

μ_2 -Acetato- $\kappa^2O:O'$ -tris(μ_2 -ferrocenecarboxylato- $\kappa^2O:O'$)bis[(*N,N*-dimethylformamide- κO)copper(II)]. Corrigendum

Jian-Hai Luo, Chang-Cang Huang,* Xi-He Huang and Jin-Gen Wang

Department of Chemistry, Fuzhou University, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: cchuang@fzu.edu.cn

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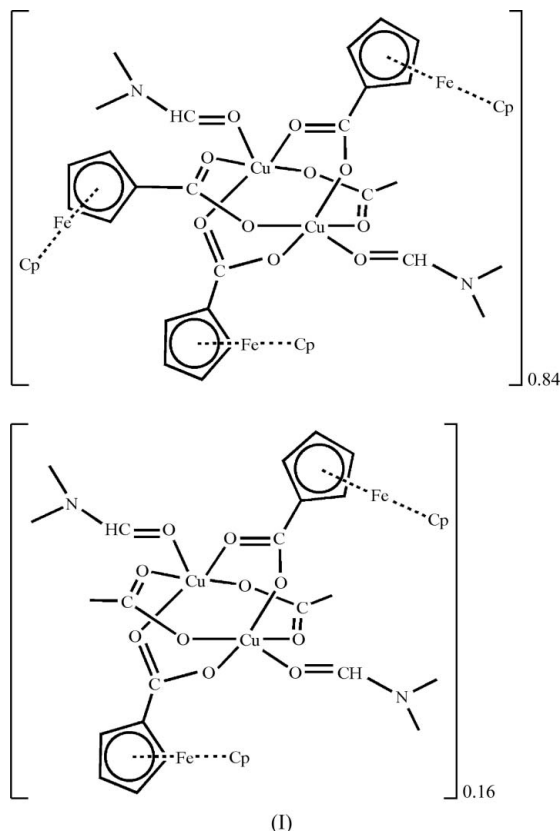
In the paper by Luo, Huang, Huang & Wang [*Acta Cryst.* (2008), **C64**, m121–m122], the structure reported as $[\text{Cu}_2\text{Fe}_3(\text{C}_5\text{H}_5)_3(\text{C}_2\text{H}_3\text{O}_2)(\text{C}_6\text{H}_4\text{O}_2)_3(\text{C}_3\text{H}_7\text{NO})_2]$ is actually a cocrystal in which one of the ferrocenecarboxylate ligands in about 16% of the molecules has been replaced with acetate. The correct structure of $[\text{Cu}_2\text{Fe}_3(\text{C}_5\text{H}_5)_3(\text{C}_2\text{H}_3\text{O}_2)(\text{C}_6\text{H}_4\text{O}_2)_3(\text{C}_3\text{H}_7\text{NO})_2]_{0.84}\cdot[\text{Cu}_2\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_6\text{H}_4\text{O}_2)_2(\text{C}_3\text{H}_7\text{NO})_2]_{0.16}$ is now reported.

Comment

This corrigendum is to correct the report of the crystal structure of μ_2 -acetato- $\kappa^2O:O'$ -tris(μ_2 -ferrocenecarboxylato- $\kappa^2O:O'$)bis[(*N,N*-dimethylformamide- κO)copper(II)] (Luo *et al.*, 2008). Examination of difference electron-density maps and atomic displacement parameters suggested that the ferrocenecarboxylate ligand centred around atom Fe3 was not fully occupied. Refinement of site-occupation factors of the atoms of this ligand indicated that atom Fe3 and the C atoms of the two ferrocene rings have an occupancy of about 0.84, while the acetate part of the ligand has full occupancy. This reveals that in about 16% of the molecules, the ferrocenecarboxylate ligand centred around atom Fe3 has been replaced by acetate. Thus, the reported compound is a cocrystal of composition μ_2 -acetato- $\kappa^2O:O'$ -tris(μ_2 -ferrocenecarboxylato- $\kappa^2O:O'$)bis[(*N,N*-dimethylformamide- κO)copper(II)]-bis(μ_2 -acetato- $\kappa^2O:O'$)bis(μ_2 -ferrocenecarboxylato- $\kappa^2O:O'$)bis[(*N,N*-dimethylformamide- κO)copper(II)] (0.84/0.16), (I).

Refinement of the site-occupation factors of the other ferrocenecarboxylate ligands indicated that these sites were fully occupied. The corrected refinement results are presented here.

The presence of an additional acetate ligand in some of the molecules is understandable given that $\text{Cu}(\text{OAc})_2\cdot\text{H}_2\text{O}$ was used in the synthesis and the cocrystal has apparently arisen because of inadequate purification of the product prior to crystallization.



Experimental

Crystal data

$[\text{Cu}_2\text{Fe}_3(\text{C}_5\text{H}_5)_3(\text{C}_2\text{H}_3\text{O}_2)(\text{C}_6\text{H}_4\text{O}_2)_3(\text{C}_3\text{H}_7\text{NO})_2]_{0.84}\cdot[\text{Cu}_2\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_6\text{H}_4\text{O}_2)_2(\text{C}_3\text{H}_7\text{NO})_2]_{0.16}$	$\alpha = 108.96 (3)^\circ$
$M_r = 992.40$	$\beta = 94.57 (3)^\circ$
Triclinic, $P\bar{1}$	$\gamma = 110.33 (3)^\circ$
$a = 10.948 (2) \text{ \AA}$	$V = 2032.3 (10) \text{ \AA}^3$
$b = 13.548 (3) \text{ \AA}$	$Z = 2$
$c = 15.828 (3) \text{ \AA}$	Mo $K\alpha$ radiation
	$\mu = 2.08 \text{ mm}^{-1}$
	$T = 298 \text{ K}$
	$0.30 \times 0.26 \times 0.26 \text{ mm}$

Data collection

Rigaku R-Axis RAPID diffractometer	19821 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	9106 independent reflections
$T_{\min} = 0.567, T_{\max} = 0.607$	6613 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$	488 parameters
$wR(F^2) = 0.155$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\max} = 0.86 \text{ e \AA}^{-3}$
9106 reflections	$\Delta\rho_{\min} = -0.76 \text{ e \AA}^{-3}$

H atoms bonded to C atoms were allowed for in idealized positions using the riding-model approximation, with C–H = 0.93 [cyclopentadienyl (Cp)] or 0.96 Å (methyl) and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the Cp rings and $1.5U_{\text{eq}}(\text{C})$ for the methyl groups. The ferrocenecarboxylate ligand centred around atom Fe3 is disordered with an acetate ligand at the same site. Refinement of a common site-occupation factor for atom Fe3 and the C atoms of the two associated Cp rings, except atom C24, which also belongs to the acetate ligand, led to a value of 0.841 (3). The site-occupation factors of the methyl H atoms of the minor-component acetate ligand were refined with a complementary value of 0.159 (3). Atoms C29, C30, C31, C32 and C33 of one Cp group were refined with the same anisotropic displacement parameters using the EADP instruction in *SHELXL97* (Sheldrick, 2008). The same type of constraint was also applied to the four methyl C atoms of the dimethylformamide ligands (C37, C38, C40 and C41).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO* (Rigaku, 1998); data reduction: *RAPID-AUTO*

(Rigaku, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: LN3142). Services for accessing these data are described at the back of the journal.

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