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Tetrakis(trimethylammonioacetato-*O*)copper(II) bis(hexafluorophosphate)

Yang-Yi Yang,[a] Xiao-Ming Chen[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Chemical Engineering, Zhongshan University, Guangzhou 510275, People's Republic of China, and [b]Institute of Postgraduate Studies, University of Malaya, 50603 Kuala Lumpar, Malaysia

Correspondence e-mail: h1nswen@umcsd.um.edu.my

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.027
wR factor = 0.071
Data-to-parameter ratio = 6.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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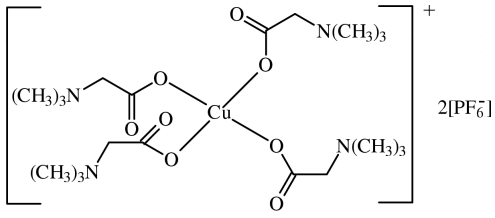
The Cu atom in the title compound, $[Cu(C_5H_{11}NO_2)_4](PF_6)_2$, shows square-planar coordination. The asymmetric unit comprises one eighth of the molecular formula.

Comment

The title compound, (I), is isomorphous with the bis-(perchlorate) (Ng *et al.*, 1998). In both compounds, the Cu atom is four-coordinate in a square-planar geometry; there is no covalent interaction between the anions and cations. The asymmetric unit comprises one eighth of the molecular formula of the title compound with the following atoms on special positions: Cu1 on $\bar{4}2m$; O1, O2, N1, C1, C2 and C4 on . .*m*; P1 on 222; F1 on 2..; and F2 and F3 on the .2. position.



(I)

Experimental

Trimethylammonioacetate and copper nitrate hexahydrate, in a 4:1 molar stoichiometry, were dissolved in a small volume of water. The solution was briefly warmed to 323 K, and and the equivalent amount of potassium hexafluorophosphate was added. The mixture was filtered; deep-blue polyhedral crystals separated from solution after a week. Analysis calculated for $C_{20}H_{44}CuF_{12}N_4O_8P_2$: C 29.41, H 5.45, N 6.65%; found: C 29.22, H 5.29, N 6.82%. IR data (cm^{-1}) in KBr: 3433 (*w br*), 3052 (*w*), 2964 (*w*), 1655 (*vs*), 1499 (*w*), 1475 (*m*), 1455 (*w*), 1398 (*s*), 1320 (*s*), 1238 (*w*), 1128 (*w*), 903 (*m*), 858 (*s*), 805 (*s*), 558 (*m*).

Crystal data

$[Cu(C_5H_{11}NO_2)_4](PF_6)_2$
M_r = 822.07
Tetragonal, $I\bar{4}2m$
a = 11.831 (6) Å
c = 11.760 (8) Å
V = 1646 (2) Å^3
Z = 2
D_x = 1.659 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 7–15°
μ = 0.88 mm^{-1}
T = 298 (2) K
Polyhedron, blue
0.50 × 0.40 × 0.30 mm

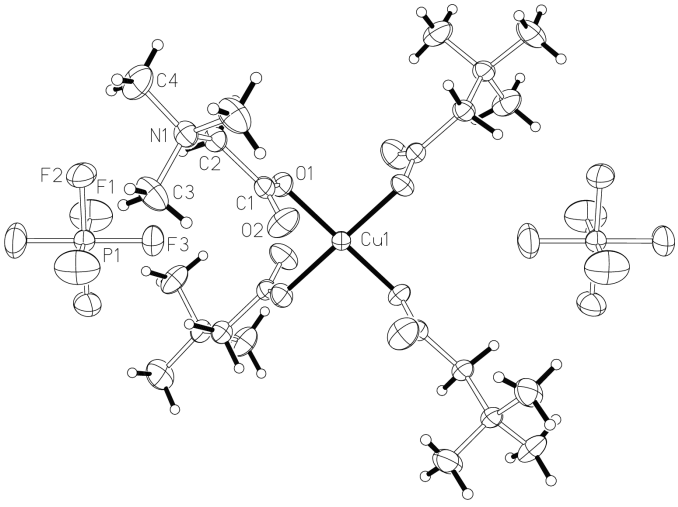


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title salt with ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Data collection

Siemens *R*3*m* four-circle diffractometer
ω scans
Absorption correction: empirical ψ scan (North *et al.*, 1968)
T_{min} = 0.657, T_{max} = 0.742
1035 measured reflections
544 independent reflections
514 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.0°
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 14$
$l = -1 \rightarrow 14$
2 standard reflections
every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.071
S = 1.04
544 reflections
89 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack & Schwarzenbach (1988)
Flack parameter = −0.01 (3), 506 Friedel pairs

Data collection: *R*3*m Software* (Siemens, 1990); cell refinement: *R*3*m Software*; data reduction: *R*3*m Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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