Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[μ_2-acetato-diacetonitrile[μ_2-*N*,*N*′-bis(2-hydroxyphenyl)pyridine-2,6-dicarboxamide]potassium(I)]

Yolanda Pérez,[a] Andrew L. Johnson[b] and Paul R. Raithby[b,c]*

[a]Departamento de Química Inorgánica y Analítica, ESCET, Universidad Rey Juan Carlos, 28933 Móstoles (Madrid), Spain, [b]Department of Chemistry, University of Bath, Bath BA2 7AY, England, and [c]CCLRC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England

Correspondence e-mail: p.r.raithby@bath.ac.uk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.062
wR factor = 0.183
Data-to-parameter ratio = 13.1

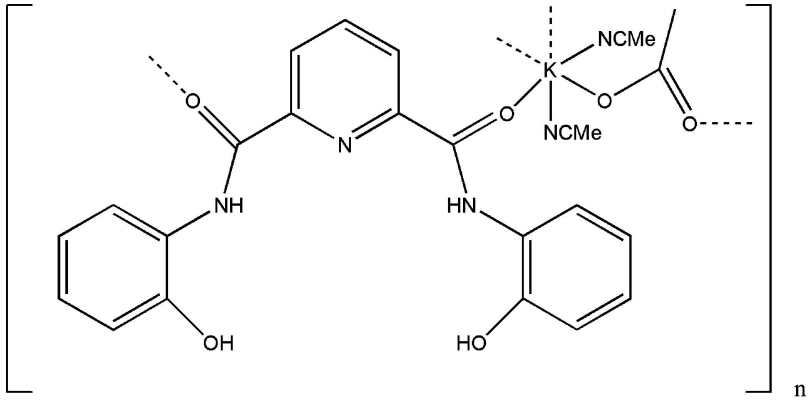
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 18 August 2006
Accepted 22 August 2006

The title compound, $[K(C_2H_3O_2)(C_2H_3N)_2(C_{19}H_{15}N_3O_4)]$, is polymeric. Each K^+ ion adopts a distorted octahedral geometry, being linked to two 2,6-pyridinedicarboxamide ligands through carbonyl O atoms and to two acetate groups also through O atoms. The potassium coordination is completed by the N atoms of two acetonitrile ligands. The 2,6-pyridinedicarboxamide ligands are also involved in O—H···O hydrogen bonds.

Comment

Many derivatives of 2,6-pyridinecarboxamide show anti-inflammatory, antipyretic and analgesic activities (Singha & Sathyanarayana, 1997, and references therein). A series of Cu^{II}, Fe^{III}, Co^{III} and Ni^{II} (Chavez *et al.*, 1996, 1998; Marlin *et al.*, 1999; Hiratani & Taguchi, 1990) complexes containing 2,6-pyridinedicarboxamide ligands has been synthesized during the last two decades. The derivative *N*,*N*′-bis(2-hydroxyphenyl)pyridine-2,6-dicarboxamide has been synthesized previously (Marlin *et al.*, 2000). Several complexes of this ligand have been reported, two of which consist of the fully deprotonated pentadentate ligand with an Fe^{III} atom in the equatorial plane of the ligand, the coordination being completed by two monodentate ligands in axial sites (Marlin *et al.*, 2000). We are continuing to investigate the coordination properties of this ligand with a range of heavier main group and transition metals.



(I)

In this paper, we report the synthesis and crystal structure of the title polymeric potassium complex of *N*,*N*′-bis(2-hydroxyphenyl)pyridine-2,6-dicarboxamide, (I) (Fig. 1), where the ligand links two K^+ ions through the two carbonyl groups. The coordination environment of each K^+ centre is completed by coordination of one O atom of each of two acetate groups, and two terminal acetonitrile ligands. The

acetate groups act as linker groups between adjacent K^+ centres.

The K^+ centres display a distorted octahedral coordination geometry. The two K—O(carbonyl) distances (average 2.75 Å) are similar in length to the two K—O(acetate) distances (average 2.72 Å), and these four distances are significantly shorter than the two K—N(acetonitrile) distances (average 3.11 Å). The K—O(ethoxy) distances are similar to the average value of 2.67 Å previously reported for an ethanol-solvated dimeric potassium calixarene complex (Clague *et al.*, 1999).

In addition, the *N*,*N*′-bis(2-hydroxyphenyl)pyridine-2,6-dicarboxamide ligands are involved in O—H···O hydrogen bonds from the two hydroxyl groups to the linking acetate groups (Table 1).

Experimental

Compound (I) was synthesized by mixing solutions of *N*,*N*′-bis(2-hydroxyphenyl)pyridine-2,6-dicarboxamide and KO^{t}Bu, in the presence of potassium acetate (as a potential deprotonation reagent), in acetonitrile, in a 1:2 molar ratio, and stirring the resulting mixture for 2 h. Orange needles of (I) suitable for X-ray analysis were grown by slow diffusion of ethyl acetate into a dimethylformamide solution of (I).

Crystal data

$[K(C_2H_3O_2)(C_2H_3N)_2(C_{19}H_{15}N_3O_4)]$
M_r = 529.59
Orthorhombic, *Pbca*
a = 13.6100 (2) Å
b = 21.1060 (3) Å
c = 17.5730 (3) Å
V = 5047.89 (13) Å^3
Z = 8
D_x = 1.394 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 150 (2) K
Block, orange
0.17 × 0.13 × 0.1 mm

Data collection

Bruker NoniusKappa CCD area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.919, T_{max} = 0.974
30810 measured reflections
4445 independent reflections
3751 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.183
S = 1.05
4445 reflections
339 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0943P)^2 + 9.313P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4O···O6^{i}	0.84	1.8	2.638 (3)	174
O1—H1O···O5^{i}	0.84	1.78	2.618 (3)	175

Symmetry code: (i) $-x+\frac{1}{2}, -y+1, z+\frac{1}{2}$.

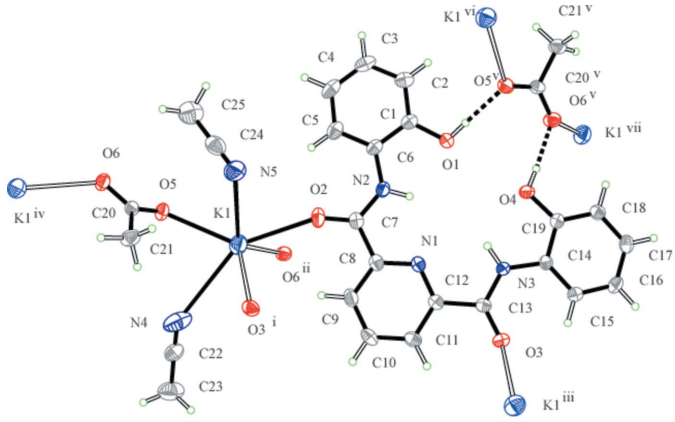


Figure 1
A view of (I), with 50% probability displacement ellipsoids, showing the polymeric nature of the structure. [Symmetry codes: (i) $\frac{1}{2}+x, \frac{3}{2}-y, 1-z$; (ii) $x-\frac{1}{2}, y, \frac{1}{2}-z$; (iii) $\frac{1}{2}-x, \frac{3}{2}-y, 1-z$; (iv) $\frac{1}{2}+x, y, \frac{1}{2}-z$; (v) $\frac{1}{2}-x, 1-y, \frac{1}{2}+z$; (vi) $\frac{1}{2}-x, 1-y, \frac{1}{2}+z$; (vii) $-x, 1-y, 1-z$.]

H atoms were constrained as riding atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H, and C—H =0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H, and with N—H = 0.88 Å and U_{iso}(H) = 1.2U_{eq}(N), and O—H = 0.84 Å and U_{iso}(H) = 1.2U_{eq}(O). There was no residual electron density above 0.5 e Å^3. The deepest hole is located 0.45 Å from atom K1.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors are grateful to the EPSRC, the Nuffield Foundation and the Universidad Rey Juan Carlos for funding.

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supporting information

Acta Cryst. (2006). E**62**, m2359–m2360 [https://doi.org/10.1107/S1600536806033678]

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$c = 17.5730$ (3) Å
$V = 5047.89$ (13) Å^3
$Z = 8$
$F(000) = 2208$
$D_x = 1.394$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 48840 reflections
$\theta = 2.9$–$25.0°$
$\mu = 0.26$ mm^{-1}
$T = 150$ K
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0.17 × 0.13 × 0.1 mm

Data collection

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4445 independent reflections
3751 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.6°$
$h = -16 \rightarrow 14$
$k = -25 \rightarrow 24$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.183$
$S = 1.05$
4445 reflections
339 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0943P)^2 + 9.313P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -1.04$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
K1	0.32899 (6)	0.63984 (4)	0.32048 (5)	0.0393 (3)

O1	0.03601 (16)	0.46047 (10)	0.61597 (12)	0.0260 (5)
H1O	0.0245	0.4377	0.6542	0.031*
O2	0.21897 (17)	0.59656 (12)	0.44330 (14)	0.0370 (6)
O3	−0.18735 (16)	0.74268 (10)	0.61676 (13)	0.0277 (5)
O4	−0.14184 (15)	0.52344 (10)	0.69281 (13)	0.0268 (5)
H4O	−0.1462	0.4862	0.7094	0.032*
O5	0.49403 (15)	0.60471 (10)	0.24059 (12)	0.0265 (5)
O6	0.65655 (16)	0.59633 (10)	0.23424 (13)	0.0294 (5)
N1	0.00694 (18)	0.64723 (11)	0.54463 (13)	0.0203 (5)
N2	0.11790 (19)	0.54268 (12)	0.52490 (14)	0.0233 (6)
H2N	0.0635	0.5472	0.5514	0.028*
N3	−0.14907 (18)	0.63872 (11)	0.63950 (14)	0.0212 (6)
H3N	−0.1019	0.6108	0.633	0.025*
N4	0.3715 (3)	0.7545 (2)	0.2052 (2)	0.0638 (11)
N5	0.4598 (3)	0.58325 (18)	0.4408 (2)	0.0512 (9)
C1	0.1195 (2)	0.44041 (14)	0.58171 (16)	0.0230 (7)
C2	0.1607 (2)	0.38097 (16)	0.59291 (19)	0.0294 (7)
H2	0.1313	0.3521	0.6276	0.035*
C3	0.2448 (3)	0.36378 (16)	0.55337 (19)	0.0337 (8)
H3	0.2729	0.3231	0.561	0.04*
C4	0.2878 (3)	0.40571 (17)	0.5028 (2)	0.0353 (8)
H4	0.3452	0.3934	0.4758	0.042*
C5	0.2486 (2)	0.46531 (17)	0.49105 (18)	0.0299 (7)
H5	0.2788	0.4939	0.4564	0.036*
C6	0.1638 (2)	0.48308 (15)	0.53076 (17)	0.0237 (7)
C7	0.1456 (2)	0.59359 (15)	0.48446 (17)	0.0245 (7)
C8	0.0810 (2)	0.65075 (15)	0.49447 (17)	0.0233 (7)
C9	0.1018 (2)	0.70516 (16)	0.45264 (19)	0.0307 (7)
H9	0.1543	0.7056	0.417	0.037*
C10	0.0446 (3)	0.75849 (16)	0.46388 (19)	0.0321 (8)
H10	0.0575	0.7963	0.4364	0.038*
C11	−0.0316 (2)	0.75581 (15)	0.51580 (18)	0.0264 (7)
H11	−0.0716	0.7919	0.5251	0.032*
C12	−0.0483 (2)	0.69926 (13)	0.55413 (16)	0.0203 (6)
C13	−0.1347 (2)	0.69564 (13)	0.60721 (16)	0.0209 (6)
C14	−0.2309 (2)	0.61816 (14)	0.68278 (16)	0.0204 (6)
C15	−0.3139 (2)	0.65442 (15)	0.69736 (18)	0.0256 (7)
H15	−0.3174	0.6969	0.6796	0.031*
C16	−0.3917 (2)	0.62870 (16)	0.73790 (19)	0.0290 (7)
H16	−0.4486	0.6535	0.7474	0.035*
C17	−0.3868 (2)	0.56729 (15)	0.76450 (18)	0.0287 (7)
H17	−0.4403	0.5499	0.7923	0.034*
C18	−0.3037 (2)	0.53074 (15)	0.75074 (18)	0.0255 (7)
H18	−0.3002	0.4886	0.7697	0.031*
C19	−0.2254 (2)	0.55555 (14)	0.70935 (16)	0.0216 (6)
C20	0.5794 (2)	0.62540 (14)	0.25225 (17)	0.0223 (7)
C21	0.5892 (3)	0.68904 (15)	0.2908 (2)	0.0349 (8)
H21A	0.5745	0.6846	0.3451	0.052*

H21B	0.5429	0.7191	0.2678	0.052*
H21C	0.6564	0.7048	0.2844	0.052*
C22	0.3376 (3)	0.79010 (18)	0.1655 (2)	0.0359 (8)
C23	0.2917 (4)	0.8356 (2)	0.1151 (3)	0.0617 (13)
H23A	0.2528	0.8131	0.0767	0.092*
H23B	0.3425	0.861	0.0899	0.092*
H23C	0.2486	0.8635	0.1446	0.092*
C24	0.5035 (3)	0.5437 (2)	0.4138 (2)	0.0417 (9)
C25	0.5612 (4)	0.4924 (2)	0.3796 (2)	0.0561 (11)
H25A	0.6299	0.5058	0.3748	0.084*
H25B	0.5349	0.4824	0.3291	0.084*
H25C	0.5575	0.4547	0.4121	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0324 (5)	0.0411 (5)	0.0445 (5)	−0.0007 (3)	0.0030 (3)	−0.0026 (3)
O1	0.0257 (11)	0.0253 (11)	0.0269 (11)	0.0016 (9)	0.0042 (9)	0.0048 (9)
O2	0.0299 (13)	0.0408 (14)	0.0402 (14)	−0.0016 (11)	0.0153 (11)	0.0023 (11)
O3	0.0285 (12)	0.0220 (11)	0.0326 (12)	0.0049 (9)	0.0016 (10)	0.0015 (9)
O4	0.0223 (11)	0.0207 (11)	0.0374 (13)	0.0026 (9)	0.0038 (10)	0.0068 (10)
O5	0.0198 (11)	0.0289 (11)	0.0306 (12)	−0.0021 (9)	0.0029 (9)	−0.0063 (9)
O6	0.0211 (11)	0.0257 (11)	0.0413 (14)	−0.0006 (9)	0.0036 (10)	−0.0047 (10)
N1	0.0186 (12)	0.0228 (12)	0.0195 (12)	−0.0044 (10)	−0.0023 (10)	0.0002 (10)
N2	0.0200 (13)	0.0274 (14)	0.0227 (13)	0.0018 (11)	0.0021 (10)	−0.0004 (10)
N3	0.0189 (12)	0.0194 (12)	0.0253 (13)	0.0027 (10)	0.0029 (10)	0.0023 (10)
N4	0.081 (3)	0.065 (2)	0.045 (2)	0.039 (2)	−0.007 (2)	−0.0071 (19)
N5	0.0345 (18)	0.049 (2)	0.070 (2)	0.0018 (17)	−0.0036 (18)	0.0115 (19)
C1	0.0216 (15)	0.0265 (16)	0.0210 (15)	0.0015 (13)	−0.0064 (12)	−0.0042 (12)
C2	0.0325 (18)	0.0269 (16)	0.0289 (17)	0.0026 (14)	−0.0092 (14)	−0.0035 (14)
C3	0.0335 (18)	0.0325 (18)	0.0352 (18)	0.0119 (15)	−0.0115 (16)	−0.0093 (15)
C4	0.0273 (17)	0.045 (2)	0.0340 (18)	0.0117 (16)	−0.0036 (15)	−0.0141 (16)
C5	0.0238 (16)	0.0391 (19)	0.0266 (16)	0.0029 (14)	−0.0017 (14)	−0.0069 (14)
C6	0.0207 (15)	0.0279 (16)	0.0225 (15)	0.0031 (13)	−0.0052 (12)	−0.0054 (12)
C7	0.0234 (16)	0.0295 (17)	0.0206 (15)	−0.0032 (13)	−0.0018 (13)	−0.0015 (13)
C8	0.0206 (15)	0.0272 (16)	0.0220 (15)	−0.0053 (13)	−0.0024 (12)	0.0000 (12)
C9	0.0269 (17)	0.0340 (18)	0.0313 (17)	−0.0056 (14)	0.0053 (14)	0.0057 (14)
C10	0.0366 (19)	0.0261 (17)	0.0335 (18)	−0.0095 (15)	0.0028 (15)	0.0072 (14)
C11	0.0299 (17)	0.0209 (15)	0.0285 (16)	−0.0043 (13)	−0.0028 (14)	0.0008 (13)
C12	0.0192 (14)	0.0218 (15)	0.0198 (14)	−0.0049 (12)	−0.0054 (12)	−0.0001 (12)
C13	0.0212 (15)	0.0215 (15)	0.0201 (14)	−0.0002 (12)	−0.0049 (12)	0.0004 (12)
C14	0.0190 (15)	0.0224 (14)	0.0197 (14)	−0.0021 (12)	0.0002 (11)	−0.0002 (12)
C15	0.0249 (16)	0.0239 (16)	0.0280 (16)	0.0036 (13)	0.0001 (13)	0.0016 (13)
C16	0.0204 (16)	0.0327 (17)	0.0340 (18)	0.0048 (13)	0.0037 (14)	−0.0020 (14)
C17	0.0227 (16)	0.0339 (17)	0.0295 (17)	−0.0051 (14)	0.0037 (13)	−0.0004 (14)
C18	0.0265 (16)	0.0222 (15)	0.0276 (15)	−0.0028 (13)	0.0012 (13)	0.0015 (13)
C19	0.0201 (15)	0.0241 (15)	0.0205 (15)	0.0000 (12)	−0.0009 (12)	−0.0017 (12)
C20	0.0244 (17)	0.0212 (15)	0.0212 (15)	0.0003 (13)	0.0029 (12)	−0.0010 (12)

C21	0.0324 (19)	0.0246 (17)	0.048 (2)	0.0021 (14)	−0.0034 (16)	−0.0084 (15)
C22	0.037 (2)	0.0362 (19)	0.0347 (19)	0.0065 (16)	−0.0003 (16)	−0.0090 (16)
C23	0.087 (4)	0.051 (3)	0.047 (2)	0.023 (3)	0.000 (2)	0.007 (2)
C24	0.039 (2)	0.047 (2)	0.039 (2)	−0.0073 (19)	−0.0100 (17)	0.0143 (18)
C25	0.070 (3)	0.062 (3)	0.037 (2)	0.008 (2)	−0.005 (2)	−0.003 (2)

Geometric parameters (Å, º)

K1—O6^{i}	2.697 (2)	C5—C6	1.400 (5)
K1—O3^{ii}	2.723 (2)	C5—H5	0.95
K1—O5	2.751 (2)	C7—C8	1.503 (4)
K1—O2	2.781 (2)	C8—C9	1.392 (4)
K1—N5	3.011 (4)	C9—C10	1.382 (5)
K1—N4	3.209 (4)	C9—H9	0.95
O1—C1	1.354 (4)	C10—C11	1.383 (5)
O1—H1O	0.84	C10—H10	0.95
O2—C7	1.234 (4)	C11—C12	1.389 (4)
O3—C13	1.236 (4)	C11—H11	0.95
O3—K1^{iii}	2.723 (2)	C12—C13	1.503 (4)
O4—C19	1.356 (4)	C14—C15	1.388 (4)
O4—H4O	0.84	C14—C19	1.404 (4)
O5—C20	1.258 (4)	C15—C16	1.387 (5)
O6—C20	1.257 (4)	C15—H15	0.95
O6—K1^{iv}	2.697 (2)	C16—C17	1.379 (5)
N1—C8	1.341 (4)	C16—H16	0.95
N1—C12	1.341 (4)	C17—C18	1.391 (5)
N2—C7	1.342 (4)	C17—H17	0.95
N2—C6	1.408 (4)	C18—C19	1.392 (4)
N2—H2N	0.88	C18—H18	0.95
N3—C13	1.343 (4)	C20—C21	1.510 (4)
N3—C14	1.417 (4)	C21—H21A	0.98
N3—H3N	0.88	C21—H21B	0.98
N4—C22	1.123 (5)	C21—H21C	0.98
N5—C24	1.129 (5)	C22—C23	1.449 (6)
C1—C2	1.388 (4)	C23—H23A	0.98
C1—C6	1.406 (5)	C23—H23B	0.98
C2—C3	1.387 (5)	C23—H23C	0.98
C2—H2	0.95	C24—C25	1.467 (6)
C3—C4	1.384 (5)	C25—H25A	0.98
C3—H3	0.95	C25—H25B	0.98
C4—C5	1.382 (5)	C25—H25C	0.98
C4—H4	0.95		
O6^{i}—K1—O3^{ii}	112.54 (7)	C10—C9—H9	120.6
O6^{i}—K1—O5	115.90 (7)	C8—C9—H9	120.6
O3^{ii}—K1—O5	121.26 (7)	C9—C10—C11	118.9 (3)
O6^{i}—K1—O2	72.33 (8)	C9—C10—H10	120.6
O3^{ii}—K1—O2	86.60 (7)	C11—C10—H10	120.6

O5—K1—O2	138.35 (7)	C10—C11—C12	118.6 (3)
O6^{i}—K1—N5	129.03 (9)	C10—C11—H11	120.7
O3^{ii}—K1—N5	97.19 (9)	C12—C11—H11	120.7
O5—K1—N5	76.62 (9)	N1—C12—C11	123.4 (3)
O2—K1—N5	69.09 (9)	N1—C12—C13	118.3 (2)
O6^{i}—K1—N4	100.86 (10)	C11—C12—C13	118.2 (3)
O3^{ii}—K1—N4	65.38 (8)	O3—C13—N3	125.2 (3)
O5—K1—N4	74.58 (8)	O3—C13—C12	119.8 (3)
O2—K1—N4	146.57 (9)	N3—C13—C12	114.9 (3)
N5—K1—N4	129.49 (11)	C15—C14—C19	120.1 (3)
C1—O1—H1O	109.5	C15—C14—N3	124.7 (3)
C7—O2—K1	155.1 (2)	C19—C14—N3	115.1 (3)
C13—O3—K1^{iii}	137.67 (19)	C14—C15—C16	120.0 (3)
C19—O4—H4O	109.5	C14—C15—H15	120
C20—O5—K1	125.27 (18)	C16—C15—H15	120
C20—O6—K1^{iv}	130.59 (19)	C17—C16—C15	120.4 (3)
C8—N1—C12	117.3 (3)	C17—C16—H16	119.8
C7—N2—C6	129.0 (3)	C15—C16—H16	119.8
C7—N2—H2N	115.5	C16—C17—C18	120.1 (3)
C6—N2—H2N	115.5	C16—C17—H17	120
C13—N3—C14	128.0 (3)	C18—C17—H17	120
C13—N3—H3N	116	C17—C18—C19	120.3 (3)
C14—N3—H3N	116	C17—C18—H18	119.8
C22—N4—K1	145.3 (4)	C19—C18—H18	119.8
C24—N5—K1	108.0 (3)	O4—C19—C18	124.5 (3)
O1—C1—C2	124.0 (3)	O4—C19—C14	116.4 (3)
O1—C1—C6	116.3 (3)	C18—C19—C14	119.2 (3)
C2—C1—C6	119.8 (3)	O6—C20—O5	124.1 (3)
C3—C2—C1	119.9 (3)	O6—C20—C21	118.3 (3)
C3—C2—H2	120	O5—C20—C21	117.6 (3)
C1—C2—H2	120	C20—C21—H21A	109.5
C4—C3—C2	120.2 (3)	C20—C21—H21B	109.5
C4—C3—H3	119.9	H21A—C21—H21B	109.5
C2—C3—H3	119.9	C20—C21—H21C	109.5
C5—C4—C3	121.0 (3)	H21A—C21—H21C	109.5
C5—C4—H4	119.5	H21B—C21—H21C	109.5
C3—C4—H4	119.5	N4—C22—C23	178.6 (5)
C4—C5—C6	119.2 (3)	C22—C23—H23A	109.5
C4—C5—H5	120.4	C22—C23—H23B	109.5
C6—C5—H5	120.4	H23A—C23—H23B	109.5
C5—C6—C1	120.0 (3)	C22—C23—H23C	109.5
C5—C6—N2	124.6 (3)	H23A—C23—H23C	109.5
C1—C6—N2	115.4 (3)	H23B—C23—H23C	109.5
O2—C7—N2	125.3 (3)	N5—C24—C25	179.2 (5)
O2—C7—C8	120.1 (3)	C24—C25—H25A	109.5
N2—C7—C8	114.6 (3)	C24—C25—H25B	109.5
N1—C8—C9	123.0 (3)	H25A—C25—H25B	109.5
N1—C8—C7	118.2 (3)	C24—C25—H25C	109.5

C9—C8—C7	118.8 (3)	H25A—C25—H25C	109.5
C10—C9—C8	118.8 (3)	H25B—C25—H25C	109.5
O6^{i}—K1—O2—C7	−53.9 (5)	C12—N1—C8—C7	178.4 (2)
O3^{ii}—K1—O2—C7	61.1 (5)	O2—C7—C8—N1	−174.4 (3)
O5—K1—O2—C7	−163.2 (5)	N2—C7—C8—N1	3.6 (4)
N5—K1—O2—C7	160.1 (5)	O2—C7—C8—C9	4.3 (4)
N4—K1—O2—C7	29.0 (6)	N2—C7—C8—C9	−177.6 (3)
O6^{i}—K1—O5—C20	172.2 (2)	N1—C8—C9—C10	1.0 (5)
O3^{ii}—K1—O5—C20	29.7 (3)	C7—C8—C9—C10	−177.6 (3)
O2—K1—O5—C20	−95.6 (2)	C8—C9—C10—C11	−0.5 (5)
N5—K1—O5—C20	−60.7 (2)	C9—C10—C11—C12	−0.7 (5)
N4—K1—O5—C20	77.4 (2)	C8—N1—C12—C11	−0.9 (4)
O6^{i}—K1—N4—C22	25.3 (5)	C8—N1—C12—C13	177.1 (2)
O3^{ii}—K1—N4—C22	−84.7 (5)	C10—C11—C12—N1	1.4 (5)
O5—K1—N4—C22	139.4 (5)	C10—C11—C12—C13	−176.7 (3)
O2—K1—N4—C22	−49.0 (6)	K1^{iii}—O3—C13—N3	114.6 (3)
N5—K1—N4—C22	−163.2 (5)	K1^{iii}—O3—C13—C12	−67.2 (4)
O6^{i}—K1—N5—C24	79.2 (3)	C14—N3—C13—O3	8.1 (5)
O3^{ii}—K1—N5—C24	−153.9 (3)	C14—N3—C13—C12	−170.2 (3)
O5—K1—N5—C24	−33.4 (3)	N1—C12—C13—O3	−179.6 (3)
O2—K1—N5—C24	122.5 (3)	C11—C12—C13—O3	−1.4 (4)
N4—K1—N5—C24	−90.1 (3)	N1—C12—C13—N3	−1.2 (4)
O1—C1—C2—C3	177.9 (3)	C11—C12—C13—N3	177.0 (3)
C6—C1—C2—C3	−0.5 (4)	C13—N3—C14—C15	2.1 (5)
C1—C2—C3—C4	0.1 (5)	C13—N3—C14—C19	179.9 (3)
C2—C3—C4—C5	0.4 (5)	C19—C14—C15—C16	−0.3 (5)
C3—C4—C5—C6	−0.3 (5)	N3—C14—C15—C16	177.4 (3)
C4—C5—C6—C1	−0.2 (4)	C14—C15—C16—C17	0.6 (5)
C4—C5—C6—N2	178.7 (3)	C15—C16—C17—C18	0.0 (5)
O1—C1—C6—C5	−177.9 (3)	C16—C17—C18—C19	−0.8 (5)
C2—C1—C6—C5	0.6 (4)	C17—C18—C19—O4	−179.6 (3)
O1—C1—C6—N2	3.1 (4)	C17—C18—C19—C14	1.0 (5)
C2—C1—C6—N2	−178.4 (3)	C15—C14—C19—O4	−179.9 (3)
C7—N2—C6—C5	−2.6 (5)	N3—C14—C19—O4	2.2 (4)
C7—N2—C6—C1	176.3 (3)	C15—C14—C19—C18	−0.5 (4)
K1—O2—C7—N2	151.0 (4)	N3—C14—C19—C18	−178.4 (3)
K1—O2—C7—C8	−31.2 (7)	K1^{iv}—O6—C20—O5	142.5 (2)
C6—N2—C7—O2	0.7 (5)	K1^{iv}—O6—C20—C21	−37.9 (4)
C6—N2—C7—C8	−177.3 (3)	K1—O5—C20—O6	156.2 (2)
C12—N1—C8—C9	−0.3 (4)	K1—O5—C20—C21	−23.4 (4)

Symmetry codes: (i) $x-1/2, y, -z+1/2$; (ii) $x+1/2, -y+3/2, -z+1$; (iii) $x-1/2, -y+3/2, -z+1$; (iv) $x+1/2, y, -z+1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*O*···O6^{v}	0.84	1.8	2.638 (3)	174

O1—H1*O*···O5^{v}	0.84	1.78	2.618 (3)	175

Symmetry code: (v) −*x*+1/2, −*y*+1, *z*+1/2.