

C(61)	-0.1465 (7)	0.2684 (6)	0.0860 (5)	0.040
C(62)	-0.1637 (9)	0.3702 (7)	0.0603 (6)	0.071
C(63)	-0.1502 (11)	0.3965 (9)	-0.0323 (7)	0.097
C(64)	-0.1239 (10)	0.3191 (10)	-0.0987 (6)	0.083
C(65)	-0.1056 (8)	0.2195 (8)	-0.0740 (6)	0.064
C(66)	-0.1173 (7)	0.1939 (7)	0.0189 (6)	0.050

Table 2. Selected geometric parameters (Å, °) for (1)

Pd(1)—Br(1)	2.517 (2)	P(1)—C(21)	1.836 (8)
Pd(1)—P(1)	2.322 (2)	P(1)—C(31)	1.811 (8)
Pd(1)—P(2)	2.319 (2)	P(2)—C(41)	1.829 (8)
Pd(1)—C(1)	1.991 (8)	P(2)—C(51)	1.834 (8)
P(1)—C(11)	1.820 (8)	P(2)—C(61)	1.818 (7)
Br(1)—Pd(1)—P(1)	92.9 (1)	C(21)—P(1)—C(31)	104.8 (4)
Br(1)—Pd(1)—P(2)	89.9 (1)	Pd(1)—P(2)—C(41)	108.4 (3)
Br(1)—Pd(1)—C(1)	170.9 (3)	Pd(1)—P(2)—C(51)	121.2 (3)
P(1)—Pd(1)—P(2)	175.9 (1)	Pd(1)—P(2)—C(61)	114.3 (3)
P(1)—Pd(1)—C(1)	87.2 (3)	C(41)—P(2)—C(51)	103.5 (4)
P(2)—Pd(1)—C(1)	90.6 (3)	C(41)—P(2)—C(61)	105.3 (4)
Pd(1)—P(1)—C(11)	114.1 (3)	C(51)—P(2)—C(61)	102.6 (4)
Pd(1)—P(1)—C(21)	118.6 (3)	Pd(1)—C(1)—C(2)	125.0 (7)
Pd(1)—P(1)—C(31)	110.5 (3)	Pd(1)—C(1)—C(6)	116.6 (7)
C(11)—P(1)—C(21)	101.3 (4)	C(2)—C(1)—C(6)	118.4 (9)
C(11)—P(1)—C(31)	106.4 (4)		
C(1)—Pd(1)—P(1)—C(11)	-152.6 (4)	C(1)—Pd(1)—P(2)—C(41)	144.1 (4)
C(1)—Pd(1)—P(1)—C(21)	-33.4 (4)	C(1)—Pd(1)—P(2)—C(51)	24.8 (4)
C(1)—Pd(1)—P(1)—C(31)	87.6 (4)	C(1)—Pd(1)—P(2)—C(61)	-98.8 (4)

The orientation of the methyl group was determined from a difference synthesis. All H atoms rode on their parent C atoms with C—H = 0.96 Å and $U(\text{H}) \approx 1.2 U(\text{C})$.

Data collection: CAD-4 EXPRESS (Enraf–Nonius, 1992). Cell refinement: CAD-4 EXPRESS. Data reduction: MolEN (Fair, 1990). Program(s) used to solve structure: GX (Mallinson & Muir, 1985). Program(s) used to refine structure: GX. Molecular graphics: CAMERON (Pierce & Watkin, 1994). Software used to prepare material for publication: GX.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HA1125). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Cross, R. J., Kennedy, A. R. & Muir, K. W. (1994). *J. Organomet. Chem.* In the press.
- Enraf–Nonius (1992). CAD-4 EXPRESS. Enraf–Nonius, Delft, The Netherlands.
- Fair, C. K. (1990). MolEN. An Interactive Intelligent System for Crystal Structure Analysis. Enraf–Nonius, Delft, The Netherlands.
- Graaf, W. de, van Wegen, J., Boersma, J., Spek, A. L. & van Koten, G. (1989). *Recl Trav. Chim. Pays-Bas*, **108**, 275–277.
- Hursthouse, M. B., Sloan, O. D., Thornton, P. & Walker, N. P. C. (1986). *Polyhedron*, **5**, 1475–1478.
- Hutton, A. T., Pringle, P. G. & Shaw, B. L. (1985). *J. Chem. Soc. Dalton Trans.* pp. 1677–1687.
- Isobe, K., Kai, E., Nakamura, Y., Nishimoto, K., Miwa, T., Kawaguchi, S., Kinoshita, K. & Nakatsu, K. (1980). *J. Am. Chem. Soc.* **102**, 2475–2476.
- Mallinson, P. R. & Muir, K. W. (1985). *J. Appl. Cryst.* **18**, 51–53.
- Orpen, A. G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989). *J. Chem. Soc. Dalton Trans.* pp. S1–S83.

Pierce, L. J. & Watkin, D. (1994). CAMERON. A Program for Molecular Graphics. Crystallographic Laboratory, Univ. of Oxford, England.

Rieger, A. L., Carpenter, G. B. & Rieger, P. H. (1993). *Organometallics*, **12**, 842–847.

Roe, D. M., Bailey, P. M., Moseley, K. & Maitlis, P. M. (1972). *J. Chem. Soc. Chem. Commun.* pp. 1273–1274.

Terheijden, J., van Koten, G., Vinke, I. C. & Spek, A. L. (1985). *J. Am. Chem. Soc.* **107**, 2891–2898.

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Bis(dimethylglyoximato)(phenylacetylido)-(triphenylphosphine)rhodium(III) Dichloromethane, [Rh(C₄H₇N₂O₂)₂-(C₈H₅)(C₁₈H₁₅P)].CH₂Cl₂

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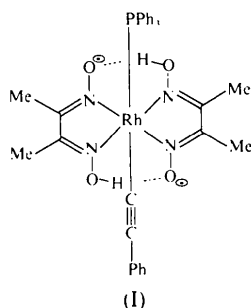
Abstract

The title structure {alternative name: bis[2,3-butanedial dioximato(1-)-N,N'](phenylethynyl)(triphenylphosphine-P)rhodium(III) dichloromethane solvate} consists of discrete complexes [Rh(dmgH)₂(PPh₃)R] (R = C≡CPh and dmgH = dimethylglyoximato, C₄H₇N₂O₂⁻) in which the Rh atom displays distorted octahedral coordination with the two dimethylglyoximato ligands in the equatorial plane and the phenylacetylido and triphenylphosphine groups in axial positions. The Rh atom is displaced by 0.073 (1) Å from the mean plane through the four oxime N-atom donors. The average Rh—N distance is 1.971 (2) Å, while the axial Rh—P and Rh—C distances are 2.409 (1) and 1.991 (3) Å, respectively.

Comparison of the results with those obtained previously for the ethyl and vinyl analogues ($R = \text{Et}$, $\text{CH}=\text{CH}_2$) indicates a lower *trans* influence of the phenylacetylide ligand in the P—Rh—C fragment, in accordance with its *sp*-hybridized C atom.

Comment

This work is part of a more general study aimed at understanding the mutual influence of ligands in organometallic compounds (Steinborn, 1992). The *trans* influence of σ -organo ligands is of particular interest. In previous papers in this series we have demonstrated (Steinborn & Ludwig, 1993a,b; Kettmann, Dunaj-Jurčo, Steinborn & Ludwig, 1994; Dunaj-Jurčo, Kettmann, Steinborn & Ludwig, 1994) that in the complexes $[\text{Rh}(\text{dmgH})_2(\text{PPh}_3)R]$ (dmgH is the monoanion of dimethylglyoxime, R is an organo group) the *trans* influence of R is reflected by the magnitude of the $^1J(^{103}\text{Rh}-^{31}\text{P})$ coupling constants and the Rh—P bond distance. Thus, the complexes with $R = \text{Et}$ and $R = \text{CH}=\text{CH}_2$ gave approximately the same coupling constants and the X-ray diffraction data revealed only slight, though significant, differences in the Rh—P bond distances. In contrast, a considerably larger $^1J(\text{Rh}-\text{P})$ coupling constant was found for the σ -phenylacetylide ($R = \text{C}\equiv\text{CPh}$) complex, where the ligating C atom is *sp* hybridized, thereby establishing the phenylacetylide group as a ligand with a weaker *trans* influence. A similarly low position of the $\text{C}\equiv\text{CPh}$ group in the *trans*-influence series has been found for other complexes, irrespective of the type of metal and the rest of the ligand system (Steinborn, Taube & Radeglia, 1988; Steinborn, 1992; Appleton, Clark & Manzer, 1973). In order to investigate further the *trans* influence of R as determined by NMR spectroscopy and structural analysis, an X-ray study was undertaken. Single crystals of the title complex (I) were obtained by slow evaporation of a dichloromethane solution at room temperature. The molecular structure and the numbering scheme are shown in Fig. 1.



The crystal structure consists of discrete molecules of the complex $[\text{Rh}(\text{dmgH})_2(\text{PPh}_3)(\text{C}\equiv\text{CPh})]$ and dichloromethane molecules. The geometry around

the central Rh atom is distorted octahedral with four oxime N-atom donors in equatorial positions. The two dimethylglyoxime ligands are present as monoanionic species and are stabilized by two intramolecular hydrogen bonds: $\text{O}(1)\cdots\text{O}(4) = 2.609$ (4) and $\text{O}(2)\cdots\text{O}(3) = 2.718$ (4) Å. On the basis of the H-atom positions (not refined) determined from a $\Delta\rho$ map, both hydrogen bridges in the $\text{Rh}(\text{dmgH})_2$ unit are unsymmetrical [$\text{O}(4)-\text{H} = 0.98$, $\text{O}(1)\cdots\text{H} = 1.70$ Å; $\text{O}(2)-\text{H} = 0.69$, $\text{O}(3)\cdots\text{H} = 2.03$ Å].

The four Rh—N bond distances range from 1.957 (2) to 1.980 (2) Å, with a mean of 1.971 (2) Å. This value is intermediate between those found in the vinyl and ethyl complexes [1.957 (2) and 1.955 (6) Å, respectively (Dunaj-Jurčo, Kettmann, Steinborn & Ludwig, 1994; Kettmann, Dunaj-Jurčo, Steinborn & Ludwig, 1994)], and in the closely related complex $[\text{Rh}(\text{dmgH})_2(\text{PPh}_3)\text{Cl}]$ [1.992 (4) Å (Cotton & Norman, 1971)].

Each dmgH⁻ ligand is planar to within ± 0.05 Å but the $\text{Rh}(\text{dmgH})_2$ system as a whole deviates from

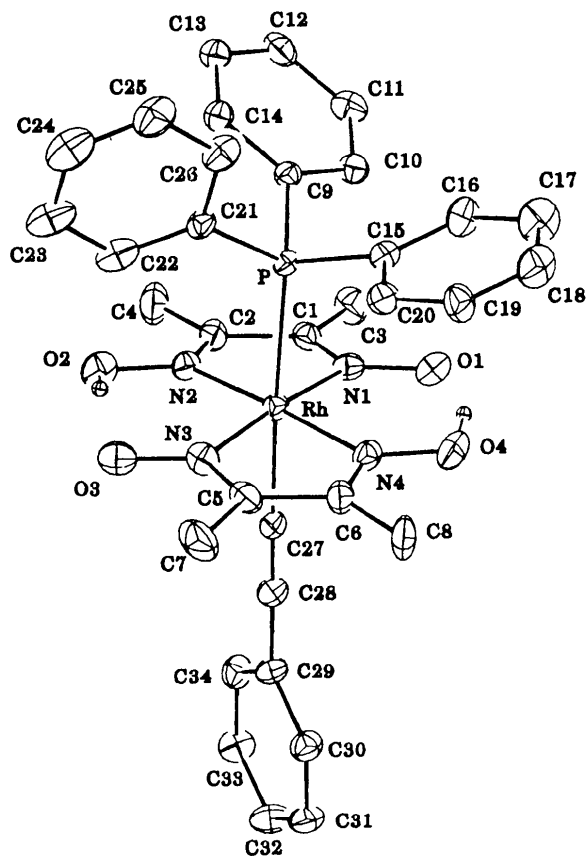


Fig. 1. Perspective drawing of the title compound with atom-numbering scheme. For clarity, only polar H atoms (involved in intramolecular hydrogen bonds) are shown. Displacement ellipsoids are plotted at the 50% probability level.

planarity since the dmgH⁻ ligands twist away from the bulky triphenylphosphine group so that the dihedral angle between the dmgH planes is 6.2 (2)°. As a result, although the four oxime N-atom donors are coplanar to within ±0.01 Å, the Rh atom is displaced by 0.073 (1) Å from their mean plane, towards the P atom. This displacement is smaller than in the corresponding ethyl [0.130 (1) Å] and vinyl [0.123 (1) Å] complexes (Kettmann, Dunaj-Jurčo, Steinborn & Ludwig, 1994; Dunaj-Jurčo, Kettmann, Steinborn & Ludwig, 1994).

As mentioned above, the coordination of the axial C≡CPh and PPh₃ ligands is of special interest here. The Rh—P and Rh—C bond lengths are 2.409 (1) and 1.991 (3) Å, respectively, and the P—Rh—C angle is 176.6 (1)°. The Rh—C bond distance is considerably shorter than those found previously for the ethyl [2.064 (7) Å] and vinyl [2.035 (3) Å] analogues, in agreement with the decreasing covalent radius in the series C_{sp³} > C_{sp²} > C_{sp}. With regard to the Rh—P bond length, X-ray data support the assignment (based on NMR) of the *trans* influence; in the present structure, the Rh—P bond distance is ca 0.04 Å shorter than those found in the corresponding ethyl and vinyl analogues. This shows clearly the lower *trans* influence of the phenylacetylide ligand compared to the ethyl and vinyl ligands. This can be explained using the rules of Bent (1961) by taking into account the lower demand of the donor orbital on C≡CPh for the rhodium 5s electron density when forming the Rh—C bond.

We found twofold positional disorder for the C atom and one Cl atom of the dichloromethane molecule. This disorder was clearly detectable by observation of the difference electron-density maps based on accurately refined coordinates for the rest of the molecule. It can be explained by pivoting of the solvent molecule about the ordered Cl(1) atom, each site being occupied approximately 60% [C(35),Cl(2)] or 40% [C(36),Cl(3)] of the time.

Experimental

Crystal data

[Rh(C₄H₇N₂O₂)₂(C₈H₅)-
(C₁₈H₁₅P)].CH₂Cl₂

M_r = 781.48

Monoclinic

*P*2₁/*c*

a = 20.378 (9) Å

b = 9.914 (5) Å

c = 17.272 (8) Å

β = 103.00 (6)°

V = 3400 (2) Å³

Z = 4

D_s = 1.527 Mg m⁻³

D_m = 1.53 (1) Mg m⁻³

Mo Kα radiation

λ = 0.71069 Å

Cell parameters from 15

reflections

θ = 6–17°

μ = 0.74 mm⁻¹

T = 293 K

Prisms

0.4 × 0.3 × 0.25 mm

Brownish yellow

Data collection

Syntax *P*2₁ diffractometer

ω/2θ scans

Absorption correction:

none

6388 measured reflections

6022 independent reflections

4478 observed reflections

[*I* ≥ 2σ(*I*)]

*R*_{int} = 0.024

θ_{max} = 25°

h = 0 → 24

k = 0 → 11

l = -20 → 20

2 standard reflections

frequency: 90 min

intensity decay: ±4%

Refinement

Refinement on *F*

R = 0.045

wR = 0.056

S = 1.34

4478 reflections

442 parameters

H-atom parameters not

refined

w = 1 if *|F|* < 60 and

w = 60/*|F|* if *|F|* ≥ 60

(Δ/σ)_{max} = 0.13

Δρ_{max} = 0.28 e Å⁻³

Δρ_{min} = -0.32 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 displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq}
Rh(1)	0.2109	0.0431	0.0049	2.43 (1)
P(1)	0.2764	0.0669 (1)	0.1388	2.08 (2)
O(1)	0.0993 (1)	0.1604 (2)	0.0560 (1)	3.42 (6)
O(2)	0.2394 (1)	-0.2462 (2)	0.0042 (2)	3.92 (7)
O(3)	0.3173 (1)	-0.0722 (3)	-0.0574 (1)	3.84 (7)
O(4)	0.1759 (1)	0.3272 (2)	-0.0005 (2)	4.16 (7)
N(1)	0.1270 (1)	0.0466 (3)	0.0443 (1)	2.74 (6)
N(2)	0.1967 (1)	-0.1508 (3)	0.0206 (2)	2.68 (7)
N(3)	0.2900 (1)	0.0411 (3)	-0.0440 (2)	3.12 (8)
N(4)	0.2193 (1)	0.2354 (3)	-0.0167 (2)	3.01 (8)
C(1)	0.1030 (2)	-0.0702 (4)	0.0591 (2)	2.93 (8)
C(2)	0.1443 (2)	-0.1838 (3)	0.0459 (2)	3.18 (9)
C(3)	0.0399 (2)	-0.0857 (5)	0.0874 (3)	4.59 (12)
C(4)	0.1273 (2)	-0.3248 (4)	0.0595 (3)	5.00 (13)
C(5)	0.3095 (2)	0.1579 (4)	-0.0650 (2)	3.63 (10)
C(6)	0.2680 (2)	0.2692 (4)	-0.0506 (2)	3.70 (10)
C(7)	0.3679 (2)	0.1701 (6)	-0.1028 (3)	5.97 (16)
C(8)	0.2801 (3)	0.4113 (5)	-0.0706 (3)	5.92 (15)
C(9)	0.2391 (2)	-0.0214 (3)	0.2104 (2)	2.33 (7)
C(10)	0.1758 (2)	0.0113 (4)	0.2215 (2)	2.97 (9)
C(11)	0.1459 (2)	-0.0647 (4)	0.2714 (2)	3.84 (9)
C(12)	0.1793 (2)	-0.1739 (4)	0.3104 (2)	3.95 (11)
C(13)	0.2415 (2)	-0.2071 (4)	0.2995 (2)	3.65 (10)
C(14)	0.2720 (2)	-0.1314 (3)	0.2506 (2)	3.08 (9)
C(15)	0.2852 (2)	0.2423 (3)	0.1659 (2)	2.55 (8)
C(16)	0.2465 (2)	0.3088 (4)	0.2097 (2)	3.83 (11)
C(17)	0.2521 (2)	0.4466 (4)	0.2220 (3)	5.23 (14)
C(18)	0.2960 (2)	0.5179 (4)	0.1872 (3)	4.91 (13)
C(19)	0.3354 (2)	0.4537 (4)	0.1453 (2)	4.33 (11)
C(20)	0.3298 (2)	0.3164 (4)	0.1337 (2)	3.42 (9)
C(21)	0.3636 (1)	0.0082 (3)	0.1651 (2)	2.69 (8)
C(22)	0.3846 (2)	-0.0933 (4)	0.1244 (2)	4.34 (11)
C(23)	0.4493 (2)	-0.1446 (5)	0.1495 (3)	5.61 (15)
C(24)	0.4911 (2)	-0.0945 (5)	0.2158 (3)	5.64 (14)
C(25)	0.4696 (2)	0.0051 (5)	0.2581 (3)	5.09 (13)
C(26)	0.4057 (2)	0.0583 (4)	0.2331 (2)	3.93 (11)
C(27)	0.1519 (2)	0.0266 (3)	-0.1035 (2)	2.72 (8)
C(28)	0.1144 (2)	0.0152 (4)	-0.1664 (2)	3.09 (9)
C(29)	0.0684 (2)	-0.0017 (3)	-0.2415 (2)	2.77 (8)
C(30)	0.0641 (2)	0.0935 (4)	-0.3011 (2)	3.44 (9)
C(31)	0.0190 (2)	0.0780 (4)	-0.3727 (2)	3.82 (11)
C(32)	-0.0217 (2)	-0.0335 (4)	-0.3865 (2)	3.85 (9)
C(33)	-0.0184 (2)	-0.1276 (4)	-0.3287 (2)	3.59 (10)

$$B_{eq} = (4/3) \sum_i \sum_j \beta_{ij} a_i \cdot a_j$$

C(34)	0.0265 (2)	-0.1117 (4)	-0.2561 (2)	3.35 (9)
Cl(1)	0.5053 (1)	-0.1832 (4)	-0.0813 (2)	16.31 (15)
Cl(2)*	0.4081 (2)	-0.3497 (4)	-0.0478 (3)	12.45 (17)
Cl(3)†	0.4627 (32)	-0.4120 (5)	-0.0170 (3)	9.71 (16)
C(35)*	0.4345 (6)	-0.2230 (12)	-0.1074 (9)	11.86 (52)
C(36)†	0.4406 (8)	-0.2640 (25)	-0.0729 (14)	12.21 (88)

* Occupancy 0.6.

† Occupancy 0.4.

Table 2. Selected geometric parameters (Å, °)

Rh(1)—P(1)	2.409 (1)	N(1)—O(1)	1.298 (3)
Rh(1)—C(27)	1.991 (3)	N(2)—O(2)	1.358 (3)
Rh(1)—N(1)	1.976 (2)	N(3)—O(3)	1.298 (4)
Rh(1)—N(2)	1.972 (2)	N(4)—O(4)	1.343 (3)
Rh(1)—N(3)	1.980 (2)	N(1)—C(1)	1.305 (4)
Rh(1)—N(4)	1.957 (2)	N(2)—C(2)	1.284 (4)
P(1)—C(9)	1.815 (3)	N(3)—C(5)	1.302 (4)
P(1)—C(15)	1.800 (3)	N(4)—C(6)	1.304 (4)
P(1)—C(21)	1.827 (3)	C(1)—C(2)	1.454 (4)
C(27)—C(28)	1.184 (4)	C(5)—C(6)	1.445 (5)
C(28)—C(29)	1.429 (4)		
N(1)—Rh(1)—N(2)	78.8 (1)	Rh(1)—C(27)—C(28)	176.9 (2)
N(3)—Rh(1)—N(4)	79.3 (1)	Rh(1)—P(1)—C(9)	112.3 (1)
P(1)—Rh(1)—N(1)	90.2 (1)	Rh(1)—P(1)—C(15)	110.2 (1)
P(1)—Rh(1)—N(2)	91.7 (1)	Rh(1)—P(1)—C(21)	120.4 (1)
P(1)—Rh(1)—N(3)	94.7 (1)	C(9)—P(1)—C(15)	108.7 (1)
P(1)—Rh(1)—N(4)	91.9 (1)	C(9)—P(1)—C(21)	102.1 (1)
P(1)—Rh(1)—C(27)	176.6 (1)	C(15)—P(1)—C(21)	102.1 (1)
C(27)—C(28)—C(29)	178.5 (3)		

All H atoms, except those of the dichloromethane molecule, were located from difference Fourier maps and included as fixed contributors to the structure factors with B set 0.5 \AA^2 higher than B_{eq} of the corresponding C atoms.

All calculations were performed with a local version of the NRC program system (Ahmed & Singh, 1973).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and least-squares-planes data have been deposited with the IUCr (Reference: MU1107). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Ahmed, F. R. & Singh, P. (1973). *J. Appl. Cryst.* **6**, 309–346.
 Appleton, T. G., Clark, H. C. & Manzer, L. E. (1973). *Coord. Chem. Rev.* **10**, 335–357.
 Bent, H. A. (1961). *Chem. Rev.* **61**, 275–311.
 Cotton, F. A. & Norman, J. G. (1971). *J. Am. Chem. Soc.* **93**, 80–82.
 Dunaj-Jurčo, M., Kettmann, V., Steinborn, D. & Ludwig, M. (1994). *Acta Cryst.* **C50**, 1427–1430.
 Kettmann, V., Dunaj-Jurčo, M., Steinborn, D. & Ludwig, M. (1994). *Acta Cryst.* **C50**, 1239–1241.
 Steinborn, D. (1992). *Angew. Chem.* **104**, 392–412; *Angew. Chem. Int. Ed. Engl.* **31**, 401–421.
 Steinborn, D. & Ludwig, M. (1993a). *Proceedings of the Eighteenth Conference on Coordination Chemistry*, pp. 343–348. Bratislava: Smolenice.
 Steinborn, D. & Ludwig, M. (1993b). *J. Organomet. Chem.* **463**, 65–71.
 Steinborn, D., Taube, R. & Radeaglia, R. (1988). *Mitt. Chem. Ges. DDR.* **35**, 278–284.

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L'hydrogénocarbonate de Bis(*N,N*-diméthylbiguanide) Cuivre(II), [Cu(C₄H₁₁N₅)₂]2HCO₃

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Abstract

The structure of bis(*N*¹,*N*¹-dimethylbiguanide-*N*²,*N*⁴)copper(II) bis(hydrogencarbonate) consists of a [Cu(C₄H₁₁N₅)₂]²⁺ cation and two HCO₃⁻ anions. The Cu atom is at a centre of symmetry and forms a square-planar structure with four N atoms belonging to two *N,N*-dimethylbiguanide (metformin) groups. The metformin ligand is planar, allowing delocalization of the π electrons in the metal–ligand ring. The hydrogencarbonate anions are hydrogen bonded to N(1), N(2) and N(3).

Commentaire

La biguanide et ses dérivés *N*-substitués sont des ligands susceptibles de chélater de nombreux ions métalliques en particulier ceux appartenant aux éléments de la première série de transition (Ray, 1961). Par ailleurs, plusieurs biguanides comme la phenformine, la buformine et la metformine (*N,N*-diméthylbiguanide) présentent des propriétés hypoglycémiantes actives par voie orale. Dans un précédent mémoire, nous avons décrit la synthèse et la structure cristalline du tétrachlorocuprate(II) de metformine obtenu par action du chlorure de cuivre sur le chlorhydrate de metformine en milieu acide (Lemoine, Tomas, Viossat & Dung, 1994). Poursuivant notre étude, nous avons modifié ce mode opératoire afin de synthétiser un véritable composé de coordination entre cuivre(II) et la metformine.