Crystal structure of bis(1-phenyl-5-cyclohexyl-pentane-1,3-dionato) copper(II), $[\text{Cu}(\text{C}_{17}\text{H}_{21}\text{O}_2)_2]$

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Received June 21, 1996, CSD-No. 402542

Source of material: The complex was prepared by the reaction of copper acetate with 1-phenyl-5-cyclohexyl-pentane-1,3-dione in ethanol (see ref. 2). The compounds were purified in chloroform and the crystals can be obtained from hexane.

The unexpected *cis*-configuration of a complex isolated from an extraction process was recently reported (see ref. 1). For the further study of this effect crystals of a long-chain β -diketone copper complex were now prepared by reaction in homogeneous solution. The ligands are in a square planar arrangement around Cu and a *cis*-configuration was confirmed as well.

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

Crystal:	dark-green prism, size 0.23 x 0.53 x 0.65 mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	7.51 cm ⁻¹
Diffraction:	Stoe STADI-4
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	298 K
$2\theta_{\text{max}}$:	64°
$N(hkl)_{\text{unique}}$:	3540
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	360
Program:	SHELXL-93

$\text{C}_{34}\text{H}_{42}\text{CuO}_4$, monoclinic, $P2_1/c$ (No. 14), $a = 17.698(5)$ Å, $b = 9.778(5)$ Å, $c = 19.37(1)$ Å, $\beta = 114.55(2)^\circ$, $V = 3049.0$ Å³, $Z = 4$, $R(F) = 0.042$, $R_w(F^2) = 0.117$.

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

Atom	Site	x	y	z	U_{iso}
H(2A)	4e	0.447(2)	0.241(4)	0.541(2)	0.04(1)
H(5A)	4e	0.6961(3)	0.3408(5)	0.6019(3)	0.073
H(6A)	4e	0.7943(3)	0.2242(6)	0.7034(3)	0.092
H(7A)	4e	0.7636(3)	0.0136(6)	0.7377(3)	0.089
H(8A)	4e	0.6341(3)	-0.0765(6)	0.6745(3)	0.093
H(9A)	4e	0.5326(3)	0.0439(5)	0.5786(3)	0.076
H(10A)	4e	0.3035(3)	0.2559(6)	0.4758(3)	0.088
H(10B)	4e	0.2997(3)	0.4157(6)	0.4733(3)	0.088
H(11A)	4e	0.2429(3)	0.2475(6)	0.3467(3)	0.098
H(11B)	4e	0.2414(3)	0.4072(6)	0.3428(3)	0.098
H(12A)	4e	0.1517(3)	0.2701(5)	0.4123(3)	0.079
H(13A)	4e	0.1034(3)	0.1818(7)	0.2913(4)	0.118
H(13B)	4e	0.0862(3)	0.3294(7)	0.2567(4)	0.118
H(14A)	4e	-0.0390(3)	0.2366(7)	0.2467(4)	0.125
H(14B)	4e	-0.0011(3)	0.2055(7)	0.3341(4)	0.125
H(15A)	4e	-0.0793(3)	0.3960(8)	0.3122(4)	0.134
H(15B)	4e	-0.0321(3)	0.4632(8)	0.2680(4)	0.134
H(16A)	4e	0.0354(3)	0.4146(8)	0.4250(4)	0.152
H(16B)	4e	0.0175(3)	0.5591(8)	0.3862(4)	0.152
H(17A)	4e	0.1224(3)	0.5316(6)	0.3457(4)	0.112
H(17B)	4e	0.1603(3)	0.5032(6)	0.4333(4)	0.112
H(19A)	4e	0.545(3)	0.737(5)	0.250(3)	0.08(2)
H(22A)	4e	0.6644(3)	0.8147(4)	0.2796(3)	0.067
H(23A)	4e	0.8001(3)	0.8628(5)	0.3030(3)	0.080
H(24A)	4e	0.9061(3)	0.7264(6)	0.3811(3)	0.091
H(25A)	4e	0.8767(3)	0.5351(6)	0.4354(3)	0.086
H(26A)	4e	0.7428(3)	0.4882(5)	0.4159(2)	0.072
H(27A)	4e	0.3389(3)	0.7304(6)	0.2105(3)	0.098
H(27B)	4e	0.4014(3)	0.7815(6)	0.1776(3)	0.098
H(28A)	4e	0.3364(3)	0.5182(6)	0.1496(3)	0.105
H(28B)	4e	0.3838(3)	0.5918(6)	0.1077(3)	0.105
H(29A)	4e	0.2690(3)	0.7370(5)	0.0458(3)	0.092
H(30A)	4e	0.2323(4)	0.4575(6)	0.0226(3)	0.110
H(30B)	4e	0.2782(4)	0.5440(6)	-0.0164(3)	0.110
H(31A)	4e	0.1583(4)	0.6650(7)	-0.0853(3)	0.121
H(31B)	4e	0.1399(4)	0.5082(7)	-0.0999(3)	0.121
H(32A)	4e	0.0750(4)	0.5048(8)	-0.0177(4)	0.138
H(32B)	4e	0.0330(4)	0.6176(8)	-0.0797(4)	0.138
H(33A)	4e	0.0634(4)	0.7021(8)	0.0441(4)	0.133
H(33B)	4e	0.1077(4)	0.7891(8)	0.0036(4)	0.133
H(34A)	4e	0.2055(4)	0.7427(6)	0.1268(3)	0.113
H(34B)	4e	0.1860(4)	0.5860(6)	0.1161(3)	0.113

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

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cu	4e	0.49865(3)	0.45798(5)	0.38747(3)	0.0476(4)	0.0433(4)	0.0454(3)	0.0012(2)	0.0199(2)	0.0084(2)
C(1)	4e	0.5397(3)	0.2827(4)	0.5156(2)	0.048(3)	0.038(3)	0.046(3)	0.004(2)	0.023(2)	0.001(2)
C(2)	4e	0.4589(3)	0.2799(5)	0.5065(3)	0.051(4)	0.062(3)	0.050(3)	0.005(2)	0.026(2)	0.018(2)
C(3)	4e	0.3917(3)	0.3401(4)	0.4477(2)	0.045(3)	0.057(3)	0.055(3)	−0.001(2)	0.023(2)	0.008(2)
C(4)	4e	0.6038(3)	0.2050(4)	0.5791(2)	0.052(3)	0.044(3)	0.045(2)	0.008(2)	0.025(2)	0.008(2)
C(5)	4e	0.6825(3)	0.2574(5)	0.6169(3)	0.052(3)	0.059(3)	0.069(3)	0.008(2)	0.022(2)	0.013(2)
C(6)	4e	0.7418(3)	0.1865(6)	0.6771(3)	0.053(3)	0.094(4)	0.069(3)	0.011(3)	0.012(2)	0.006(3)
C(7)	4e	0.7234(3)	0.0618(6)	0.6981(3)	0.075(4)	0.083(4)	0.062(3)	0.028(3)	0.026(3)	0.026(3)
C(8)	4e	0.6464(3)	0.0090(6)	0.6607(3)	0.087(4)	0.070(4)	0.072(4)	0.014(3)	0.031(3)	0.034(3)
C(9)	4e	0.5858(3)	0.0801(5)	0.6024(3)	0.062(3)	0.059(3)	0.065(3)	0.005(2)	0.023(2)	0.019(2)
C(10)	4e	0.3066(3)	0.3354(6)	0.4471(3)	0.048(4)	0.104(4)	0.067(3)	−0.003(3)	0.024(2)	0.028(3)
C(11)	4e	0.2371(3)	0.3296(6)	0.3722(3)	0.060(4)	0.100(4)	0.083(4)	−0.002(3)	0.028(3)	0.000(3)
C(12)	4e	0.1502(3)	0.3302(5)	0.3712(3)	0.042(3)	0.075(4)	0.077(3)	0.009(2)	0.023(2)	0.014(3)
C(13)	4e	0.0871(3)	0.2736(7)	0.2984(4)	0.073(4)	0.101(5)	0.118(5)	−0.008(3)	0.037(3)	−0.039(4)
C(14)	4e	−0.0001(3)	0.2691(7)	0.2961(4)	0.058(4)	0.123(6)	0.125(5)	−0.024(4)	0.031(3)	−0.039(4)
C(15)	4e	−0.0256(3)	0.4035(8)	0.3101(4)	0.053(4)	0.135(6)	0.118(5)	0.012(4)	0.006(3)	−0.031(4)
C(16)	4e	0.0348(3)	0.4665(8)	0.3822(4)	0.047(4)	0.170(7)	0.148(6)	0.008(4)	0.025(4)	−0.072(5)
C(17)	4e	0.1217(3)	0.4690(6)	0.3843(4)	0.068(4)	0.098(5)	0.098(4)	−0.007(3)	0.017(3)	−0.025(3)
C(18)	4e	0.6024(3)	0.6090(4)	0.3342(2)	0.061(3)	0.041(3)	0.046(3)	0.000(2)	0.028(2)	−0.003(2)
C(19)	4e	0.5337(3)	0.6699(5)	0.2780(3)	0.057(4)	0.061(3)	0.068(3)	−0.004(2)	0.026(2)	0.020(2)
C(20)	4e	0.4522(3)	0.6345(5)	0.2598(3)	0.065(4)	0.062(3)	0.059(3)	0.006(2)	0.020(2)	0.016(2)
C(21)	4e	0.6884(3)	0.6452(4)	0.3460(2)	0.050(3)	0.047(3)	0.043(2)	−0.005(2)	0.026(2)	−0.006(2)
C(22)	4e	0.7069(3)	0.7586(4)	0.3117(3)	0.068(4)	0.046(3)	0.062(3)	−0.003(2)	0.036(2)	−0.006(2)
C(23)	4e	0.7882(3)	0.7868(5)	0.3256(3)	0.076(4)	0.060(3)	0.082(4)	−0.024(3)	0.050(3)	−0.016(3)
C(24)	4e	0.8514(3)	0.7055(6)	0.3718(3)	0.061(4)	0.099(5)	0.077(4)	−0.017(3)	0.038(3)	−0.016(3)
C(25)	4e	0.8339(3)	0.5924(6)	0.4047(3)	0.052(4)	0.098(4)	0.070(3)	0.004(3)	0.030(2)	0.003(3)
C(26)	4e	0.7537(3)	0.5639(5)	0.3924(2)	0.062(4)	0.070(3)	0.054(3)	0.002(2)	0.031(2)	0.003(2)
C(27)	4e	0.3811(3)	0.7011(6)	0.1940(3)	0.078(4)	0.074(4)	0.078(4)	0.001(3)	0.018(3)	0.031(3)
C(28)	4e	0.3442(3)	0.6057(6)	0.1298(3)	0.101(4)	0.069(4)	0.081(4)	0.011(3)	0.027(3)	0.018(3)
C(29)	4e	0.2603(3)	0.6492(5)	0.0658(3)	0.077(4)	0.069(4)	0.070(3)	0.007(3)	0.017(3)	0.019(3)
C(30)	4e	0.2355(4)	0.5473(6)	0.0027(3)	0.084(4)	0.085(4)	0.090(4)	0.002(3)	0.021(3)	0.002(3)
C(31)	4e	0.1534(4)	0.5798(7)	−0.0619(3)	0.089(5)	0.110(5)	0.081(4)	0.008(4)	0.011(3)	−0.009(3)
C(32)	4e	0.0839(4)	0.5922(8)	−0.0369(4)	0.076(5)	0.130(6)	0.111(5)	−0.003(4)	0.011(4)	0.003(4)
C(33)	4e	0.1058(4)	0.6999(8)	0.0248(4)	0.093(5)	0.123(6)	0.111(5)	0.023(4)	0.037(4)	0.000(4)
C(34)	4e	0.1911(4)	0.6684(6)	0.0905(3)	0.122(5)	0.086(4)	0.069(4)	0.006(4)	0.033(4)	0.006(3)
O(1)	4e	0.5663(2)	0.3498(3)	0.4736(2)	0.048(2)	0.052(2)	0.052(2)	0.005(1)	0.024(1)	0.014(1)
O(2)	4e	0.3982(2)	0.4060(3)	0.3933(2)	0.039(2)	0.068(2)	0.059(2)	0.001(1)	0.018(1)	0.017(2)
O(3)	4e	0.5970(2)	0.5181(3)	0.3800(2)	0.043(2)	0.053(2)	0.050(2)	0.000(1)	0.022(1)	0.009(1)
O(4)	4e	0.4289(2)	0.5447(3)	0.2947(2)	0.053(2)	0.073(2)	0.058(2)	−0.002(2)	0.017(1)	0.025(2)

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