Feng Yi-Min and Tai Xi-Shi*

Crystal structure of 2-(1*H*-indol-3-yl)ethan-1-aminium 2-(4-acetylphenoxy)acetate, C₂₀H₂₂N₂O₄

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Abstract

C₂₀H₂₂N₂O₄, monoclinic, *P*₂₁/*c* (no. 14), *a* = 18.1092(12) Å, *b* = 8.4026(6) Å, *c* = 11.6983(8) Å, β = 92.582(7)°, *V* = 1778.3(2) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0456, *wR*_{ref}(*F*²) = 0.1137, *T* = 200.00(10) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title salt was prepared by the following steps: 0.194 g 4-acetyl-phenoxyacetic acid (1.0 mmol), 0.1602 g

Table 1: Data collection and handling.

Crystal:	Bronze block
Wavelength:	Size 0.14 × 0.11 × 0.10 mm
μ:	Mo Kα radiation (0.71073 Å)
Diffractometer, scan mode:	0.09 mm ⁻¹
θ _{max} , completeness:	SuperNova, ω
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	25.0°, >99%
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	7718, 3108, 0.035
<i>N</i> (<i>param</i>) _{refined} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2477
Programs:	252
	Bruker [1], Olex2 [2], SHELX [3],
	Diamond [4]

tryptamine (1.0 mmol), 0.040 g NaOH (1.0 mmol), and 0.1225 g manganese acetate tetrahydrate (0.5 mmol) were dissolved in 25 mL *N,N*-dimethylformamide-water solution-ethanol (v:v = 1:2:2). The mixture was stirred for 4 h at 70 °C, and then continually stirred for 3 h at room temperature. The colorless crystals of the title salt were received from the filtrate after 22 days.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93–0.97 Å and N–H = 0.85–0.99 Å). Their *U*_{iso} values were set to 1.2*U*_{eq} or 1.5*U*_{eq} of the parent atoms.

Comment

Aminium compounds based on organic carboxylates exhibit applications in cement grinding aids [5], antirust [6], supramolecular assemblies [7]. Our goal was to synthesize a manganese complex of a Schiff base, however, unfortunately, neither the Schiff base ligand nor the manganese complex was formed. Only a new salt compound has been obtained by 4-acetyl-phenoxyacetic acid, tryptamine, NaOH, and manganese acetate tetrahydrate as raw materials.

The title compound consists of one (4-acetyl-phenoxy)-acetate anion and one 2-(1*H*-indol-3-yl)-ethyl-ammonium cation (the Figure). The bond distances of C–O are 1.220(2) Å (C7–O1), 1.368(2) Å (C4–O2), 1.425(2) Å (C9–O2), 1.253(2) Å (C10–O3), 1.254(2) Å (C10–O4), respectively, indicating that

*Corresponding author: Tai Xi-Shi, College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P. R. China, E-mail: taixs@wfu.edu.cn. <https://orcid.org/0000-0002-0050-1900>

Feng Yi-Min, College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P. R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} */U _{eq}
O1	0.54252 (8)	0.5713 (2)	0.68117 (15)	0.0720 (6)
O2	0.20651 (6)	0.63334 (14)	0.50218 (10)	0.0285 (3)
O3	0.10967 (7)	0.69689 (14)	0.23523 (10)	0.0289 (3)
O4	0.07386 (6)	0.59419 (14)	0.39999 (10)	0.0306 (3)
C1	0.41219 (10)	0.5781 (2)	0.67014 (17)	0.0329 (5)
C2	0.40832 (10)	0.6213 (2)	0.55554 (17)	0.0363 (5)
H2	0.451954	0.635271	0.517780	0.044*
C3	0.34144 (10)	0.6442 (2)	0.49571 (17)	0.0331 (5)
H3	0.340210	0.673656	0.419024	0.040*
C4	0.27613 (9)	0.62248 (19)	0.55190 (15)	0.0248 (4)
C5	0.27915 (10)	0.5831 (2)	0.66746 (15)	0.0281 (4)
H5	0.235562	0.572034	0.705815	0.034*
C6	0.34596 (10)	0.5602 (2)	0.72545 (16)	0.0311 (4)
H6	0.347096	0.532535	0.802479	0.037*
C7	0.48516 (11)	0.5494 (3)	0.72966 (19)	0.0433 (5)
C8	0.48752 (12)	0.4936 (3)	0.8512 (2)	0.0590 (7)
H8A	0.537656	0.470042	0.875539	0.089*
H8B	0.457869	0.399533	0.856964	0.089*
H8C	0.468558	0.575547	0.898958	0.089*
C9	0.19985 (9)	0.6734 (2)	0.38376 (15)	0.0267 (4)
H9A	0.232219	0.605637	0.341314	0.032*
H9B	0.215290	0.782859	0.373500	0.032*
C10	0.12087 (9)	0.65352 (18)	0.33698 (15)	0.0223 (4)
N1	0.12482 (10)	0.52622 (19)	1.01261 (15)	0.0353 (4)
H1	0.1139 (11)	0.591 (2)	1.0647 (19)	0.044 (6)*
N2	0.07292 (9)	0.50832 (17)	0.62536 (14)	0.0239 (4)
H2A	0.0216 (12)	0.495 (2)	0.6287 (17)	0.034 (5)*
H2B	0.0790 (11)	0.550 (2)	0.547 (2)	0.044 (6)*
H2C	0.0899 (10)	0.585 (2)	0.6805 (17)	0.032 (5)*
C11	0.10797 (10)	0.3497 (2)	0.64127 (15)	0.0275 (4)
H11A	0.161174	0.360252	0.638093	0.033*
H11B	0.090976	0.279562	0.579680	0.033*
C12	0.08921 (10)	0.2774 (2)	0.75503 (16)	0.0313 (4)
H12A	0.035858	0.270648	0.758032	0.038*
H12B	0.108512	0.169748	0.758725	0.038*
C13	0.11864 (10)	0.36713 (19)	0.85832 (15)	0.0258 (4)
C14	0.08117 (11)	0.4742 (2)	0.92154 (17)	0.0320 (5)
H14	0.032832	0.507200	0.905096	0.038*
C15	0.19231 (11)	0.4523 (2)	1.01027 (16)	0.0294 (4)
C16	0.19060 (10)	0.35208 (19)	0.91338 (15)	0.0260 (4)
C17	0.25354 (10)	0.2606 (2)	0.89255 (18)	0.0348 (5)
H17	0.254463	0.195592	0.828305	0.042*
C18	0.31375 (11)	0.2684 (3)	0.9682 (2)	0.0464 (6)
H18	0.355271	0.206958	0.955413	0.056*
C19	0.31343 (12)	0.3677 (3)	1.0644 (2)	0.0504 (6)
H19	0.354618	0.370034	1.114856	0.060*
C20	0.25353 (12)	0.4618 (2)	1.08584 (18)	0.0424 (5)
H20	0.253971	0.529478	1.148761	0.051*

the C7–O1 bond is double bond. The bond distances of C–N are 1.369(3) Å (C14–N1), 1.372(3) Å (C15–N1) and 1.484(2) Å (C11–N2), respectively. The bond distances of C–O and C–N

are consistent with Refs. [8–10]. The ring 1 (C13–C14–N1–C15–C16) and ring 2 (C15–C16–C17–C18–C19–C20) are coplanar with a dihedral angle of 2.3°. The ring 3 (C1–C2–C3–C4–C5–C6) and ring 2 (C15–C16–C17–C18–C19–C20) are not coplanar with a dihedral angle of 54.2°. The title compound forms a layered structure by N–H···O hydrogen bonds.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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