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# Poly[[diaquabis($\mu_3$-maleato-$\kappa^4O^1:O^{1'},O^4:O^{4'}$)dicopper(II)] trihydrate]

**Gregory A. Farnum and Robert L. LaDuca***

Lyman Briggs College, Department of Chemistry, Michigan State University, East Lansing, MI 48825, USA
Correspondence e-mail: laduca@msu.edu

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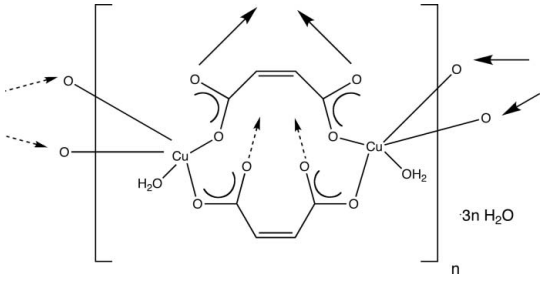
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.023; $wR$ factor = 0.055; data-to-parameter ratio = 11.1.

In the title compound, $\{[Cu_2(C_4H_2O_4)_2(H_2O)_2]\cdot 3H_2O\}_n$, $Cu^{II}$ ions with square-pyramidal coordination are bridged by exotridentate maleate dianions into $[Cu_2(maleate)_2(H_2O)_2]_n$ layers coincident with the *bc* crystal plane. The interlamellar regions contain hydrogen-bonded cyclic water hexamers which facilitate layer stacking into a pseudo-three-dimensional crystal structure. The water hexamers themselves are formed by the operation of crystallographic inversion centers on sets of three crystallographically distinct water molecules of hydration.

## Related literature

For recent dpa coordination polymers, see: Brown *et al.* (2008). For the preparation of dpa, see: Zapf *et al.* (1998). For the determination of the $\tau$ factor for five-coordinate geometries, see: Addison *et al.* (1984).




## Experimental

### Crystal data

$[Cu_2(C_4H_2O_4)_2(H_2O)_2]\cdot 3H_2O$
$M_r$ = 445.27
Monoclinic, $P2_1/c$
$a$ = 8.8835 (14) Å
$b$ = 8.7700 (14) Å
$c$ = 18.814 (3) Å
$\beta$ = 97.994 (3)°
$V$ = 1451.5 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 3.00 mm$^{-1}$
$T$ = 173 (2) K
0.30 × 0.28 × 0.05 mm

### Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.470, $T_{max}$ = 0.860
9585 measured reflections
2643 independent reflections
2331 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.055
$S$ = 1.03
2643 reflections
238 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$WA$···O5 | 0.878 (16) | 2.034 (17) | 2.910 (3) | 175 (3) |
| O1$W$—H1$WB$···O2$W$ | 0.864 (16) | 2.034 (18) | 2.863 (3) | 161 (3) |
| O2$W$—H2$WA$···O7 | 0.861 (16) | 1.967 (17) | 2.827 (3) | 177 (3) |
| O2$W$—H2$WB$···O3$W$ | 0.851 (16) | 2.014 (18) | 2.854 (3) | 169 (3) |
| O3$W$—H3$WA$···O2$^{i}$ | 0.871 (16) | 1.995 (19) | 2.847 (2) | 166 (3) |
| O3$W$—H3$WB$···O1$W^{i}$ | 0.857 (16) | 2.17 (2) | 2.928 (3) | 148 (2) |
| O9—H9$A$···O1$W^{ii}$ | 0.853 (16) | 1.987 (18) | 2.831 (3) | 170 (3) |
| O9—H9$B$···O10$^{iii}$ | 0.851 (16) | 2.023 (19) | 2.855 (3) | 165 (2) |
| O10—H10$A$···O2$W^{iv}$ | 0.867 (16) | 1.943 (17) | 2.797 (3) | 168 (3) |
| O10—H10$B$···O3$W$ | 0.846 (16) | 2.059 (18) | 2.879 (3) | 163 (2) |

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+1, -z$; (iii) $x+1, y+1, z$; (iv) $-x+1, -y, -z$.

Data collection: *COSMO* (Bruker, 2006); cell refinement: *APEX2* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalMaker* (Palmer, 2007); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2520).

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