

Data collection

Enraf–Nonius CAD-4 diffractometer	1582 reflections with $I > 3\sigma(I)$
$\omega/2\theta$ scans	$R_{\text{int}} = 0.041$
Absorption correction: Gaussian (<i>Xtal3.4</i> ; Hall <i>et al.</i> , 1995)	$\theta_{\text{max}} = 28.02^\circ$ $h = 0 \rightarrow 16$ $k = 0 \rightarrow 16$ $l = -43 \rightarrow 43$
$T_{\text{min}} = 0.779$, $T_{\text{max}} = 0.836$	
6562 measured reflections	3 standard reflections
2990 independent reflections	every 100 reflections intensity decay: 0.40%

Refinement

Refinement on F	$(\Delta/\sigma)_{\text{max}} = 0.009$
$R = 0.027$	$\Delta\rho_{\text{max}} = 1.33 \text{ e } \text{\AA}^{-3}$
$wR = 0.028$	$\Delta\rho_{\text{min}} = -2.23 \text{ e } \text{\AA}^{-3}$
$S = 0.976$	Extinction correction: none
1582 reflections	Scattering factors from <i>International Tables for X-ray Crystallography</i> (Vol. IV)
145 parameters	
H atoms not refined	
Weighting scheme: see below	

Table 1. Selected geometric parameters (\AA , $^\circ$)

Mo1—Mo2	2.570 (1)	Mo2—O2	1.664 (4)
Mo1—O1	1.682 (4)	Mo2—O3	1.936 (4)
Mo1—O3	1.916 (4)	Mo2—O4	1.929 (4)
Mo1—O4	1.926 (4)	Mo2—O5 ⁱ	2.040 (4)
Mo1—O5	2.138 (4)	Mo2—O6 ⁱ	2.017 (4)
Mo1—O6	2.220 (4)	O5—C5 ^o	1.423 (8)
Mo1—N	2.255 (5)	O6—C6 ^o	1.414 (9)
O1—Mo1—O3	109.8 (2)	O2—Mo2—O3	111.5 (2)
O1—Mo1—O4	108.7 (2)	O2—Mo2—O4	109.5 (2)
O1—Mo1—O5	93.4 (2)	O2—Mo2—O5 ⁱ	106.1 (2)
O1—Mo1—O6	156.1 (2)	O2—Mo2—O6 ⁱ	106.0 (2)
O1—Mo1—N	89.2 (2)	O3—Mo2—O4	92.3 (2)
O3—Mo1—O4	93.1 (2)	O3—Mo2—O6 ⁱ	140.9 (2)
O3—Mo1—O5	155.7 (2)	O3—Mo2—O5 ⁱ	85.8 (2)
O3—Mo1—O6	88.1 (2)	O4—Mo2—O6 ⁱ	85.3 (2)
O3—Mo1—N	86.4 (2)	O4—Mo2—O5 ⁱ	142.4 (2)
O4—Mo1—O5	86.0 (2)	O6 ⁱ —Mo2—O5 ⁱ	73.4 (1)
O4—Mo1—O6	85.1 (1)	Mo1—O3—Mo2	83.7 (1)
O4—Mo1—N	161.0 (2)	Mo1—O4—Mo2	83.6 (2)
O5—Mo1—O6	67.6 (1)	Mo1—O5—Mo2 ⁱⁱ	110.6 (2)
O5—Mo1—N	86.8 (2)	Mo1—O6—Mo2 ⁱⁱ	108.2 (2)
O6—Mo1—N	75.9 (2)		

Symmetry codes: (i) $\frac{1}{4} + y, \frac{7}{4} - x, \frac{3}{4} - z$; (ii) $\frac{7}{4} - y, x - \frac{1}{4}, \frac{3}{4} - z$.

The weighting scheme used was $w = W_F W_S$, where $W_F (F_o < 90) = (F_o/90)^2$, $W_F (F_o > 160) = (160/F_o)^{1.5}$ and $W_F (90 < F_o < 160) = 1$, and $W_S (\sin\theta < 0.42) = (\sin\theta/0.42)^2$, $W_S (\sin\theta > 0.55) = (0.55/\sin\theta)^4$ and $W_S (0.42 < \sin\theta < 0.55) = 1$. Of the four peaks exceeding $1.0 \text{ e } \text{\AA}^{-3}$ in the final difference Fourier map, one ($1.194 \text{ e } \text{\AA}^{-3}$) is located on an S_4 special position in the middle of the octanuclear ring. The other three peaks (1.33 , 1.091 and $1.035 \text{ e } \text{\AA}^{-3}$) lie closest to O6 [$1.385(3) \text{\AA}$], O4 [$1.296(4) \text{\AA}$] and O2 [$0.561(5) \text{\AA}$], respectively. The two deepest holes, with values of -2.232 and $-2.191 \text{ e } \text{\AA}^{-3}$, are found on the Mo1 and Mo2 positions. The remaining 11 holes, with values ranging from -1.466 to $-1.014 \text{ e } \text{\AA}^{-3}$, lie close to Mo1 and Mo2. The relatively high number of peaks and holes results from the high symmetry of the space group.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *Xtal3.4* (Hall *et al.*, 1995). Program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994). Program(s) used to refine

structure: *Xtal3.4*. Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *Xtal3.4*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1365). Services for accessing these data are described at the back of the journal.

References

- Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
- Chae, H. K., Klemperer, W. G. & Marquart, T. A. (1993). *Coord. Chem. Rev.* **128**, 209–224.
- Chen, Q., Liu, S. & Zubieta, J. (1988). *Angew. Chem. Int. Ed. Engl.* **27**, 1724–1725.
- Chen, Q., Liu, S. & Zubieta, J. (1989). *Inorg. Chem.* **28**, 4434–4436.
- Chisholm, M. H., Huffman, J. C., Kirkpatrick, C. C., Leonelli, J. & Foltling, K. (1981). *J. Am. Chem. Soc.* **103**, 6093–6099.
- Cotton, F. A. & Ilsley, W. H. (1982). *Inorg. Chim. Acta*, **59**, 213–217.
- Darensbourg, D. J., Gray, R. L. & Delord, T. (1985). *Inorg. Chim. Acta*, **98**, L39–42.
- Douglas, B., McDaniel, D. & Alexander, J. (1994). *Concepts and Models of Inorganic Chemistry*, p. 102. New York: Wiley.
- El-Essawi, M. M., Weller, F., Stahl, K., Kersting, M. & Dehnicke, K. (1986). *Z. Anorg. Allg. Chem.* **542**, 175–181.
- Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
- Hall, S. R., King, G. S. D. & Stewart, J. M. (1995). Editors. *Xtal3.4 User's Manual*. University of Western Australia, Australia.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Khan, M. I. & Zubieta, J. (1995). *Prog. Inorg. Chem.* **43**, 1–149.
- Modc, B., Brenčić, J. V. & Leban, I. (1998). *Inorg. Chem. Commun.* **1**, 161–163.
- Spivack, B. & Dori, Z. (1975). *Coord. Chem. Rev.* **17**, 99–136.
- Stiefel, E. I. (1977). *Prog. Inorg. Chem.* **22**, 1–223.

Acta Cryst. (1998). **C54**, 1575–1578

Ferrocenium Tetrachloroferrate Revisited, and Ferrocenium Tetrachloroaluminate

F. ALBERT COTTON, LEE M. DANIELS AND ISABEL PASCUAL

Laboratory for Molecular Structure and Bonding, Department of Chemistry, Texas A&M University, PO Box 30012, College Station, TX 77842-3012, USA. E-mail: cotton@tamu.edu

(Received 9 March 1998; accepted 19 May 1998)

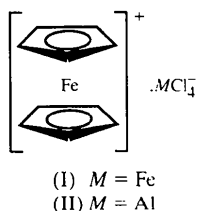
Abstract

The structure of the title compound, $[\text{Fe}(\text{Cp})_2][\text{FeCl}_4]$ (Cp = cyclopentadienyl, C_5H_5), was reported in 1978 in the non-centrosymmetric space group $Pna2_1$ at room

temperature [Paulus & Schäfer (1978). *J. Organomet. Chem.* **144**, 205–213]. A low-temperature data set indicates a phase transition from the non-centrosymmetric space group to the centrosymmetric space group *Pnma*. Crystals of [Fe(Cp)₂][AlCl₄] have also been studied at low temperature and are isomorphous with the FeCl₄⁻ complex.

Comment

[Fe(Cp)₂][FeCl₄], (I), was characterized in 1978 by X-ray crystallography at room temperature, in space group *Pna2*₁ (Paulus & Schäfer, 1978). Data have now been collected on this compound at a moderately low temperature (213 K), and the results are reported here.



Statistical tests performed on the (highly redundant) area-detector data set of (I) strongly indicated centrosymmetry, with a mean $|E^2 - 1| = 0.935$ (with expected values of 0.968 for centrosymmetric and 0.736 for non-centrosymmetric). As a check, the structure was refined in both *Pnma* and *Pna2*₁. Refinement in the non-centrosymmetric group resulted in substantial correlation between atoms that would be related by mirror symmetry in the centrosymmetric group, with correlation coefficients ranging from 0.80 to 0.93. Fully anisotropic treatment in space group *Pna2*₁ was therefore not possible, since the refinement would not converge. Refinement in *Pnma* also gave better residuals, even with only slightly more than half the number of parameters, *i.e.* 0.084 *versus* 0.088 (not converged) in *Pna2*₁ (weighted *R*, calculated on *F*² using all data).

To assess our choice of space group further, we crystallized [Fe(Cp)₂][AlCl₄], (II), an isomorphous species that had not been characterized by X-ray diffraction. Data were collected from a regular crystal, also at a temperature of 213 K. Evidence of centrosymmetry was analogous to that for (I), *i.e.* the mean $|E^2 - 1| = 1.050$; there are correlation problems in *Pna2*₁, and the residuals are lower in *Pnma* (0.144 *versus* 0.153).

Ferrocenium salts of 'innocent' counter-ions, such as SbF₆⁻ (Hendrickson *et al.*, 1996), PF₆⁻ (Martinez & Tiripicchio, 1990), TcO₄⁻ (Grigoriev & Krytchov, 1993), SbCl₄⁻ (Yamin *et al.*, 1996) or FeBr₄⁻ (Evans *et al.*, 1992), among others, have various conformations (staggered, *gauche* or eclipsed) at room temperature. Crystals of [Fe(Cp)₂]PF₆ exhibit a phase change at high temperature, from *P2*₁/*c* (staggered disordered at 295 K) to *Pm3* (eclipsed at 360 K; Webb *et al.*, 1992).

The structure reported by Paulus & Schäfer (1978) was deduced from data collected at room temperature, where the space group is *Pna2*₁ and the Cp ligands are rotated 11(2)° away from the eclipsed conformation. At the lower temperature of the present study, the average structure has mirror symmetry and the space group is *Pnma*. Similar behavior for ferrocene has been thoroughly studied at different temperatures using X-rays (Seiler & Dunitz, 1979*a,b*, 1982) and neutrons (Takusagawa & Koetzle, 1979).

It is apparent that the structures of both (I) and (II) are significantly affected by rigid-body motion, most noticeably the Cp rings. In fact, it is precisely the conformation of the rings that determines whether or not the mirror planes in *Pnma* are present. The C—C bond distances in both compounds were analyzed for rigid-body motion (Schomaker & Trueblood, 1968) and were found to suffer significant librational shortening. In our analysis, the [FeCp₂]⁺ groups were treated independently of the [MCl₄]⁻ ions, and the H atoms were removed. Before the corrections, the average C—C distance was 1.385(7) Å for (I) and 1.387(6) Å for (II). The corrections for the C—C distances range from 0.032 to 0.035 Å, and bring the average C—C distance to 1.42(2) Å for both (I) and (II), which is essentially the expected value for the C—C distance of cyclopentadienyl ligands (Seiler & Dunitz, 1979*b*).

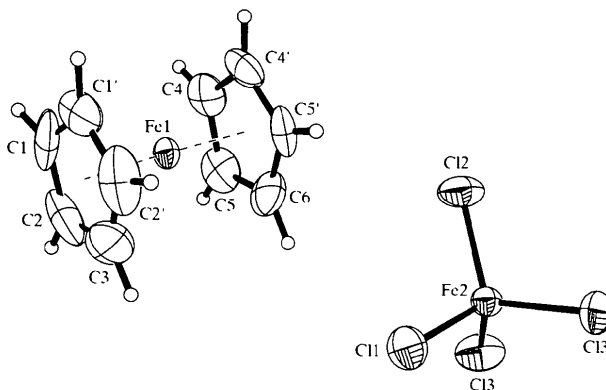


Fig. 1. The molecular structure of (I), drawn with 50% probability displacement ellipsoids and with H atoms shown as arbitrarily sized spheres.

The five atoms making up each Cp ring are planar, to within 0.008 Å for (I) and 0.004 Å for (II). In compound (I), atom Fe1 is 1.701(2) Å from the least-squares plane defined by atoms C1–C3, and 1.695(2) Å from the least-squares plane defined by atoms C4–C6. The planes make an angle of 1.6(2)°. In (II), the Fe atom is 1.698(4) Å from the least-squares plane defined by atoms C1–C3, and 1.695(4) Å from the least-squares plane defined by atoms C4–C6. The two planes form an angle of 1.8(3)°.

The weighted average Fe—Cl bond distance in (I) is 2.184 (2) Å, and the weighted average Al—Cl bond distance in (II) is 2.124 (2) Å. These are essentially equal to the average values in the Cambridge Structural Database (Allen & Kennard, 1993): 2.18 (1) Å for unassociated Fe^{III}Cl₄ (97 structures) and 2.12 (1) Å for unassociated AlCl₄ (103 structures).

Experimental

Compounds (I) and (II) were prepared in diethyl ether by stirring stoichiometric amounts of Fe(Cp)₂ and PhICl₂ with FeCl₃ [for (I)] or AlCl₃ [for (II)]. Crystals of both compounds were grown by slow diffusion of hexanes into dichloromethane solutions.

Compound (I)

Crystal data

[Fe(C ₅ H ₅) ₂][FeCl ₄]	Mo K α radiation
$M_r = 383.68$	$\lambda = 0.71073 \text{ \AA}$
Orthorhombic	Cell parameters from 250 reflections
<i>Pnma</i>	$\theta = 9.1\text{--}20.8^\circ$
$a = 13.7463 (8) \text{ \AA}$	$\mu = 2.755 \text{ mm}^{-1}$
$b = 8.6401 (4) \text{ \AA}$	$T = 213 (2) \text{ K}$
$c = 11.9943 (12) \text{ \AA}$	Prism
$V = 1424.6 (2) \text{ \AA}^3$	$0.22 \times 0.19 \times 0.12 \text{ mm}$
$Z = 4$	Dark red
$D_x = 1.789 \text{ Mg m}^{-3}$	
D_m not measured	

Data collection

Nonius FAST diffractometer	1252 reflections with
ω scans	$I > 2\sigma(I)$
Absorption correction:	$R_{\text{int}} = 0.045$
multi-scan (Blessing,	$\theta_{\text{max}} = 25.29^\circ$
1995)	$h = -16 \rightarrow 16$
$T_{\text{min}} = 0.546, T_{\text{max}} = 0.722$	$k = -10 \rightarrow 10$
7402 measured reflections	$l = -12 \rightarrow 14$
1348 independent reflections	

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.035$	$\Delta\rho_{\text{max}} = 0.692 \text{ e \AA}^{-3}$
$wR(F^2) = 0.084$	$\Delta\rho_{\text{min}} = -0.445 \text{ e \AA}^{-3}$
$S = 1.179$	Extinction correction: none
1348 reflections	Scattering factors from
82 parameters	<i>International Tables for</i>
H atoms not refined	<i>Crystallography</i> (Vol. C)
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2$	
$+ 2.2P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

Compound (II)

Crystal data

[Fe(C ₅ H ₅) ₂][AlCl ₄]	Mo K α radiation
$M_r = 354.81$	$\lambda = 0.71073 \text{ \AA}$

Orthorhombic

Pnma

$a = 13.788 (6) \text{ \AA}$
$b = 8.643 (2) \text{ \AA}$
$c = 12.009 (6) \text{ \AA}$
$V = 1431.1 (10) \text{ \AA}^3$
$Z = 4$
$D_x = 1.647 \text{ Mg m}^{-3}$
D_m not measured

Cell parameters from 250 reflections

$\theta = 9.1\text{--}20.8^\circ$
$\mu = 1.831 \text{ mm}^{-1}$
$T = 213 (2) \text{ K}$
Block
$0.27 \times 0.21 \times 0.19 \text{ mm}$
Dark blue

Data collection

Nonius FAST diffractometer	1146 reflections with
ω scans	$I > 2\sigma(I)$
Absorption correction:	$R_{\text{int}} = 0.055$
multi-scan (Blessing,	$\theta_{\text{max}} = 25.08^\circ$
1995)	$h = -16 \rightarrow 16$
$T_{\text{min}} = 0.591, T_{\text{max}} = 0.717$	$k = -10 \rightarrow 10$
6947 measured reflections	$l = -14 \rightarrow 11$
1351 independent reflections	

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.059$	$\Delta\rho_{\text{max}} = 0.939 \text{ e \AA}^{-3}$
$wR(F^2) = 0.144$	$\Delta\rho_{\text{min}} = -0.492 \text{ e \AA}^{-3}$
$S = 1.146$	Extinction correction: none
1351 reflections	Scattering factors from
82 parameters	<i>International Tables for</i>
H atoms not refined	<i>Crystallography</i> (Vol. C)
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2$	
$+ 5.1P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

H atoms were located in difference maps, but their positions were not included as refined parameters. Each H atom was allowed to 'ride' on the attached C atom at a distance of 0.94 Å, with an isotropic displacement parameter set at 1.2 times the equivalent isotropic parameter of the C atom.

For both compounds, data collection: *MADNES* (Pflugrath & Messerschmidt, 1992); cell refinement: *MADNES*; data reduction: *SHELXTL* (Sheldrick, 1996); program(s) used to solve structures: *SHELXTL*; program(s) used to refine structures: *SHELXL93* (Sheldrick, 1993); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL93*.

We are grateful to the National Science Foundation for support of this work.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG1462). Services for accessing these data are described at the back of the journal.

References

- Allen, F. H. & Kennard, O. (1993). *Chem. Des. Autom. News*, **8**, 31–37.
- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
- Evans, P. J. M., Fitzsimmons, B. W., Marshall, W. G., Golder, A. J., Larkworthy, L. F., Smith, G. W. & Povey, D. C. (1992). *J. Chem. Soc. Dalton Trans.* pp. 1065–1068.
- Grigoriev, M. S. & Kryuchkov, S. V. (1993). *Radiochim. Acta*, **63**, 187–193.
- Hendrickson, D., Rheingold, A. L. & Allen, M. B. (1996). Private communication.

- Martinez, R. & Tiripicchio, A. (1990). *Acta Cryst.* **C46**, 202–205.
 Paulus, E. F. & Schäfer, L. (1978). *J. Organomet. Chem.* **144**, 205–213.
 Pflugrath, J. W. & Messerschmidt, A. (1992). *MADNES. Munich Area Detector Systems*. Delft Instruments, Delft, The Netherlands.
 Schomaker, V. & Trueblood, K. N. (1968). *Acta Cryst.* **B24**, 63–76.
 Seiler, P. & Dunitz, J. D. (1979a). *Acta Cryst.* **B35**, 1068–1074.
 Seiler, P. & Dunitz, J. D. (1979b). *Acta Cryst.* **B35**, 2020–2032.
 Seiler, P. & Dunitz, J. D. (1982). *Acta Cryst.* **B38**, 1741–1745.
 Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
 Sheldrick, G. M. (1996). *SHELXTL. Structure Determination Programs*. Version 5.05. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Takusagawa, F. & Koetzle, T. F. (1979). *Acta Cryst.* **B35**, 1074–1079.
 Webb, R. J., Lowery, M. D., Shiomi, Y., Sorai, M., Wittebort, R. J. & Hendrickson, D. N. (1992). *Inorg. Chem.* **31**, 5211–5219.
 Yamin, B. M., Fun, H.-K., Sivakumar, K., Yip, B.-C. & Shawkataly, O. B. (1996). *Acta Cryst.* **C52**, 600–602.

Acta Cryst. (1998). **C54**, 1578–1580

Aqua(4,4'-dicarbomethoxy-2,2'-bipyridine-*N,N'*)(3,6-dichloro-4,5-dihydroxy-1,2-benzoquinonato-*O*⁴,*O*⁵)copper(II) Acetonitrile Hemisolvate†

LI-MIN ZHENG,^a HELMUT W. SCHMALLE,^b SYLVIE FERLAY^c AND SILVIO DECURTINS^c

^aState Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China,

^bInstitute of Inorganic Chemistry, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland,

and ^cDepartment für Chemie und Biochemie, Universität Bern, Freiestrasse 3, CH-3012 Bern 9, Switzerland. E-mail: schmalle@aci.unizh.ch

(Received 12 February 1998; accepted 5 May 1998)

Abstract

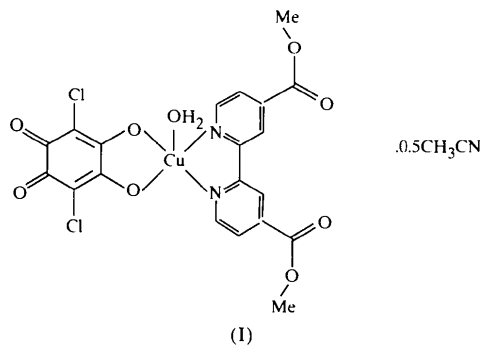
The title compound, [Cu(C₆Cl₂O₄)(C₁₄H₁₂N₂O₄)(H₂O)].0.5CH₃CN, adopts a slightly distorted square-pyramidal geometry around the five-coordinated Cu^{II} atoms, where the bidentate benzoquinone anion and the bidentate bipyridine ligand form the basal plane. The elongated apical position is occupied by a water molecule. The acetonitrile solvate molecule is disordered.

Comment

Attempts to build new metallic molecular materials using the oxalate ligand leads to three- and two-

† Systematic name: aqua(3,6-dichloro-4,5-dihydroxy-1,2-benzoquinonato-*O*⁴,*O*⁵)(dimethyl 2,2'-bipyridine-4,4'-dicarboxylato-*N,N'*)copper(II) acetonitrile hemisolvate.

dimensional compounds (Decurtins *et al.*, 1994; Pellaux *et al.*, 1997), while the 3,6-dichloro-4,5-dihydroxy-1,2-benzoquinone ligand (CA²⁻) has the potential for building up one-dimensional or two-dimensional transition metal polymers. The structures of several such polymers have been determined. Among these are the one-dimensional structures of [Cu(CA)(H₂O)₂]_n (Cueto *et al.*, 1992), {[Cu(CA)(H₂O)_m](G)}_n (*m* = 2, *G* = 2,5-dimethylpyrazine and phenazine; *m* = 1, *G* = 1,2,3,4,6,7,8,9-octahydrophenazine; Kawata *et al.*, 1996) and [Cu(CA)(CH₃OH)₂]_n (Kawata *et al.*, 1994), and the two-dimensional sheet structure of [Cu(CA)(pyz)]_n (pyz = pyrazine; Kawata *et al.*, 1994). We have recently succeeded in synthesizing the two chain compounds [Mn(bipy)(CA)]_n (bipy = 2,2'-bipyridine; Zheng *et al.*, 1996) and [Cu(DCMB)(CA)]_n (DCMB = 3,3'-dicarbomethoxy-2,2'-bipyridine) (Decurtins, Schmale, Zheng & Enslin, 1996). In our attempt to build new one- or two-dimensional bimetallic systems from an analogous precursor, [Cu(4-DCMB)]²⁺ (4-DCMB = 4,4'-dicarbomethoxy-2,2'-bipyridine), and a manganese(II) salt, a mononuclear compound, (I), was obtained.



The molecular structure of (I) is shown in Fig. 1. It exhibits a slightly distorted square-pyramidal coordination geometry about the Cu^{II} atom. Two N atoms from the 4-DCMB ligand [Cu—N = 1.984(2) and 1.985(2) Å, N1A—Cu—N1B = 81.7(1)°] and two O atoms from the CA²⁻ ligand [Cu—O = 1.938(2) and 1.947(2) Å, O1—Cu—O2 = 84.0(1)°] occupy the basal plane. All four atoms deviate by 0.007(1) Å from this plane. The Cu atom is pulled out of this least-squares plane [0.218(1) Å] towards the apically coordinated O11 atom [Cu—O11 = 2.216(2) Å]. The structure could be closely related to the mononuclear compound [Cu(DHBQ)(bipym)(H₂O)].5H₂O (DHBQ is the dianion of 2,5-dihydroxy-1,4-benzoquinone and bipym = 2,2'-bipyrimidine; Decurtins, Schmale, Schneuwly & Zheng, 1996), where the bond lengths Cu—N [1.983(3) and 2.004(3) Å] and Cu—O [1.928(3) and 1.947(3) Å] are comparable to those in the title compound, and the bond angles N—Cu—N [82.1(1)°] and O—Cu—O [85.1(1)°] are only slightly larger. The two pyridine