

plane of the ring. The fold about the Cr—Cr line is  $156^\circ$  whereas the corresponding angle for the  $\text{Cr}_2\text{N}_2$  ring of *cis*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})\text{NMe}_2]_2$  is  $178^\circ$ . The greater puckering of the methoxo complex can be attributed to its less symmetrical pattern of steric strain, for the methoxo complex has methyl groups on only one side of the  $\text{Cr}_2\text{O}_2$  ring and the dimethylamido complex has pairs of methyl groups above and below its  $\text{Cr}_2\text{N}_2$  ring. Several related *trans* complexes have crystallographic centres of symmetry and their  $\text{Cr}_2\text{X}_2$  rings are therefore necessarily planar, *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})\text{SPh}]_2$  (McPhail & Sim, 1968), *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})\text{NMe}_2]_2$  (Bush & Sim, 1970), and *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})_2]_2$  (Calderón, Fontana, Frauendorfer & Day, 1974).

The Cr—Cr separation in the methoxo-bridged complex is 2.882 (2) Å. This is appreciably greater than the 2.62 Å in *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})_2]_2$ , 2.67 Å in *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})\text{NMe}_2]_2$ , and 2.72 Å in *cis*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})\text{NMe}_2]_2$  but is shorter than the 2.95 Å in *trans*- $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})\text{SPh}]_2$ . Unbridged Cr—Cr single-bond distances are 2.97 Å in the binuclear  $[\text{Cr}_2(\text{CO})_{10}]^{2-}$  anion (Handy, Ruff & Dahl, 1970) and 3.28 Å in  $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{CO})_3]_2$  (Adams, Collins & Cotton, 1974).

The  $M-M'$ ,  $M-X$ ,  $M-X-M'$ , and  $X-M-X'$  lengths and angles of a central  $M_2X_2$  ring are not independent and the metal—metal separation must be considered in relation to the other dimensions of the ring. Since the single-bond covalent radii of S,  $sp^3\text{-N}$  and O are *ca* 1.04, 0.71, and 0.66 Å, the mean Cr—S, Cr—N, and Cr—O distances of 2.32, 2.01, and 1.96 Å in the complexes  $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})X]_2$  are clearly consistent. The  $X-M-X'$  angles in the S-, N- and O-bridged complexes are 101, 95, and  $83^\circ$ , respectively, while the  $M-X-M'$  angles are 79, 84, and  $95^\circ$ , respectively. The smaller  $X-M-X'$  angles in the dimethylamido and methoxo complexes serve to counterbalance to some extent the reductions in the Cr—Cr distance that would result from the replacement of the S atom in the  $\text{Cr}_2\text{S}_2$  fragment by the distinctly smaller N or O atoms. The appreciable difference between the

ring angles in the dimethylamido and methoxo complexes, together with the concomitant difference in the Cr—Cr distance, is surprising, however.

It has been noted that when the angle at the metal atom in an  $M_2X_2$  ring is obtuse and that at the bridging ligand is acute, the ring generally has a metal—metal bond and, conversely, when the ring lacks a metal—metal bond this arrangement of angles is reversed (Dahl, de Gil & Feltham, 1969; Connelly & Dahl, 1970; Simon & Dahl, 1973). If this test is applied to the  $[(\eta^5\text{-C}_5\text{H}_5)\text{Cr}(\text{NO})X]_2$  complexes, the angular pattern suggests that the O-bridged complex differs from the S- and N-bridged complexes by lacking a direct metal—metal bond. Nevertheless, all these complexes are diamagnetic and metal—metal spin coupling must be a common feature. It is possible, of course, that superexchange interaction through the bridging ligands may be important in the methoxo complex.

We thank Dr G. R. Knox for a sample of the complex and the Science Research Council for financial assistance.

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## The Structure of Dichloro-DL-ethioninepalladium(II)

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**Abstract.**  $\text{Pd}(\text{C}_6\text{H}_{13}\text{NO}_2\text{S})\text{Cl}_2$ ,  $M_r = 340.547$ , monoclinic,  $P2_1/n$ ,  $a = 11.065$  (11),  $b = 14.539$  (12),  $c = 7.138$  (4) Å,  $\beta = 97.60$  (4) $^\circ$ ,  $U = 1138$  (2) Å<sup>3</sup>,  $Z = 4$ ,

$D_m = 1.96$ ,  $D_c = 1.98$  Mg m<sup>-3</sup>,  $\mu = 2.20$  mm<sup>-1</sup>. The structure was solved by Patterson and Fourier methods and refined by block-diagonal least squares to  $R =$

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0.031 for 2093 observed reflexions. The amino acid molecule acts as a bidentate ligand and the coordination around palladium is distorted square-planar. The centrosymmetric molecules of the complex are associated in dimers through hydrogen bonds involving the carboxyl groups. In addition there is a hydrogen bond  $N-H \cdots Cl = 3.380 \text{ \AA}$  which is relevant for packing.

**Introduction.** Ethionine,  $CH_3CH_2SCH_2CH_2CH(NH_2)COOH$ , is a methionine antagonist (Dyer, 1938; Roblin, Lampen, English, Cole & Vaughan, 1945), inhibiting its metabolism. The stability constants ( $\log \beta_2$ ) of the DL-ethionine metal chelates are approximately  $10^2$  higher than those of DL-methionine chelates (Lenz & Martell, 1964). Due to the greater stability of its chelates, ethionine successfully competes with methionine when metal coordination is involved in enzyme reactions. The crystal structure of dichloro-DL-ethioninepalladium(II) has been investigated in order to contribute to the definition of the chelating properties of the sulphur-containing amino acids. A similar structure determined by X-ray diffraction is that of the analogous DL-methionine complex (Warren, McConnell & Stephenson, 1970) which suffered from radiation damage, but the ethionine complex is stable to radiation. The present analysis shows that DL-ethionine behaves as a bidentate ligand. The carboxyl group is not involved in coordination, as was also deduced from IR spectra (Livingstone & Nolan, 1968), as in DL-methionine and S-methyl-L-cysteine palladium chelates (Battaglia, Bonamartini Corradi, Grasselli Palmieri, Nardelli & Vidoni Tani, 1973).

The compound, prepared following Livingstone & Nolan (1968), occurs as prismatic bright-orange crystals. Crystal data were determined from rotation and Weissenberg photographs and from diffractometer measurements ( $Zr$ -filtered  $Mo K\alpha$  radiation,  $\lambda = 0.71069 \text{ \AA}$ ); space group  $P2_1/n$  from systematic absences.

Table 1. *Final atomic fractional coordinates* ( $\times 10^4$ ) *with e.s.d.'s for non-hydrogen atoms*

	x	y	z
Pd	446 (0)	602 (0)	3085 (1)
Cl(1)	823 (1)	-941 (1)	2463 (2)
Cl(2)	2449 (1)	884 (1)	4276 (2)
S	195 (1)	2126 (1)	3552 (2)
O(1)	-3528 (3)	-226 (3)	386 (5)
O(2)	-4516 (3)	886 (3)	1699 (5)
N	-1309 (3)	318 (3)	1938 (6)
C(1)	-3536 (4)	453 (3)	1390 (6)
C(2)	-2364 (4)	866 (3)	2412 (7)
C(3)	-2260 (4)	1878 (3)	1917 (7)
C(4)	-1400 (4)	2410 (3)	3391 (7)
C(5)	601 (6)	2632 (4)	1350 (8)
C(6)	639 (6)	3671 (4)	1496 (8)

Table 2. *Final atomic fractional coordinates* ( $\times 10^3$ ) *and isotropic thermal parameters with e.s.d.'s for hydrogen atoms*

	x	y	z	B ( $\text{\AA}^2$ )
H(1)	-144 (5)	-25 (4)	209 (8)	4.8 (1.4)
H(2)	-127 (5)	33 (4)	53 (7)	4.2 (1.3)
H(3)	-239 (4)	77 (3)	388 (7)	3.3 (1.1)
H(4)	-528 (5)	64 (4)	88 (7)	4.0 (1.2)
H(5)	-319 (5)	209 (4)	193 (8)	4.8 (1.4)
H(6)	-203 (5)	193 (4)	55 (7)	3.7 (1.2)
H(7)	-164 (5)	234 (4)	467 (7)	3.8 (1.2)
H(8)	-149 (5)	300 (4)	317 (7)	3.9 (1.2)
H(9)	-2 (5)	240 (4)	25 (8)	4.8 (1.3)
H(10)	135 (5)	235 (4)	105 (8)	4.6 (1.3)
H(11)	80 (5)	393 (4)	32 (8)	5.1 (1.4)
H(12)	-15 (5)	386 (4)	162 (8)	5.4 (1.5)
H(13)	126 (5)	382 (4)	254 (8)	5.8 (1.6)

The intensity data were collected on an 'on-line' Siemens AED single-crystal diffractometer. An  $\omega/2\theta$  scan ( $2\theta_{\max} = 58^\circ$ ) was used. The intensities of 3022 independent reflexions were measured excluding those with  $I < 2\sigma(I)$ . 2093 reflexions were used in the structure determination. Corrections for Lorentz and polarization effects were applied, but none for absorption.

The structure was solved by Patterson and Fourier methods. The refinement was carried out by block-diagonal least squares, first with isotropic, then with anisotropic thermal parameters. The hydrogen atoms were located from a difference Fourier synthesis. Further least-squares cycles were computed including the hydrogen atoms with isotropic thermal parameters. Unit weights were assumed for all the reflexions. The final conventional  $R$  value was 3.1%. The atomic scattering factors of Cromer & Mann (1968) were used for non-hydrogen atoms and those of Stewart, Davidson & Simpson (1965) for the hydrogen atoms.

All the calculations were carried out on the CDC 6600 computer of the Centro di Calcolo Elettronico Interuniversitario dell'Italia Nord-Orientale (Bologna) with programs written by Immirzi (1967).

Atomic coordinates are given in Tables 1 and 2.\*

**Discussion.** A clinographic projection of the structure is shown in Fig. 1. Bond distances and angles are given in Table 3. Coordination around palladium is slightly distorted square-planar (Fig. 2) and involves the sulphur and nitrogen atoms of the amino acid and the two chlorine atoms. An additional long contact  $Pd \cdots Pd(\bar{x}, \bar{y}, 1 - z) = 3.497 \text{ \AA}$  gives the coordination an elongated tetragonal-pyramidal shape. The amino

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34332 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

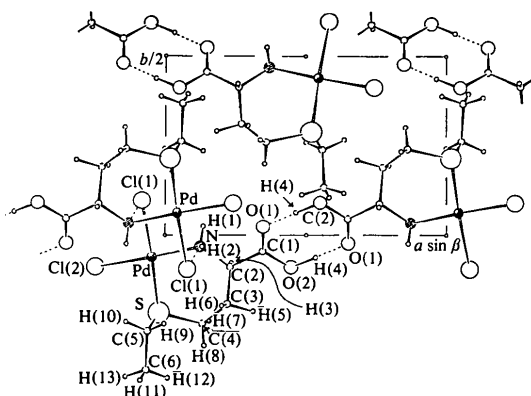


Fig. 1. Clinographic projection of the structure.

Table 3. *Interatomic distances (Å) and bond angles (°)*

## (a) In the coordination polyhedron

Pd—Cl(1)	2.335 (3)	Pd—S	2.263 (3)
Pd—Cl(2)	2.303 (3)	Pd—N	2.047 (4)
Cl(1)—Pd—Cl(2)	93.1 (1)	S—Pd—N	97.4 (2)
Cl(1)—Pd—S	175.6 (25)	Pd—S—C(4)	110.7 (3)
Cl(1)—Pd—N	85.1 (2)	Pd—S—C(5)	102.5 (4)
Cl(2)—Pd—S	84.4 (1)	Pd—N—C(2)	122.1 (6)
Cl(2)—Pd—N	177.6 (15)		

## (b) In the amino acid molecule

C(1)—O(1)	1.221 (6)	C(2)—H(3)	1.06 (5)
C(1)—O(2)	1.298 (6)	O(2)—H(4)	1.03 (5)
C(1)—C(2)	1.525 (6)	C(3)—H(5)	1.08 (6)
C(2)—N	1.489 (6)	C(3)—H(6)	1.04 (5)
C(2)—C(3)	1.521 (6)	C(4)—H(7)	0.99 (5)
C(3)—C(4)	1.532 (6)	C(4)—H(8)	0.88 (6)
C(4)—S	1.801 (5)	C(5)—H(9)	1.03 (5)
S—C(5)	1.844 (6)	C(5)—H(10)	0.97 (6)
C(5)—C(6)	1.514 (8)	C(6)—H(11)	0.96 (6)
N—H(1)	0.85 (6)	C(6)—H(12)	0.93 (6)
N—H(2)	1.01 (5)	C(6)—H(13)	0.97 (5)
O(1)—C(1)—O(2)	124.3 (9)	C(2)—C(3)—H(6)	108.8 (55)
O(1)—C(1)—C(2)	121.9 (8)	C(4)—C(3)—H(6)	113.6 (55)
O(2)—C(1)—C(2)	113.9 (7)	H(5)—C(3)—H(6)	109.8 (98)
C(1)—C(2)—N	108.9 (6)	C(3)—C(4)—H(7)	111.3 (54)
C(3)—C(2)—N	112.3 (7)	C(3)—C(4)—H(8)	109.0 (62)
C(1)—C(2)—C(3)	110.8 (6)	S—C(4)—H(7)	107.3 (52)
C(2)—C(3)—C(4)	112.8 (7)	S—C(4)—H(8)	108.9 (58)
C(3)—C(4)—S	116.3 (6)	H(7)—C(4)—H(8)	103.2 (99)
C(4)—S—C(5)	101.6 (5)	S—C(5)—H(9)	107.8 (51)
S—C(5)—C(6)	110.3 (6)	S—C(5)—H(10)	109.3 (57)
H(1)—N—C(2)	109.9 (67)	C(6)—C(5)—H(9)	112.9 (60)
H(2)—N—C(2)	110.8 (58)	C(6)—C(5)—H(10)	114.7 (67)
H(1)—N—H(2)	100.0 (97)	H(9)—C(5)—H(10)	101.3 (88)
N—C(2)—H(3)	106.2 (48)	C(5)—C(6)—H(11)	109.8 (63)
C(1)—C(2)—H(3)	106.8 (45)	C(5)—C(6)—H(12)	106.5 (60)
C(3)—C(2)—H(3)	111.7 (50)	C(5)—C(6)—H(13)	106.6 (56)
C(1)—O(2)—H(4)	112.2 (62)	H(11)—C(6)—H(12)	104.6 (107)
C(2)—C(3)—H(5)	100.0 (49)	H(11)—C(6)—H(13)	113.0 (111)
C(4)—C(3)—H(5)	111.0 (55)	H(12)—C(6)—H(13)	116.1 (115)

acid acts as a bidentate ligand forming a six-membered chelate ring. The comparison of the environment of Pd with that in the methionine complex shows that the arrangement is similar in the two cases, the angular

difference for corresponding directions being not greater than  $1^\circ$ . This is indicated also by the ring-puckering parameters calculated following Cremer & Pople (1975) for the chelating rings (in DL-methionine complex:  $q_2 = 0.352 \text{ \AA}$ ,  $\phi_2 = 17.5^\circ$ ,  $q_3 = -0.422 \text{ \AA}$ ,  $Q = 0.550 \text{ \AA}$ ,  $\theta_2 = 140.2^\circ$ ; in DL-ethionine complex:  $q_2 = 0.313 \text{ \AA}$ ,  $\phi_2 = 17.9^\circ$ ,  $q_3 = -0.466 \text{ \AA}$ ,  $Q = 0.561 \text{ \AA}$ ,  $\theta_2 = 146.1^\circ$ ) which correspond to a half-boat conformation.

The molecules of the complex related by the centre of symmetry are connected through hydrogen bonds ( $2.640 \text{ \AA}$ ) formed by the carboxyl groups (Fig. 1). The structure consists of layers parallel to (010), where the molecules are held together by hydrogen bonds  $N-H(2)\cdots Cl(1)(\bar{x}, \bar{y}, \bar{z}) = 3.380 \text{ \AA}$  along [001] and by hydrogen bonds between the carboxyl groups of two centrosymmetric molecules along [100]. Intramolecular interactions involving the O(1) and O(2) oxygen atoms and the hydrogen atoms of the  $NH_2$  group are important in determining the orientation of the carboxyl group.

In Table 4 the internal rotation angles  $\psi_1$ ,  $\psi_2$ ,  $\chi_1$ ,  $\chi_2$  and  $\chi_3$  observed in this complex, in the methionine complex and in  $\alpha$ -DL-methionine (Mathieson, 1952) are compared, showing the effects that the coordination and intramolecular contacts have on the conformation of the ligands.

The N—H distances are  $0.85 (6)$  and  $1.01 (5) \text{ \AA}$ . The C—H distances and the corresponding e.s.d.'s are in the ranges  $0.88\text{--}1.08$  and  $0.05\text{--}0.06 \text{ \AA}$  respectively.

The values of bond distances and angles are not significantly different from those observed in the methionine complex.

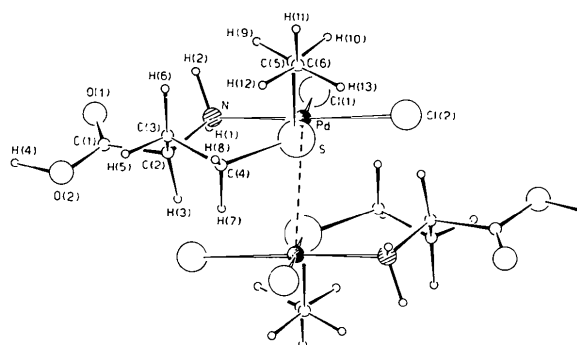


Fig. 2. Coordination around the palladium atom.

Table 4. *Internal rotation angles (°) for analogous sulphur-containing amino acid complexes*

$\psi_1$ ,  $\psi_2$  and  $\chi$  are defined according to the IUPAC rule:  $\psi_1 = \tau(N,C(2),C(1),O(1))$ ;  $\psi_2 = \tau(N,C(2),C(1),O(2))$ ;  $\chi_1 = \tau(N,C(2),C(3),C(4))$ ;  $\chi_2 = \tau(C(2),C(3),C(4),S)$ ;  $\chi_3 = \tau(C(3),C(4),S,C(5))$ .

	$\psi_1$	$\psi_2$	$\chi_1$	$\chi_2$	$\chi_3$
Dichloro-DL-ethioninepalladium(II)	0.5	-179.7	-79.2	68.2	71.8
Dichloro-DL-methioninepalladium(II)	-12.1	167.3	-81.2	68.7	76.3
$\alpha$ -DL-Methionine	-34	150	-60	177	81

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## Bis(3,5-dimethyl-1-phenylpyrazole)dinitratocopper(II)

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**Abstract.**  $\text{Cu}(\text{C}_{11}\text{H}_{12}\text{N}_2)_2(\text{NO}_3)_2$ ,  $\text{C}_{22}\text{H}_{24}\text{CuN}_6\text{O}_6$ , orthorhombic,  $P2_12_12_1$ ,  $a = 10.613(2)$ ,  $b = 13.188(3)$ ,  $c = 17.715(3)$  Å,  $V = 2479$  Å<sup>3</sup>,  $Z = 4$ ,  $D_m = 1.43$  (floatation),  $D_x = 1.42$  Mg m<sup>-3</sup>. The final  $R$  was 0.064 for 1750 observations. The  $\text{Cu}^{2+}$  is coordinated to the nitrate ions and the organic ligands in a near square-planar *cis* arrangement.

**Introduction.** Blue prismatic crystals of the title compound were prepared by Dr Cristo B. Melios *et al.* (Institute of Chemistry of Araraquara, UNESP). Chemical analysis showed a composition ratio of 1:2:2 for the  $\text{Cu}^{\text{II}}$  ions, nitrate and organic ligands (Melios, 1978). The structure determination was undertaken to study the coordination between the  $\text{Cu}^{\text{II}}$  and  $\text{NO}_3^-$  ions. Cell dimensions were refined by a least-squares fit to the setting angles of 25 reflexions on a CAD-4 automatic diffractometer. Intensity measurements were carried out up to  $\theta = 30^\circ$ , using the  $\omega$ - $2\theta$  scan mode, with graphite-monochromated Mo  $K\alpha$  radiation and a rectilinear crystal,  $0.4 \times 0.3 \times 0.6$  mm. Lorentz and polarization corrections were applied, but no absorption correction was made [ $\mu(\text{Mo } K\alpha) = 0.97$  mm<sup>-1</sup>]. Of the 2478 measured unique reflexions, 1750 were considered observed [ $F^2 \geq 2\sigma(F^2)$ ] and retained for use in the structure analysis\* and refinement.

\* Lists of structure factors, anisotropic thermal parameters, hydrogen atom parameters and bond distances and angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34236 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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The structure was solved by the heavy-atom method. It was refined by full-matrix least-squares calculations by minimization of  $\sum \omega(k|F_o| - |F_c|)^2$ , where  $\omega = [\sigma(F_o)^2 + (0.05F_o)^2]^{-1}$  for observed and  $\omega = 0$  for unobserved reflexions, until all the atomic parameter shifts were smaller than each standard deviation. The final unweighted  $R$  factor, omitting unobserved reflexions, was 0.064 and including them 0.070. Aniso-

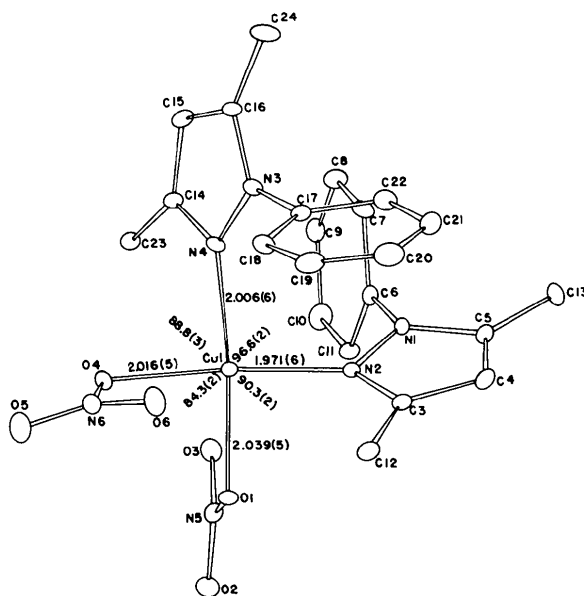


Fig. 1. Diagram of the molecule showing bond lengths (Å) and angles ( $^\circ$ ) around the copper ion and atom numbering.

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