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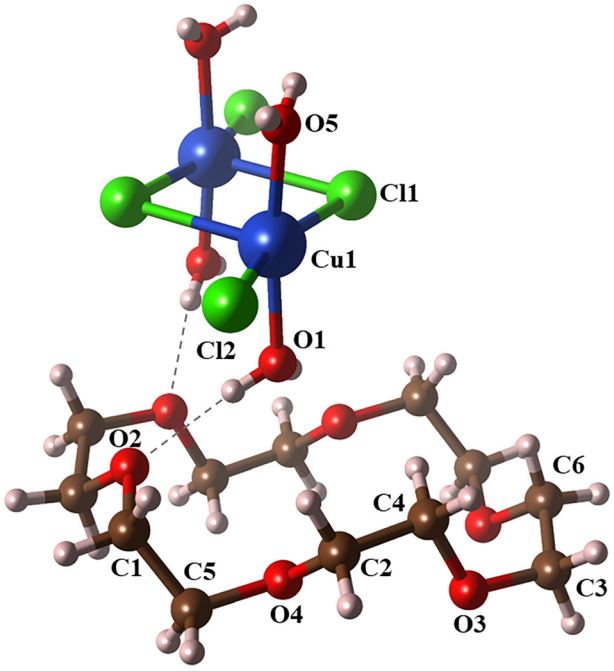
# The crystal structure of 18-crown-6 — tetraaqua-dichlorido-di-μ$_2$-chloridodicopper(II) (2/1), $C_{12}H_{32}O_{10}Cu_2Cl_4$

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**Abstract**

$C_{12}H_{32}O_{10}Cu_2Cl_4$, monoclinic, $P2_1/n$ (no. 14), $a$ = 9.0202(4) Å, $b$ = 9.5791(4) Å, $c$ = 13.6994(6) Å, $\beta$ = 92.555(1)°, $V$ = 1182.53(9) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0308, $wR_{ref}(F^2)$ = 0.0800, $T$ = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Blue block |
| Size: | 0.15 × 0.11 × 0.07 mm |
| Wavelength: | Cu *K*α radiation (1.54184 Å) |
| $\mu$: | 6.77 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker D8 Smart Apex, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 72.1°, 99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 13205, 2306, 0.038 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2278 |
| $N(param)_{refined}$: | 144 |
| Programs: | Bruker [1], SHELX [2,3], Olex2 [4] |

## 1 Source of materials

A total of 2.416 g (0.018 mol) of copper (II) chloride was dissolved in 10 mL of deionized water, followed by the addition of 1.584 g (0.006 mol) of 18-crown-6. To ensure complete dissolution, an excess of methanol was added, resulting in the formation of a transparent dark green solution. The solution was then allowed to evaporate at room temperature for 24 h, leading to the formation of transparent blue crystals of $C_{12}H_{32}O_{10}Cu_2Cl_4$.

## 2 Experimental details

Hydrogen atoms were incorporated into the calculated positions and refined as riding atoms, with a fixed C–H bond length of 0.97 Å and an isotropic displacement parameter ($U_{iso}$) value of 1.2 times the equivalent isotropic displacement parameter ($U_{eq}$) of the corresponding carbon atom for the methylene hydrogen atoms.

## 3 Comment

Crown ether supramolecular host-guest compounds have garnered significant attention due to their excellent physical properties, including ferroelectricity [5] and photoluminescence [6]. Research has revealed that this type of compound exhibit outstanding photoluminescence effects. For instance, Feldmann et al. [6] discovered rare $Zn^{2+}$-based luminescence in $ZnI_2$(18-crown-6) and observed 100 % quantum yield in $Mn_2I_4$ (18-crown-6). Nevertheless, the

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.32789 (3) | 0.59155 (3) | 0.48515 (2) | 0.03354 (14) |
| Cl1 | 0.49914 (5) | 0.53654 (5) | 0.37368 (3) | 0.04280 (16) |
| Cl2 | 0.11991 (5) | 0.67253 (5) | 0.55339 (4) | 0.04961 (18) |
| O1 | 0.41879 (17) | 0.77369 (15) | 0.50618 (12) | 0.0403 (3) |
| O2 | 0.4114 (2) | −0.1226 (2) | 0.69264 (13) | 0.0580 (4) |
| O3 | 0.30111 (19) | 0.18794 (17) | 0.36784 (14) | 0.0555 (4) |
| O4 | 0.32563 (19) | 0.10126 (17) | 0.56116 (14) | 0.0553 (4) |
| O5 | 0.2176 (2) | 0.4234 (2) | 0.4521 (2) | 0.0730 (7) |
| C1 | 0.2873 (3) | −0.0346 (3) | 0.7087 (2) | 0.0653 (7) |
| H1A | 0.276289 | −0.024564 | 0.778474 | 0.078 |
| H1B | 0.198045 | −0.078756 | 0.681262 | 0.078 |
| C2 | 0.1972 (3) | 0.0704 (3) | 0.5013 (3) | 0.0686 (8) |
| H2A | 0.123984 | 0.143654 | 0.507701 | 0.082 |
| H2B | 0.154008 | −0.016867 | 0.521987 | 0.082 |
| C3 | 0.3431 (4) | 0.1960 (3) | 0.2686 (2) | 0.0726 (8) |
| H3A | 0.374825 | 0.290679 | 0.255395 | 0.087 |
| H3B | 0.256666 | 0.176711 | 0.226066 | 0.087 |
| C4 | 0.2390 (4) | 0.0594 (3) | 0.3974 (3) | 0.0737 (9) |
| H4A | 0.310680 | −0.015148 | 0.390766 | 0.088 |
| H4B | 0.151947 | 0.037692 | 0.356078 | 0.088 |
| C5 | 0.3023 (4) | 0.1065 (3) | 0.6644(2) | 0.0687 (8) |
| H5A | 0.213169 | 0.159906 | 0.675162 | 0.082 |
| H5B | 0.385128 | 0.154609 | 0.697036 | 0.082 |
| C6 | 0.5351 (4) | −0.0976 (4) | 0.7565(2) | 0.0752 (9) |
| H6A | 0.508499 | −0.112177 | 0.823576 | 0.090 |
| H6B | 0.568227 | −0.001875 | 0.749889 | 0.090 |
| H1C | 0.492 (3) | 0.788 (3) | 0.4900 (19) | 0.041 (7) |
| H1D | 0.418 (4) | 0.800 (4) | 0.562 (3) | 0.071 (10) |
| H5C | 0.135 (4) | 0.418 (4) | 0.469 (3) | 0.074 (10) |
| H5D | 0.255 (4) | 0.365 (4) | 0.425 (2) | 0.063 (9) |

luminescence properties of Cu based materials have not been reported in the relevant literature.

In order to investigate the structural features of Cu in crown ether compounds, a new centrosymmetric crown ether material $C_{12}H_{32}O_{10}Cu_2Cl_4$ was obtained by evaporating an aqueous solution in this study. The structure of the crown ether is completely ordered, showing $D_{3d}$ structural symmetry. Two Copper (II) chloride dihydrate units are inter-connected by sharing two chlorine ions, with the bond lengths of Cu–Cl of 2.282 Å and 2.722 Å, respectively. In crown ether supermolecule host-guest compounds, the crown ethers are usually coordinated with either amino or metal cations. In this compound, however, the crown ethers are connected by water molecules in the copper(II) chloride dihydrate unit through hydrogen bonds. The bond lengths are determined to be 1.920 Å (H5D–O3), 1.945 Å (H1D–O2), respectively. Moreover, this material has luminescent properties and can emit light at 328 nm and 720 nm under excitation at a wavelength of 266 nm.

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**Research ethics:** All authors involved in the study are aware of the risks and benefits involved, including the right to withdraw.

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**Data availability:** The data and materials used in the study are open access and available for use by other researchers.

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