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Aqua(salicylidene-β-alaninato-κ^2O,O')potassium(I)

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Key indicators

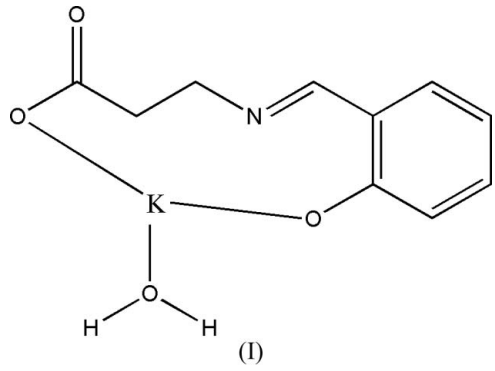
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.060
wR factor = 0.142
Data-to-parameter ratio = 16.8

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

In the molecule of the title compound, $[K(C_{10}H_9NO_3)(H_2O)]$, the dihedral angle between the planes of the salicylidene and alanine units is 73.7 (3)°. In the crystal structure, intermolecular O—H···O hydrogen bonds link the molecules into a two-dimensional layer.

Comment

The title compound, (I), is an effective material for the preparation of rare earth complexes (Parekh *et al.*, 2005). We report here the crystal structure of (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The C1–C8/N1/O1 and C9/C10/O2/O3 units are nearly planar, with r.m.s. deviations of 0.028 (2) and 0.005 (1) Å, respectively, and a dihedral angle between them of 73.7 (3)°.

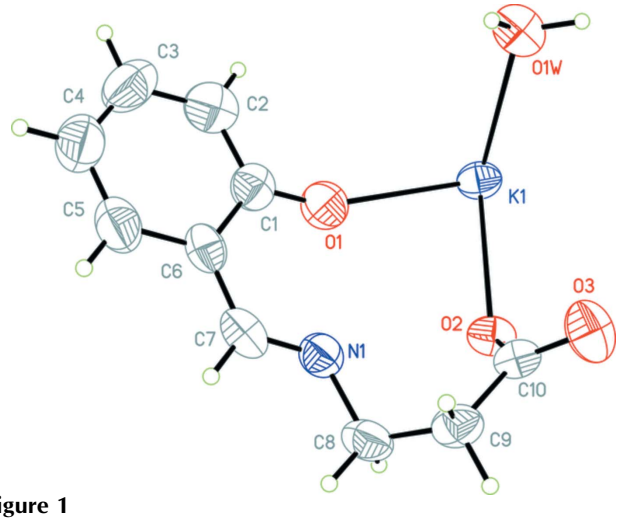


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

As can be seen from the packing diagram (Fig. 2), intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into a two-dimensional layer.

Experimental

The title compound was prepared by a literature method (Parekh *et al.*, 2005). The resulting solid was recrystallized from an ethanol–diethyl ether (1:1) mixture, giving crystals of (I) suitable for X-ray analysis (yield 66%; m. p. 447 K).

Crystal data

$[K(C_{10}H_9NO_3)(H_2O)]$
$M_r = 248.30$
Monoclinic, $P2_1/c$
$a = 17.792$ (4) Å
$b = 7.9920$ (16) Å
$c = 8.3590$ (17) Å
$\beta = 100.29$ (3)°
$V = 1169.5$ (4) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.45$ mm^{-1}
$T = 294$ (2) K
0.30 × 0.30 × 0.10 mm

Data collection

Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.876$, $T_{max} = 0.956$
2289 measured reflections
2289 independent reflections
1477 reflections with $I > 2\sigma(I)$
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.142$
$S = 1.03$
2289 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H4B···O2^{v}	0.97	2.60	3.475 (3)	150
O1W—H4A···O3^{vi}	0.97	2.15	2.741 (3)	118

Symmetry codes: (v) $-x, -y+1, -z+1$; (vi) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

H atoms were positioned geometrically, with O—H = 0.97 Å (for water) and C—H = 0.93 and 0.97 Å and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C,O)$.

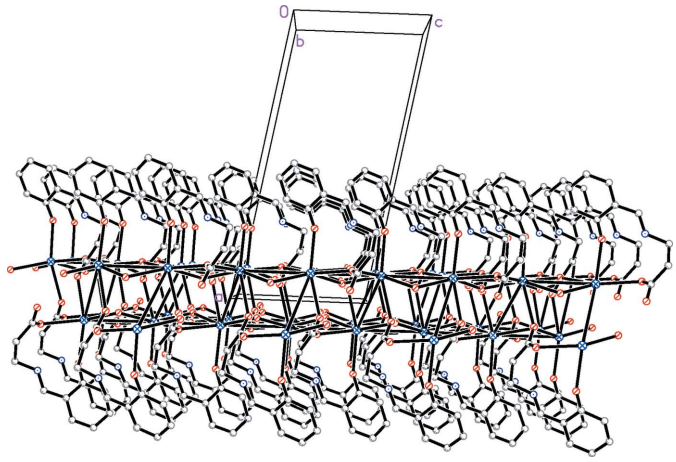


Figure 2
A packing diagram for (I). H atoms have been omitted.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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