

angle = 9.6°), one molecule being rotated in the coordination plane by ca 90° with respect to the other. However, there are no intermolecular contacts less than the sums of the van der Waals radii.

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## Bis(oxamide oximato)platinum(II)–Hydrogen Chloride (1:2), Form (II)

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**Abstract.**  $C_4H_{10}N_8O_4Pt \cdot 2HCl$ ,  $[Pt(C_2H_5N_4O_2)_2] \cdot 2HCl$ ,  $M_r = 502.17$ ,  $P\bar{1}$ ,  $a = 6.787$  (2),  $b = 8.876$  (4),  $c = 12.486$  (6) Å,  $\alpha = 112.58$  (3),  $\beta = 81.67$  (3),  $\gamma = 112.71$  (2)°,  $Z = 2$ ,  $d_c = 2.60$  Mg m<sup>-3</sup>; final  $R = 0.067$  for 4065 reflections. A H-bonded intramolecular O–Cl–O bridge exists instead of an O–H–O bridge between oxime O atoms.

**Introduction.** In preceding papers we have dealt with the structural variability of oxamide oxime (diaminoglyoxime, oaoH<sub>2</sub>) complexes of Ni and Pt. References are given in Endres & Schlicksupp (1979), where we describe how  $[Pt(oaoH)_2] \cdot 2HCl$  crystallizes simultaneously in two different modifications from HCl solution, and where we report the structure of form (I). The structure of form (II) is the subject of this communication.

A crystal 0.06 × 0.17 × 0.19 mm was used for the investigation. Rotation and Weissenberg photographs showed the crystal to be triclinic and gave an estimate for the lattice constants. Exact lattice parameters were calculated by least squares (Berdesinski & Nuber, 1966) from the  $\theta$  values of 59 reflections centred on a diffractometer. Data collection on a computer-controlled diffractometer (Siemens AED, Mo  $K\alpha$  radiation,  $\theta$ – $2\theta$  scans, five-value method,  $4 < 2\theta < 66^\circ$ ) yielded 4065 observed independent reflections with  $I > 3.0\sigma(I)$ . They were corrected for Lorentz and polarization factors. An absorption correction by numerical integration was applied.

The Pt position was derived from a Patterson synthesis, which favoured the choice of the centrosymmetric space group. Fourier syntheses showed the positions of the other atoms. Refinement by full-matrix least squares with anisotropic temperature factors converged with  $R = 0.067$  (maximum shift/error 0.009). A final difference map showed no maxima

Table 1. Positional parameters ( $\times 10^4$ ) and isotropic temperature factors equivalent to the refined anisotropic values

	x	y	z	U (Å <sup>2</sup> )
Pt	2426 (1)	4837 (1)	2039 (1)	0.034
Cl(1)	3949 (7)	8205 (5)	7888 (3)	0.054
Cl(2)	1963 (6)	1911 (4)	6195 (3)	0.045
O(1)	2076 (19)	2480 (12)	3362 (9)	0.052
O(2)	2645 (18)	8531 (11)	3307 (8)	0.048
O(3)	2673 (18)	7279 (12)	822 (8)	0.049
O(4)	2223 (19)	1108 (11)	615 (8)	0.049
N(1)	2301 (21)	4111 (12)	3363 (9)	0.041
N(2)	2478 (19)	6979 (13)	3397 (9)	0.040
N(3)	2633 (19)	5633 (12)	738 (9)	0.038
N(4)	2415 (21)	2720 (13)	634 (9)	0.042
N(5)	2404 (21)	4993 (14)	5391 (9)	0.045
N(6)	2857 (23)	8372 (15)	5407 (9)	0.049
N(7)	2436 (21)	4912 (16)	–1264 (9)	0.046
N(8)	2165 (24)	1481 (14)	–1377 (9)	0.050
C(1)	2483 (22)	5269 (16)	4419 (10)	0.040
C(2)	2636 (26)	7029 (16)	4432 (10)	0.042
C(3)	2429 (22)	4525 (16)	–323 (10)	0.038
C(4)	2309 (25)	2783 (19)	–389 (11)	0.045

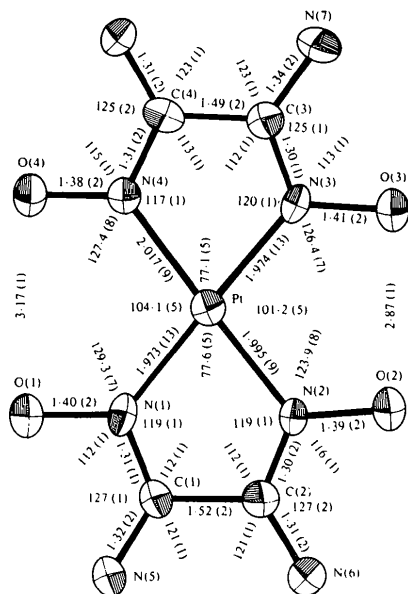


Fig. 1. The bis(oxamide oximato)platinum(II) molecule with bond distances (Å) and angles ( $^{\circ}$ ).

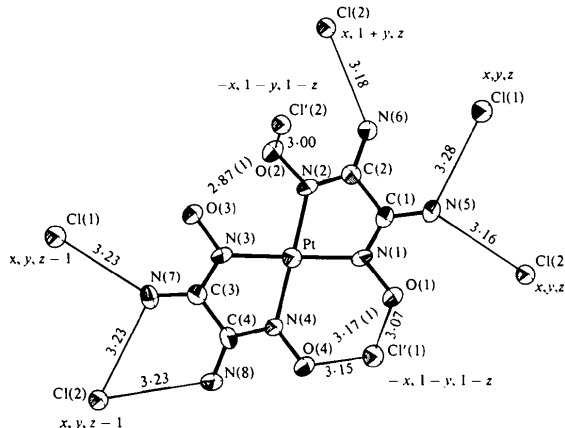


Fig. 2. The arrangement of the nearest ( $<3.3$  Å) Cl atoms around the complex molecule. The symmetry operations which generate the Cl positions are indicated. The e.s.d.'s of the distances are of the order of 0.02 Å.

attributable to solvent molecules. H atoms could not be identified.\*

Calculations were performed on an IBM 370/168 computer (Universitätsrechenzentrum Heidelberg) with the XRAY system (Stewart, Kundell & Baldwin, 1970) and scattering factors from *International Tables for X-ray Crystallography* (1974). Unit weights were used for all reflections. Plots were drawn by *ORTEP* (Johnson, 1965).

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34929 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

**Discussion.** Atomic coordinates are listed in Table 1; bond distances and angles with the numbering scheme are given in Fig. 1. The distances between the oxime O atoms indicate the absence of H bridges. Fig. 2 shows the molecule with the surrounding Cl atoms at distances  $<3.3$  Å. This limit for possible H-bonding interaction has been chosen by comparison with the N-Cl distance in crystalline  $\text{NH}_4\text{Cl}$ , 3.36 Å (Wyckoff, 1963). In particular, the short Cl-O distances indicate strong H bonding and, instead of the H bridge from O(1) to O(4), the existence of a HCl bridge has to be assumed. In neutron scattering work on the chloride of an amine oxime complex of Ni, Hussain & Schlemper (1979) found distances involving H bonding of 3.28 Å for Cl-N and 3.27 Å for Cl-OH<sub>2</sub>. As shown in Fig. 2, similar Cl-N distances to the amino groups exist in our case, and the Cl-O distances are markedly shorter. But as the H positions could not be determined, it is not clear whether H is closer to O or Cl and whether the compound should be formulated as  $[\text{Pt}(\text{oaoH})_2] \cdot 2\text{HCl}$  or as  $[\text{Pt}(\text{oaoH}_2)]^{2+} \cdot 2\text{Cl}^-$ . This also applies to the previously described form (I) of the title compound (Endres & Schlicksupp, 1979), where similar N-Cl and O-Cl distances were found. However, form (I) does not contain an intramolecular O-Cl-O bridge like that in form (II). The main differences between the two forms lie in the geometry of the molecules and in their packing in the crystal. In form (I) with one formula unit in the triclinic unit cell, the molecule is centrosymmetric. The distance between the oxime O atoms is 2.95 Å, intermediate between the two values found in form (II). In form (I) the molecules are arranged in stacks with an interplanar distance of 3.42 Å and a pronounced intermolecular overlap. The unit cell of form (II) contains two formula units. The molecule does not occupy an inversion centre and is far from centrosymmetric. No stacks are formed, in contrast to form (I), and there is no remarkable intermolecular overlap between adjacent molecules.

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