Crystal structure of bis[μ -chloro(1-platina-diethyl- β -diketone)], [Pt₂(μ -Cl)₂((COEt)₂H)₂],

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Source of material: see ref. 1.

C₁₂H₂₂Cl₂O₄Pt₂, triclinic, $P\bar{1}$ (No. 2), $a = 4.8835(6)$ Å,
 $b = 9.008(1)$ Å, $c = 10.152(1)$ Å, $\alpha = 89.66(2)^\circ$, $\beta = 76.83(1)^\circ$,
 $\gamma = 80.11(1)^\circ$, $V = 428.1$ Å³, $Z = 1$, $R(F) = 0.034$, $R_w(F^2) = 0.076$.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow, block-shaped, size 0.1 x 0.2 x 0.2 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	166.39 cm ⁻¹
Diffractometer:	Stoe STADI4
Scan mode:	profile data from $\omega/2\theta$
Temperature:	293 K
$2\theta_{\max}$:	50°
$N(hkl)_{\text{unique}}$:	1503
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	98
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2A)	2i	0.287(2)	0.970(1)	0.829(1)	0.086
H(2B)	2i	0.100(2)	0.843(1)	0.847(1)	0.086
H(3A)	2i	0.30(1)	0.852(8)	1.031(2)	0.113
H(3B)	2i	0.610(8)	0.82(1)	0.935(5)	0.113
H(3C)	2i	0.43(2)	0.696(2)	0.953(6)	0.113
H(5A)	2i	0.571(2)	0.768(2)	0.232(1)	0.100
H(5B)	2i	0.416(2)	0.632(2)	0.278(1)	0.100
H(6A)	2i	0.81(1)	0.55(1)	0.105(4)	0.118
H(6B)	2i	0.86(1)	0.470(4)	0.238(6)	0.118
H(6C)	2i	1.014(4)	0.607(6)	0.188(9)	0.118
H(1)	2i	0.73(4)	0.64(3)	0.56(3)	0.17(8)

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Pt(1)	2i	0.30858(7)	0.85831(4)	0.53211(4)	0.0362(2)	0.0450(3)	0.0345(2)	0.0038(1)	-0.0095(1)	-0.0005(2)
Cl(1)	2i	-0.0804(5)	1.0525(3)	0.6531(3)	0.048(1)	0.064(2)	0.040(1)	0.014(1)	-0.014(1)	-0.007(1)
O(1)	2i	0.668(2)	0.699(1)	0.6928(8)	0.067(5)	0.069(6)	0.049(5)	0.023(4)	-0.020(4)	0.009(4)
O(2)	2i	0.793(2)	0.619(1)	0.4578(9)	0.059(4)	0.062(5)	0.053(5)	0.026(4)	-0.014(4)	-0.008(4)
C(1)	2i	0.455(2)	0.794(1)	0.693(1)	0.050(5)	0.052(6)	0.042(5)	-0.004(5)	-0.021(4)	0.011(5)
C(2)	2i	0.295(2)	0.862(1)	0.831(1)	0.059(6)	0.062(7)	0.046(6)	0.013(5)	-0.020(5)	0.000(5)
C(3)	2i	0.420(3)	0.803(2)	0.948(1)	0.086(8)	0.11(1)	0.033(6)	0.001(7)	-0.022(6)	0.000(7)
C(4)	2i	0.597(2)	0.704(1)	0.420(1)	0.049(5)	0.042(6)	0.048(6)	-0.007(4)	-0.009(4)	-0.003(5)
C(5)	2i	0.588(2)	0.673(2)	0.278(1)	0.054(6)	0.076(9)	0.068(8)	0.013(5)	-0.028(6)	-0.002(7)
C(6)	2i	0.843(3)	0.565(2)	0.194(1)	0.069(7)	0.10(1)	0.053(7)	0.023(7)	-0.018(6)	-0.036(7)

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