2)-N(2A)	96.6 (8)	Pt(1)-Pt(2)-N(4A)	109.3 (7)	Pt(1)-Pt(2)-N(3A)	82.9 (8)
Pt(2)-Pt(1)-O(4A)	76.3 (5)	N(2)-Pt(1)-N(4)	90.7 (8)	N(2)-Pt(1)-N(3)	91.6 (7)
Pt(1)-Pt(2)-O(4)	76.8 (6)	N(2A)-Pt(2)-N(4A)	89.8 (8)	N(2A)-Pt(2)-N(3A)	179.3 (9)
N(2)-Pt(1)-O(4A)	173.6 (8)	N(4)-Pt(1)-N(3)	177.5 (6)	N(4)-Pt(1)-O(4A)	87.0 (7)
N(2A)-Pt(2)-O(4)	88.1 (7)	N(4A)-Pt(2)-N(3A)	90.9 (8)	N(4A)-Pt(2)-O(4)	173.8 (8)
N(3)-Pt(1)-O(4A)	90.6 (6)	Pt(1)-N(3)-C(2)	118 (1)	Pt(1)-N(3)-C(4)	123 (2)
N(3A)-Pt(2)-O(4)	91.3 (7)	Pt(2)-N(3A)-C(2A)	119 (1)	Pt(2)-N(3A)-C(4A)	121 (2)
Pt(1)-O(4A)-C(4A)	127 (1)	O(51)-N(5)-O(52)	121 (2)	O(51)-N(5)-O(53)	121 (3)
Pt(2)-O(4)-C(4)	130 (1)	O(61)-N(6)-O(62)	117 (4)	O(61)-N(6)-O(63)	121 (4)
O(52)-N(5)-O(53)	119 (2)				
O(61)-N(6)-O(63)	122 (2)				

^a Atoms are related to those given in Table II as follows: (i) $x, 1/2 - y, 1/2 + z$; (ii) $x, 1/2 - y, z - 1/2$; (iii) $-x, y - 1/2, 1/2 - z$; (iv) $-x, 1 - y, 1 - z$; (v) $-x, 1 - y, -z$; (vi) $1 - x, 1 - y, 1 - z$; (vii) $x, 1.5 - y, 1/2 + z$.

ammine groups form a square plane about each platinum atom which lies roughly above the square plane on the other atom. Thus the cation is very much like the 1-methylthyminato complex we have described previously.¹¹ This is portrayed even more clearly when considering details of the structures. Thus the N(3)-O(4) and N(3A)-O(4A) bite distances of 2.30 (4) and 2.30 (4) Å compare with 2.25 (2) and 2.29 (2) Å, the Pt(1)-Pt(2) distance of 2.954 (2) compares with 2.974 (1) Å, the dihedral angle between the square plane of 35.8° compares with 36.1°, and the rotation of the square planes with respect to each other about Pt(1)-Pt(2) is 17.1-21.20° compared to 13-14.5° (see Figure 1B). Indeed a bond for bond and angle for angle comparison shows no significant variation between the two structures, which is not surprisingly considering the large errors.

Despite the errors, because we have two rings on both the 1-methylthyminate and 1-methyluracilate complexes, it is possible to consider the averages for the bond lengths and angles and compare these with the average of the values for uncoordinated neutral 1-methylthymine and 1-methyluracil.¹⁹ There is no significant difference in bond lengths, except perhaps for N3-C4 which is shorter in the complexes. There are significant differences in the angles, however, with an increase in N3-C4-C5 (~5°) and N3-C4-O4 (~3°) and a decrease in C2-N3-C4 (~6°) and O4-C4-C5 (~8°). The decrease in C2-N3-C4 is expected. As Singh²⁰ has noted, removal of an exocyclic group (in this case the proton) reduces the internal ring angle and increases the adjacent ring angles. The increase in N3-C4-C5 is significant while that of N1-C2-N3 is not. Further we have noted^{21,22} that, when coor-

Table IV. X-ray Powder Diffraction Data for Bis(μ -(1-methyluracilate-*N*³,*O*⁴))-bis(*cis*-diammineplatinum(II)) Dinitrate Trihydrate

line	2 θ (obsd), deg	2 θ (calcd), deg	index	intens
1	9.80	9.81	100	10
2	10.73	10.73	020	80
3	11.23	11.19	110	100
4	12.45	12.47	12 $\bar{1}$	50
5	13.15	13.19	11 $\bar{2}$	40
6	14.78	14.89	21 $\bar{1}$	5
7	16.63	16.64	22 $\bar{1}$	10
8	18.40	18.48	031	30
9	18.90	18.91	130	30
10	19.80	19.69	200	25
11	20.45	20.43	210	25
12	21.60	21.56	040	20
13	22.48	22.48	220	55
14	23.25	23.29	041	20
15	24.20	24.23	20 $\bar{4}$	20
16	25.18	25.23	33 $\bar{2}$	15
17	25.50	25.52	40 $\bar{4}$	15
18	26.55	26.56	22 $\bar{4}$	30
19	28.00	28.06	33 $\bar{4}$	40
20	29.35	29.37	240	5
21	29.70	29.73	11 $\bar{4}$	20
22	30.50	30.52	25 $\bar{1}$	10
23	31.05	31.07	32 $\bar{5}$	5
24	31.20	31.17, 31.21	132, 12 $\bar{4}$	5

minated platinum is the new exocyclic group, the angular changes are not restored. The increase in O4-C4-C5 is expected, as it increases the bite distance (N3-O4), and the two increases will cause the observed decrease in O4-C4-C5. The

(18) We used the IUPAC nomenclature for pyrimidine rings N3,O4 etc., when we do not wish to refer to atoms in a specific ring. We use the symbols N(3), O(4A), etc., when we refer to specific atoms.

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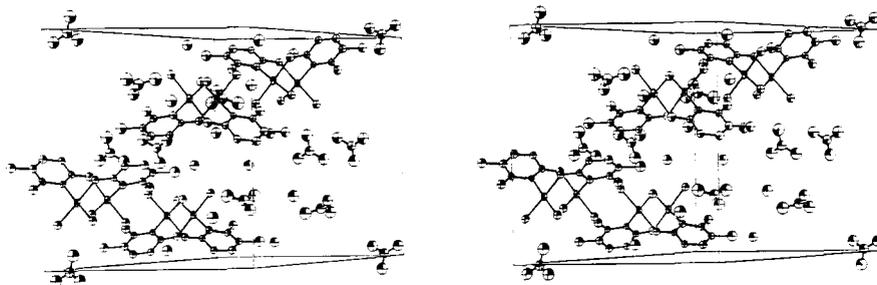


Figure 2. Packing of $[(\text{NH}_3)_2\text{Pt}(\text{C}_5\text{H}_5\text{N}_2\text{O}_2)_2\text{Pt}(\text{NH}_3)_2](\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ in the unit cell. a and b are parallel to the bottom and side of the page. The view is down c^* .

detailed calculations have been deposited.

Because the crystals originally used were blue, we considered the possibility that we had a "platinum-pyrimidine blue", but the great similarity to the yellow 1-methylthymine-platinum(II) complex¹¹ suggested that the crystals should also be yellow and were contaminated with a blue impurity. This has occurred before in structural studies of "platinblau".²³ Electron microscope pictures showed a cracked surface layer, of slightly different density, about 10000 Å thick.²⁴ The layer was amorphous. Subsequent work on new preparations gave a yellow-green product, which was clearly contaminated by blue material. We could not obtain this material as good crystals, but X-ray powder photographs showed clearly that the yellow-green material was identical with the crystalline portion of the single crystal (see Table IV). We conclude that the postulate that the "blue crystals" were yellow, contaminated with a blue noncrystalline component, is correct.

The packing within the crystal is illustrated in Figure 2. The cations are arranged in chains along c centered at roughly $1/4$, $1/4$ and $3/4$, $3/4$, adjacent cations being related by the glide plane. The cations are hydrogen bonded together through O(2)-N(4A), O(2)-N(2A), O(2A)-N(2), and O(2A)-N(4) such that the intercation Pt-Pt distance is 5.10 Å. Further long-range hydrogen bonds along the chains are provided through the N(6) nitrate ion which lies parallel to one of the pyrimidine rings of the cation. The nitrate ion is hydrogen bonded to the cation through O(62)-N(4) and O(62)-N(4A) and then to cations related by the c glide by O(63)-OH(2)-O(4A). N(6) nitrate ions related by the glide plane are themselves hydrogen bonded through O(63)-OH(1)-O(61). This same nitrate ion provides hydrogen bonding between cations related by a translation through hydrogen bonds O(61)-N(2) and O(61)-N(2A). The N(5) nitrate ions at roughly $y = 0$, $1/2$ are arranged so that they lie roughly parallel

to the ligating atoms square planes. They are hydrogen bonded directly to the cation through N(2)-O(53) and N(2a)-O(53) and to water through O(51)-OH(1) and O(51)-OH(3). Thus the prime interactions in the b direction are hydrogen bonds through cation-nitrate-water-cation as well as hydrogen bonding between the cations through OH(2)-OH(3).

We have noted above the similarity in structure of the cations of the 1-methyluracilate and 1-methylthymine complexes¹¹ which in turn are like that of the 1-methylcytosinate complex.²⁵ Despite differences in pyrimidine structure and stoichiometry of the compounds and dramatic differences in unit cell parameters, the similarities exist even in the crystal packing. The hydrogen-bonded chains of cations, one nitrate ion parallel to pyrimidine ring and hydrogen bonded to the ammine groups, and the other nitrate ion parallel to the ligating atoms square plane and bonded to the ammine groups are features found in each of the structures. Only the remaining hydrogen bonds, which determine how the chains are related to each other, differ and thus cause the overall structural difference. Hydrogen bonding is most extensive in the structure of the uracilate complex, and on the basis of volume and stoichiometry considerations, the compound has the most efficient packing in the solid state.

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Registry No. $[(\text{NH}_3)_2\text{Pt}(\text{C}_5\text{H}_5\text{N}_2\text{O}_2)_2\text{Pt}(\text{NH}_3)_2](\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$, 75790-30-6; *cis*-Pt(NH₃)₂Cl₂, 15663-27-1.

Supplementary Material Available: A table of the comparison of uracil and thymine bond lengths and angles and a listing of moduli of the observed and calculated structure factor amplitudes (22 pages). Ordering information is given on any current masthead page.

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(24) We thank Professor R. Kelly, Institute for Materials Research, McMaster University, for interpreting the electron microscope pictures.

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