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Potassium *N*-(6-oxocyclohexa-1,3-dien-5-ylidenemethyl)glycinate

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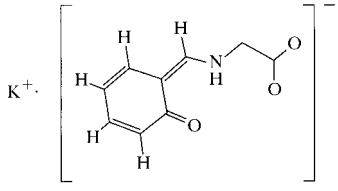
We are very interested in characterizing ligands derived from salicylaldehyde and α-amino acids. These ligands form interesting complexes with different transition metals, which are very useful for understanding some biological systems. For



(I)

Schiff bases derived from salicylaldehyde and different alkylamines or arylamines, the enol–imine form is predominant. The title compound, (I), shows bond distances which are clearly in agreement with the keto–amine form.

Experimental

Crystal data

$K^+ \cdot C_9H_8NO_3^-$
M_r = 217.26
Orthorhombic, *Pcca*
a = 13.8864 (2) Å
b = 18.4943 (7) Å
c = 6.9664 (9) Å
V = 1789.1 (2) Å^3
Z = 8
D_x = 1.613 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 18191 reflections
θ = 2.93–27.49°
μ = 0.570 mm^{-1}
T = 100 (1) K
Plate, orange
0.30 × 0.30 × 0.10 mm

Data collection

KappaCCD diffractometer
φ and ω scans with κ offsets
Absorption correction: multi-scan (*DENZO–SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.848, T_{max} = 0.945
18 191 measured reflections
2036 independent reflections
1580 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 27.49°
$h = -18 \rightarrow 18$
$k = -24 \rightarrow 24$
$l = -8 \rightarrow 8$
Intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.034
$wR(F^2)$ = 0.091
S = 1.051
2036 reflections
131 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.0850P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.312 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O3	0.91 (2)	1.91 (2)	2.6310 (19)	135.4 (18)

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL/PC*; software used to prepare material for publication: *SHELXTL/PC*.

Data were collected at the University of Toronto (where all structural calculations were carried out) on a Nonius KappaCCD purchased with funds from NSERC Canada. We would like to thank FONDECYT for funding of Project 2960043.

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