$V = 1258.0\ (9)$ Å^3
$Z = 2$
$D_x = 2.145$ Mg m^{-3}
Amber
Crystal source: recrystallized from chloroform/hexane

Data collection

Rigaku AFC-6R diffractometer
ω-2θ scans
Absorption correction: empirical (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.768$, $T_{\max} = 1.286$
2532 measured reflections
2220 independent reflections
1463 observed reflections $[I > 3\sigma(I)]$
$R_{\rm int} = 0.050$
$\theta_{\max} = 25°$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 10$
$l = -17 \rightarrow 17$
3 standard reflections monitored every 300 reflections intensity variation: ±1%

Refinement

Refinement on F
Final $R = 0.031$
$wR = 0.038$
$S = 1.55$
1463 reflections
127 parameters
H atoms riding, $B(\mathrm{H}) = 1.2\ B_{\rm eq}(\mathrm{C})$
$w = 1/[\sigma^2(F)+0.02F^2]$
$(\Delta/\sigma)_{\max} = 0.15$
$\Delta\rho_{\max} = 0.64$ e Å^{-3} (near Re)
$\Delta\rho_{\min} = -0.90$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$U_{\rm eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Re	0.35525 (3)	0.50154 (5)	0.53574 (2)	0.0370 (3)
P(1)	0.2926 (3)	0.6832 (3)	0.4195 (2)	0.053 (1)
P(2)	0.5760 (3)	0.6894 (3)	0.3539 (2)	0.051 (1)
O(1)	0.2733 (8)	0.2280 (10)	0.4078 (5)	0.090 (6)
O(2)	0.0773 (8)	0.5147 (11)	0.6080 (6)	0.088 (6)
O(3)	0.4578 (8)	0.7735 (11)	0.6604 (6)	0.092 (6)
C(1)	0.3062 (10)	0.3342 (13)	0.4532 (6)	0.054 (6)
C(2)	0.1808 (10)	0.5124 (12)	0.5801 (6)	0.051 (5)
C(3)	0.4262 (10)	0.6699 (13)	0.6143 (7)	0.060 (7)
C(4)	0.1694 (12)	0.8299 (16)	0.4506 (8)	0.103 (10)
C(5)	0.2157 (12)	0.5958 (18)	0.3134 (7)	0.096 (9)
C(6)	0.4277 (10)	0.8028 (12)	0.3805 (6)	0.057 (7)
C(7)	0.5365 (12)	0.6273 (15)	0.2364 (7)	0.081 (8)
C(8)	0.6977 (11)	0.8444 (15)	0.3375 (8)	0.089 (9)

Table 2. *Geometric parameters* (Å, °)

Re—Re$^{\rm i}$	3.126 (1)	P(1)—C(6)	1.812 (10)
Re—P(1)	2.374 (3)	P(2)—C(6)	1.829 (10)
Re—P(2$^{\rm i}$)	2.382 (3)	P(2)—C(7)	1.836 (11)
Re—C(1)	1.928 (10)	P(2)—C(8)	1.824 (12)
Re—C(2)	1.893 (9)	O(1)—C(1)	1.166 (11)
Re—C(3)	1.957 (11)	O(2)—C(2)	1.132 (12)
P(1)—C(4)	1.834 (12)	O(3)—C(3)	1.152 (12)
P(1)—C(5)	1.860 (12)		
Re$^{\rm i}$—Re—P(1)	88.10 (8)	Re—P(1)—C(5)	114.9 (5)
Re$^{\rm i}$—Re—P(2$^{\rm i}$)	89.69 (8)	Re—P(1)—C(6)	115.8 (3)
Re$^{\rm i}$—Re—C(1)	89.0 (2)	C(4)—P(1)—C(5)	104.0 (6)
Re$^{\rm i}$—Re—C(2)	177.6 (3)	C(4)—P(1)—C(6)	102.2 (5)
Re$^{\rm i}$—Re—C(3)	84.4 (2)	C(5)—P(1)—C(6)	103.5 (5)
P(1)—Re—P(2$^{\rm i}$)	176.76 (8)	Re—P(2$^{\rm i}$)—C(6$^{\rm i}$)	114.8 (3)
P(1)—Re—C(1)	89.2 (3)	Re—P(2$^{\rm i}$)—C(7$^{\rm i}$)	119.0 (4)
P(1)—Re—C(2)	90.8 (3)	Re—P(2$^{\rm i}$)—C(8$^{\rm i}$)	115.3 (4)
P(1)—Re—C(3)	90.8 (3)	C(6)—P(2)—C(7)	103.3 (5)
P(2$^{\rm i}$)—Re—C(1)	88.4 (3)	C(6)—P(2)—C(8)	100.9 (5)
P(2$^{\rm i}$)—Re—C(2)	91.5 (3)	C(7)—P(2)—C(8)	101.0 (6)
P(2$^{\rm i}$)—Re—C(3)	91.3 (3)	Re—C(1)—O(1)	175.7 (8)
C(1)—Re—C(2)	93.1 (4)	Re—C(2)—O(2)	177.9 (9)
C(2)—Re—C(3)	93.6 (4)	Re—C(3)—O(3)	174.6 (9)
C(1)—Re—C(3)	173.3 (4)	P(1)—C(6)—P(2)	112.9 (5)
Re—P(1)—C(4)	114.8 (4)		

Symmetry code: (i) $1 - x, 1 - y, 1 - z$.

Sample preparation: Milder *et al.* (1990). Scan speed: 16° min^{-1} in ω. Scan width: $(1.00 + 0.30\tan\theta)°$. Structure analysis package: *TEXSAN* (Molecular Structure Corporation, 1989). Re position: *PHASE* (subprogram of *DIRDIF*; Beurskens *et al.*, 1984).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71097 (23 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH1037]

References

Beurskens, P. T., Bosman, W. P., Doesburg, H. M., Gould, R. O., Van den Hark, T. E. M., Prick, P. A. J., Noordik, K. H., Beurskens, G., Parthasarathi, V., Bruins Slot, H. J., Haltiwanger, R. C., Strumpel, M. & Smits, J. M. M. (1984). *DIRDIF*. Technical Report 1984/1. Crystallography Laboratory, Toernooiveld, 6525 ED Nijmegen, The Netherlands.

Milder, S. J., Castellani, M. P., Weakley, T. J. R., Tyler, D. R., Miskowski, V. M. & Stiegman, A. E. (1990). *J. Phys. Chem.* **94**, 6599–6603.

Molecular Structure Corporation (1989). *TEXSAN. TEXRAY Structure Analysis Package*. Version 5.0. MSC, 3200A Research Forest Drive, The Woodlands, TX 77381, USA.

Walker, N. & Stuart, D. (1983). *Acta Cryst.* A**39**, 158–166.

Acta Cryst. (1993). C**49**, 1493–1496

Structure of Tri-μ-chloro-bis[(η^6-benzene)ruthenium(II)] Hexafluoroarsenate

FRED B. MCCORMICK* AND WILLIAM B. GLEASON†

3M Corporate Research Laboratories, St. Paul, Minnesota 55144, USA

(*Received* 16 *October* 1992; *accepted* 9 *February* 1993)

Abstract

The cationic portion of the tri-μ-chloro-bis[(η^6-benzene)ruthenium(II)] hexafluoroarsenate molecule consists of two (η^6-C_6H_6)Ru moieties [Ru to ring plane distances are 1.6392 (4) and 1.6486 (4) Å] symmetrically bridged by three Cl atoms [Ru—Cl$_{\rm av}$ = 2.423 (7) Å]. The benzene rings are planar and lie

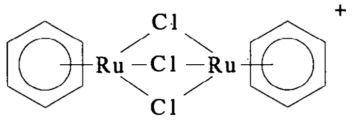
---

† Current address: Biomedical Engineering Center, University of Minnesota, Minneapolis, MN 55455, USA.

essentially perpendicular to the Ru···Ru vector. The distance between the Ru atoms [3.2754 (4) Å] indicates no bonding interaction. The octahedral AsF_6^- anion is ordered with average As—F bond lengths of 1.706 (3) Å.

Comment

The title cation, $(\mu\text{-Cl})_3\text{-}[Ru(\eta^6\text{-}C_6H_6)]_2^+$ (I), was first prepared from the reaction of $[(\eta^6\text{-}C_6H_6)Ru(Cl)_2]_2$ with ammonium hexafluorophosphate in water (Bennett & Smith, 1974). Later, the reaction of $(\eta^6\text{-arene})M(\text{pyridine})_2X^+$ with $(\eta^6\text{-arene})M(\text{pyridine})X_2$, where M is the metal and X is the halide, was found to be a general route to $(\mu\text{-}X)_3\text{-}[Ru(\eta^2\text{-arene})]_2^+$ and $(\mu\text{-}X)_3\text{-}[Os(\eta^6\text{-arene})]_2^+$ complexes (Arthur & Stephenson, 1981). The $(\mu\text{-Cl})_3[Ru(\eta^6\text{-arene})]_2^+$ salts have also been prepared from the reaction of $[(\eta^6\text{-arene})RuCl_2]_2$ with strong acids (CF_3COOH or HBF_4) and have been shown to be key intermediates in the preparation of the unsymmetrical sandwich complexes, $(\eta^6\text{-arene})\text{-}Ru(\eta^6\text{-arene}')^+$ (Rybinskaya, Kudinov & Kaganovich, 1983). Most recently, we have found $(\mu\text{-Cl})_3\text{-}[Ru(\eta^6\text{-}C_6H_6)]_2^+AsF_6^-$ to be a product of the disproportionation of $(\eta^6\text{-}C_6H_6)Ru(CH_3CN)_2\text{-}Cl^+AsF_6^-$ in nitromethane solutions (McCormick, Cox & Gleason, 1993). Due to the unexpected nature of $(\mu\text{-Cl})_3\text{-}[Ru(\eta^6\text{-}C_6H_6)]_2^+AsF_6^-$ as a disproportionation product and difficulties in its unequivocal characterization by spectroscopic techniques, we undertook a single-crystal X-ray diffraction study on this complex.



(I)

The atomic labeling scheme and a view down the Ru···Ru vector of the cation are shown as *ORTEP* (Johnson, 1965) and *PLUTO* (Motherwell & Clegg, 1978) diagrams in Figs. 1 and 2, respectively. The idealized symmetry of the cation is D_{3h} with the Ru_2Cl_3 core arranged as a trigonal bipyramid. The benzene rings are planar within experimental error and cap the Ru apices. The average C—C bond lengths [1.401 Å, range 1.375 (7) to 1.426 (8) Å, standard deviation 0.016] and C—C—C bond angles [120.0°, range 118.0 (5) to 121.2 (4)°, standard deviation 0.8] in the benzene rings appear to be normal and no systematic differences were found. The average Ru—C bond distance is 2.160 Å [range 2.132 (4) to 2.178 (4) Å, standard deviation 0.014] and, in keeping with the planarity of the benzene rings, there appears to be no systematic variation in these bond lengths. The Ru atoms are displaced from the planes of their attendant benzene rings by 1.6392 (4) and 1.6486 (4) Å and the ring planes are essentially parallel. The bridging Cl atoms form a plane which also lies essentially parallel to the benzene ring planes and all three planes are perpendicular to the Ru···Ru vector. The Ru atoms reside at 1.6423 (4) and 1.6331 (4) Å on either side of the bridging Cl plane. The separation between the Ru atoms of 3.2754 (4) Å is longer than that which is normally considered a bonding interaction (Bruce, 1982) and as both Ru centers are in the +2 oxidation state, the electron count for $(\mu\text{-Cl})_3\text{-}[Ru(\eta^6\text{-}C_6H_6)]_2^+$ does not require a Ru—Ru bond. The average Ru—Cl bond length of 2.423 Å [range 2.419 (1) to 2.438 (2) Å, standard deviation 0.007] is shorter than the bridging Ru—Cl bonds [2.460 (1) Å] found in $(\mu\text{-Cl})_2\text{-}[Ru\{\eta^6\text{-}C_6(CH_3)_6\}Cl]_2$ (McCormick & Gleason, 1988), while the bridging Cl—Ru—Cl angles are similar [79.33° average, range 78.62 (4) to 80.11 (5)°, standard deviation 0.57, for the title cation *vs.* 80.90 (2)°]. The Ru—Cl—Ru bridging angles for the title cation are considerably more

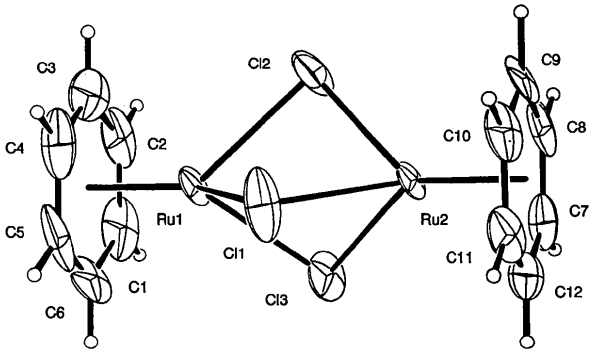


Fig. 1. Molecular configuration and atom-numbering scheme for $(\mu\text{-Cl})_3\text{-}[Ru(\eta^6\text{-}C_6H_6)]_2^+$. Thermal ellipsoids are shown at 50% probability levels and the H atoms are shown as spheres of arbitrary radii.

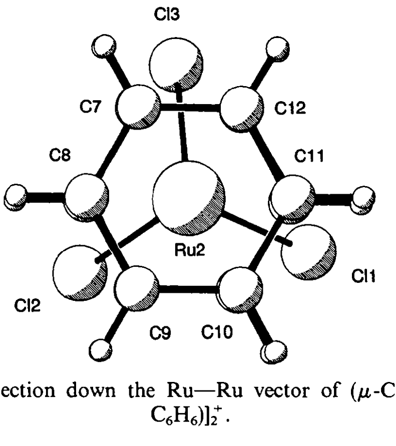


Fig. 2. Projection down the Ru—Ru vector of $(\mu\text{-Cl})_3\text{-}[Ru(\eta^6\text{-}C_6H_6)]_2^+$.

acute [84.74 (3), 85.16 (3), and 85.21 (3)° *vs.* 99.09 (2)°] than those in (μ-Cl)$_2$-[Ru{η^6-C$_6$-(CH$_3$)$_6$}Cl]$_2$ (McCormick & Gleason, 1988). The octahedral AsF_6^- anion showed no indications of disorder with average As—F distances of 1.706 Å [range 1.701 (3) to 1.711 (2) Å, standard deviation 0.003] and average F—As—F angles of 90.0° [range 89.1 (1) to 90.8 (1)°, standard deviation 0.5] and 179.2° [range 178.9 (1) to 179.6 (1)°, standard deviation 0.3].

Experimental

Crystal data

$[Ru_2Cl_3(C_6H_6)_2][AsF_6]$
M_r = 653.64
Monoclinic
$P2_1/c$
a = 10.538 (3) Å
b = 19.210 (4) Å
c = 8.686 (2) Å
β = 101.56 (4)°
V = 1722.7 Å^3
Z = 4
D_x = 2.52 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 10–15°
μ = 4.15 mm^{-1}
T = 298 K
Prism
0.34 × 0.31 × 0.15 mm
Red

Data collection

Enraf-Nonius CAD-4 diffractometer
ω scans
Absorption correction: empirical
T_{min} = 0.708, T_{max} = 1.000
6221 measured reflections
3013 independent reflections

2449 observed reflections [$I > 3\sigma(I)$]
R_{int} = 0.019
θ_{max} = 25°
$h = -12 \rightarrow 12$
$k = 0 \rightarrow 22$
$l = -10 \rightarrow 10$
3 standard reflections
frequency: 83 min
intensity variation: none

Refinement

Refinement on F
Final R = 0.041
wR = 0.052
S = 2.15
2449 reflections
218 parameters
H-atom parameters not refined
$w = 1/\sigma^2(F_o)$
$(\Delta/\sigma)_{max}$ = 0.01

$\Delta\rho_{max}$ = 1.1 e Å^{-3}
$\Delta\rho_{min}$ = −1.1 e Å^{-3}
Extinction correction: secondary
Extinction coefficient: 5.42 (2) × 10^{-7}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{eq} = (4/3)[a^2B(1,1)+b^2B(2,2)+c^2B(3,3)+ab(\cos\gamma)B(1,2)+ac(\cos\beta)B(1,3)+bc(\cos\alpha)B(2,3)].$$

	x	y	z	B_{eq}
Ru(1)	0.63828 (3)	0.13014 (2)	0.20824 (5)	2.147 (7)
Ru(2)	0.36766 (3)	0.11832 (2)	0.33749 (5)	1.926 (7)
As	1.01526 (5)	0.12541 (2)	0.77784 (6)	2.32 (1)
Cl(1)	0.4667 (1)	0.04418 (7)	0.1697 (2)	4.39 (3)
Cl(2)	0.4520 (1)	0.20586 (7)	0.1846 (2)	5.16 (3)
Cl(3)	0.5923 (1)	0.12301 (7)	0.4719 (2)	3.82 (3)
F(1)	0.8522 (3)	0.1280 (2)	0.7090 (5)	4.45 (8)
F(2)	1.1780 (3)	0.1222 (2)	0.8469 (5)	5.6 (1)
F(3)	0.9981 (4)	0.1841 (2)	0.9200 (4)	5.07 (9)
F(4)	1.0301 (3)	0.0669 (2)	0.6339 (4)	4.89 (8)
F(5)	0.9930 (4)	0.0581 (2)	0.8979 (4)	5.10 (8)
F(6)	1.0350 (4)	0.1922 (2)	0.6555 (4)	4.92 (8)
C(1)	0.8371 (5)	0.1658 (4)	0.2841 (7)	4.9 (1)
C(2)	0.7713 (5)	0.2085 (3)	0.1604 (7)	4.3 (1)
C(3)	0.7082 (6)	0.1797 (3)	0.0211 (7)	4.4 (1)
C(4)	0.7068 (6)	0.1080 (3)	−0.0014 (8)	4.8 (1)
C(5)	0.7720 (5)	0.0647 (3)	0.1156 (7)	4.8 (1)
C(6)	0.8362 (5)	0.0925 (4)	0.2588 (8)	5.3 (1)
C(7)	0.2943 (5)	0.1408 (3)	0.5465 (6)	3.6 (1)
C(8)	0.2313 (5)	0.1837 (3)	0.4263 (7)	3.6 (1)
C(9)	0.1687 (5)	0.1553 (3)	0.2812 (7)	3.9 (1)
C(10)	0.1693 (5)	0.0824 (3)	0.2588 (6)	3.7 (1)
C(11)	0.2330 (5)	0.0391 (3)	0.3829 (6)	3.4 (1)
C(12)	0.2942 (5)	0.0684 (3)	0.5232 (6)	3.4 (1)

Table 2. *Geometric parameters* (Å, °)

Ru(1)—C(1)	2.177 (4)	Ru(2)—Cl(1)	2.419 (1)
Ru(1)—C(2)	2.153 (4)	Ru(2)—Cl(2)	2.420 (1)
Ru(1)—C(3)	2.138 (4)	Ru(2)—Cl(3)	2.422 (1)
Ru(1)—C(4)	2.132 (4)	C(1)—C(2)	1.418 (7)
Ru(1)—C(5)	2.160 (4)	C(1)—C(6)	1.426 (8)
Ru(1)—C(6)	2.168 (4)	C(2)—C(3)	1.375 (7)
Ru(2)—C(7)	2.154 (4)	C(3)—C(4)	1.390 (6)
Ru(2)—C(8)	2.163 (4)	C(4)—C(5)	1.385 (7)
Ru(2)—C(9)	2.175 (4)	C(5)—C(6)	1.397 (8)
Ru(2)—C(10)	2.178 (4)	C(7)—C(8)	1.390 (7)
Ru(2)—C(11)	2.170 (3)	C(7)—C(12)	1.406 (6)
Ru(2)—C(12)	2.149 (4)	C(8)—C(9)	1.409 (7)
Ru(1)—Cl(1)	2.4221 (9)	C(9)—C(10)	1.416 (7)
Ru(1)—Cl(2)	2.419 (1)	C(10)—C(11)	1.418 (6)
Ru(1)—Cl(3)	2.438 (2)	C(11)—C(12)	1.379 (6)
As—F(1)	1.703 (3)	As—F(2)	1.701 (3)
As—F(3)	1.708 (2)	As—F(4)	1.711 (2)
As—F(5)	1.707 (2)	As—F(6)	1.705 (2)
Cl(1)—Ru(1)—Cl(2)	80.11 (5)	Cl(2)—Ru(2)—Cl(3)	78.62 (4)
Cl(1)—Ru(1)—Cl(3)	78.93 (4)	Ru(1)—Cl(1)—Ru(2)	85.16 (3)
Cl(2)—Ru(1)—Cl(3)	78.92 (4)	Ru(1)—Cl(2)—Ru(2)	85.21 (3)
Cl(1)—Ru(2)—Cl(2)	80.06 (4)	Ru(1)—Cl(3)—Ru(2)	84.74 (3)
Cl(1)—Ru(2)—Cl(3)	79.32 (4)		

Programs used: *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and *SDP* (Enraf-Nonius, 1982). The empirical absorption correction was based on ψ scans (North, Phillips & Mathews, 1968) with relative transmission coefficients from 0.708 to 1.000 having an average of 0.877. The scan width was $(0.9 + 0.35\tan\theta)$° and the scan speed was variable. The method of Zachariasen (1963) was used in the secondary- extinction correction.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry, a stereoview of the unit cell and a diagram of the AsF_6^- counterion have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71082 (40 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST1045]

References

Arthur, T. & Stephenson, T. A. (1981). *J. Organomet. Chem.* **208**, 369–387.

Bennett, M. A. & Smith, A. K. (1974). *J. Chem. Soc. Dalton Trans.* pp. 233–241.

Bruce, M. I. (1982). *Comprehensive Organometallic Chemistry*, edited by G. Wilkinson, F. G. A. Stone & E. W. Abel, Vol. 4, ch. 32.5, pp. 843–887. Oxford: Pergamon Press.

Enraf–Nonius (1982). *Structure Determination Package*. Enraf–Nonius, Delft, The Netherlands.
Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1982). *MULTAN*11/82. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.
McCormick, F. B., Cox, D. D. & Gleason, W. B. (1993). *Organometallics*, **12**, 610–612.
McCormick, F. B. & Gleason, W. B. (1988). *Acta Cryst.* C**44**, 603–605.
Motherwell, W. D. S. & Clegg, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Rybinskaya, M. I., Kudinov, A. R. & Kaganovich, V. S. (1983). *J. Organomet. Chem.* **246**, 279–285.
Zachariasen, W. H. (1963). *Acta Cryst.* **16**, 1139–1144.

Acta Cryst. (1993). C**49**, 1496–1498

Structure of Diaquabis(4-chlorobenzoato)zinc(II)

Ivan Potočňák and Michal Dunaj-Jurčo

Department of Inorganic Chemistry, Slovak Technical University, 812 47 Bratislava, Czechoslovakia

Juraj Černák

Department of Inorganic Chemistry, University of P. J. Šafárik, 041 54 Košice, Czechoslovakia

(*Received* 25 *September* 1992; *accepted* 8 *February* 1993)

Abstract

The crystal structure of the complex [Zn(4-$ClC_6H_4COO)_2(H_2O)_2$] is reported here. Molecules of the complex are bridged by hydrogen bonds forming infinite planes parallel to the *bc* plane. The coordination geometry of the Zn atom is very deformed tetrahedral with four normal Zn—O bonds [1.973 (5) (2 ×) and 1.991 (5) Å (2 ×)]. There are two additional weak interactions at longer Zn···O distances [2.456 (5) Å (2 ×)].

Comment

As part of our study on the synthesis, crystal chemistry, properties and biological activity of zinc carboxylates with and without additional ligands the title complex was isolated and its crystal structure determined. Details of preparation, identification and properties will be published elsewhere (Černák, 1993).

The Zn atom sits on a twofold axis and the coordination polyhedron around it is a very deformed tetrahedron with four normal Zn—O bonds [1.973 (5) (2 ×) and 1.991 (5) Å (2 ×)]. An interesting feature of this structure is the presence of two additional weak Zn···O interactions [2.456 (5) Å (2 ×)] involving the non-coordinated O atoms from adjacent carboxylic groups. These additional interactions may determine the orientation of the carboxylic groups. The same type of very deformed tetrahedral coordination, as well as similar additional weak interactions, was found in both the salicylato complex [Zn(2-$HOC_6H_4COO)_2$-$(H_2O)_2$] (Rissanen, Valkonen, Kokkonen & Leskelä, 1987) and the nitrobenzoato complex [Zn(4-$NO_2C_6H_4COO)_2(H_2O)_2$] (Gusejnov, Musaev, Amiraslanov, Usubaliev & Mamedov, 1983), the

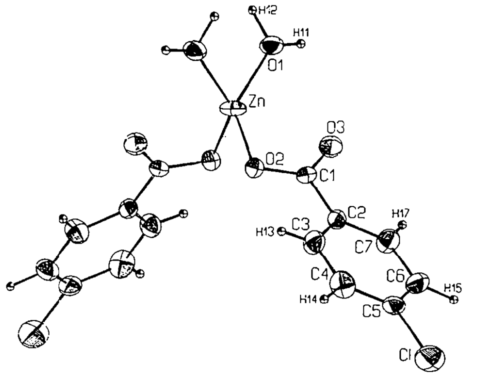


Fig. 1. *ORTEP* drawing of the title compound showing the atomic labeling scheme. Thermal ellipsoids are drawn at the 40% probability level.

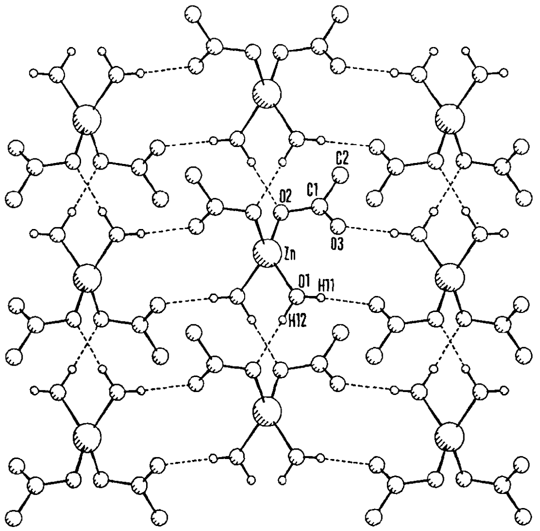


Fig. 2. Schematic drawing of the hydrogen bonding. Benzene rings are omitted for clarity.