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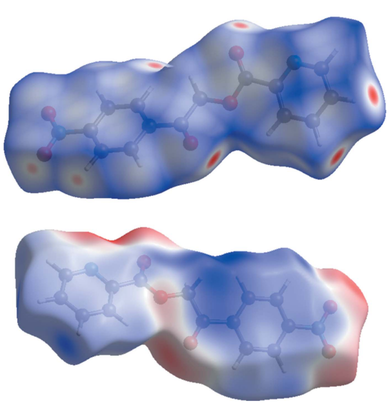
Crystal structure and Hirshfeld surface analysis of 2-(4-nitrophenyl)-2-oxoethyl picolinate

T. N. Sanjeeva Murthy,[a] C. S. Chidan Kumar,[b] S. Naveen,[c]* M. K. Veeraiah,[d] Kakarla Raghava Reddy[e] and Ismail Warad[f]*

[a]Department of Chemistry, Sri Siddhartha Academy of Higher Education, Tumkur 572 107, Karnataka, India, [b]Department of Chemistry, Vidya Vikas Institute of Engineering & Technology, Visvesvaraya Technological University, Alanahally, Mysuru 570 028, India, [c]Department of Physics, School of Engineering and Technology, Jain University, Bangalore 562 112, India, [d]Department of Chemistry, Sri Siddhartha Institute of Technology, Tumkur 572 105, Karnataka, India, [e]School of Chemical & Biomolecular Engineering, The University of Sydney, Sydney, NSW, Australia, and [f]Department of Chemistry, Science College, An-Najah National University, PO Box 7, Nablus, West Bank, Palestinian Territories. *Correspondence e-mail: s.naveen@jainuniversity.ac.in, khalil.i@najah.edu

2-(4-Nitrophenyl)-2-oxoethyl picolinate, $C_{14}H_{10}N_2O_5$, was synthesized under mild conditions. The chemical and molecular structures were confirmed by single-crystal X-ray diffraction analysis. The molecules are linked by inversion into centrosymmetric dimers *via* weak intermolecular C—H···O interactions, forming $R_2^2(10)$ ring motifs, and further strengthened by weak π–π interactions. Hirshfeld surface analyses, the d_{norm} surfaces, electrostatic potential and two-dimensional fingerprint (FP) plots were used to verify the contributions of the different intermolecular interactions within the supramolecular structure. The shape-index surface shows that two sides of the molecules are involved with the same contacts in neighbouring molecules and curvedness plots show flat surface patches that are characteristic of planar stacking.



1. Chemical context

Derivatives of phenacyl bromide have found significant application in the identification of organic acids (Rather & Reid, 1919). In organic chemistry, phenacyl benzoate is a derivative of an acid, formed by reaction between an acid and phenacyl bromide. The syntheses of phenacyl esters have many advantages in organic chemistry because they are usually solids and provide a useful means of characterizing acids and phenols. Phenacyl esters are useful for the photoremoval of protecting groups for carboxylic acids in organic synthesis and biochemistry. These compounds can be photolysed under neutral and mild conditions (Sheehan *et al.*, 1973; Ruzicka *et al.*, 2002; Literák *et al.*, 2006). They also find application in the field of synthetic chemistry, such as in the synthesis of oxazoles and imidazoles (Huang *et al.*, 1996), as well as with benzoxazepine (Gandhi *et al.*, 1995). In continuation of our work on the synthesis of these ester derivaties (Kumar *et al.*, 2014), we report herein the crystal and molecular structures of 2-(4-nitrophenyl)-2-oxoethyl picolinate.

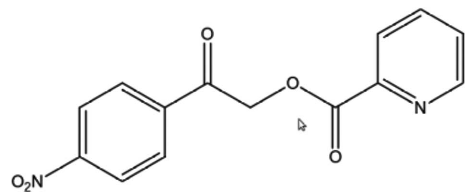


Table 1
Selected geometric parameters (Å, °).

O1—C8	1.4329 (17)	O5—N1	1.211 (2)
O1—C9	1.3374 (16)	N1—C3	1.4761 (19)
O2—C7	1.2021 (18)	N2—C10	1.3372 (18)
O3—C9	1.1969 (17)	N2—C11	1.339 (2)
O4—N1	1.205 (2)		
C8—O1—C9	116.39 (10)	O2—C7—C8	121.71 (13)
O4—N1—O5	123.38 (16)	O1—C8—C7	108.11 (11)
O4—N1—C3	118.83 (14)	O1—C9—O3	123.96 (13)
O5—N1—C3	117.79 (15)	O1—C9—C10	111.08 (11)
C10—N2—C11	115.93 (13)	O3—C9—C10	124.96 (12)
N1—C3—C2	118.29 (14)	N2—C10—C9	114.56 (12)
N1—C3—C4	118.83 (13)	N2—C10—C14	124.07 (13)
O2—C7—C6	120.57 (13)	N2—C11—C12	123.99 (16)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the pyridine and nitrophenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···O3[i]	0.93	2.55	3.2283 (18)	130
C8—H8*B*···O3[i]	0.97	2.45	3.2681 (17)	141
C12—H12*A*···O5[ii]	0.93	2.52	3.396 (3)	157
C13—H13*A*···O2[iii]	0.93	2.47	3.277 (2)	146
C9—O3···*Cg*1		3.35 (1)	3.4735 (16)	86 (1)
C7—O2···*Cg*2		3.58 (1)	3.8788 (15)	67 (1)
N1—O4···*Cg*2		3.76 (1)	3.5479 (16)	71 (1)
N1—O5···*Cg*2		3.68 (1)	3.5479 (16)	74 (1)

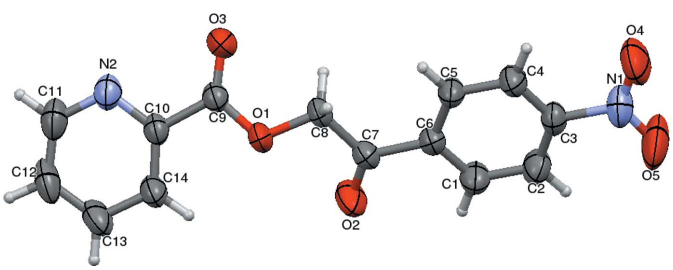


Figure 1
The molecular structure of the title compound, indicating the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1, and bond lengths and angles are listed in Table 1. The compound is composed of two aromatic rings (4-nitrophenyl and pyridine) linked by C—C(=O)—O—C(=O) bonds forming a bridge. The unique molecular conformation of this compound is characterized by three torsion angles, *viz.* τ_1 (N2—C10—C9—O3), τ_2 (C7—C8—O1—C9) and τ_3 (O2—C7—C6—C1), whereby τ_1 [−6.1 (2)°] signifies the apparent coplanarity of the mean planes of the pyridine and adjacent carbonyl rings at the connecting bridge. The torsion angle value of τ_2 = −147.02 (11)° between the two carbonyl groups indicates a *–anticlinal* conformation. Likewise, owing to a substitution on the functional group, the title compound experiences steric repulsion between the substituent and adjacent carbonyl groups, which can influence the torsion angle [τ_3 = 2.4 (2)%] and resulting in a *+synclinal* conformation. The bond lengths and angles are normal and the molecular conformation is characterized by a dihedral angle of 31.58 (8)° between the mean planes of the two aromatic rings. The nitro group lies nearly in the plane of the phenyl ring, as indicated by the torsion angle values of −4.7 (2) and −5.1 (2)° for C4—C3—N1—O4 and C2—C3—N1—O5, respectively.

3. Supramolecular features

There are no classical hydrogen bonds in the structure. However, the structure is consolidated by weak C—H···O intermolecular interactions. Specifically, singular weak intermolecular C8—H8*B*···O3(−*x*, −*y*, −*z*) interactions stabilize the supramolecular architecture by forming $R_2^2(10)$ ring motifs and chains along [011] (Fig. 2). The molecular structure is also stabilized by weak intermolecular C—O···*Cg*, N—O···*Cg*

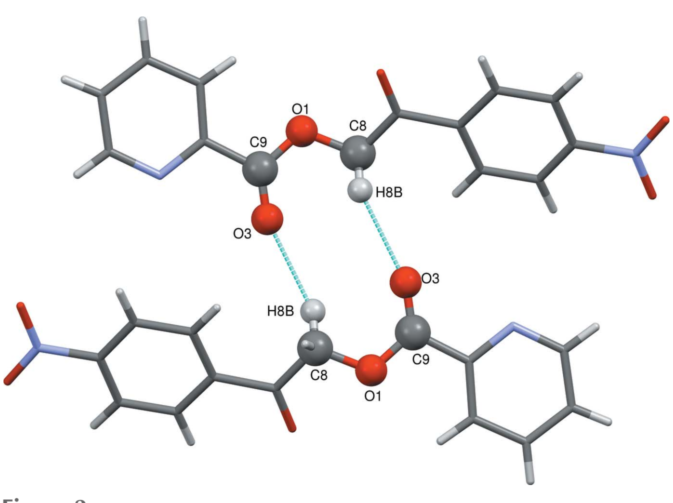


Figure 2
A view of two molecules of the title compound linked by inversion into centrosymmetric dimers by weak C8—H8*B*···O3 intermolecular interactions forming an $R_2^2(10)$ ring motif. **[See Note 1]**

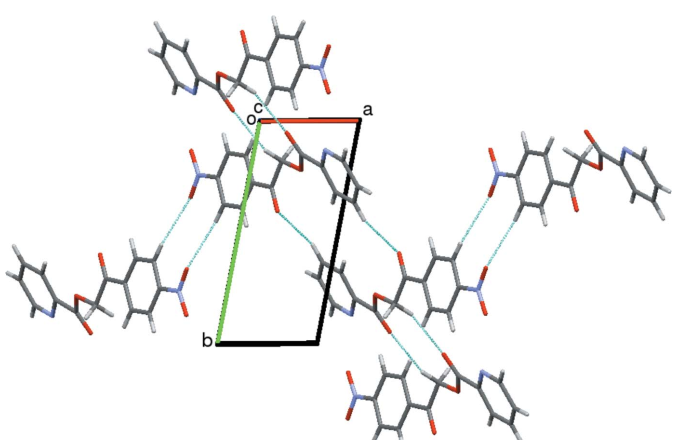


Figure 3
The packing of molecules of the title compound in the *ab* plane, viewed along the *c* axis. Cyan dashed lines indicate weak intermolecular C—H···O interactions forming $R_2^2(10)$ ring motifs.

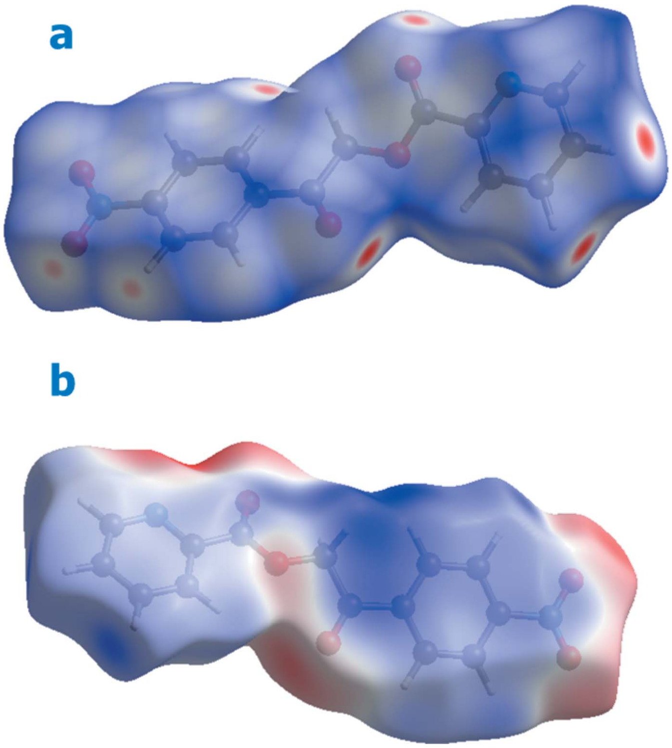


Figure 4
A view of the three-dimensional Hirshfeld surface of the title compound mapped over $d_{\rm norm}$.

and $Cg\cdots Cg$ interactions. The hydrogen-bond geometry and lone pair-π interactions are listed in Table 2. The molecule also exhibits $Cg\cdots Cg$ interactions, *i.e.* $Cg1\cdots Cg1$ [$Cg1$ is the centroid of the N2/C10/C14–C11 ring; $Cg\cdots Cg$ distance = 4.6293 (10) Å, α = 0°, β = 42.1°, the perpendicular distance of $Cg1$ on itself = 3.4332 (7) Å (symmetry code: $x - 1, y, z$)] and $Cg2\cdots Cg2$ [$Cg2$ is the centroid of the pyridine ring;; $Cg\cdots Cg$ distance = 4.6292 (10) Å, α = 0°, β = 40.3°, γ = 40.3° and the perpendicular distance of $Cg2$ on itself = 3.5322 (6) Å (symmetry code: $x + 1, y, z$)]. These weak intermolecular interactions link the molecules to form a one-dimensional chain along the c axis and the molecules exhibit layered stacking (Fig. 3).

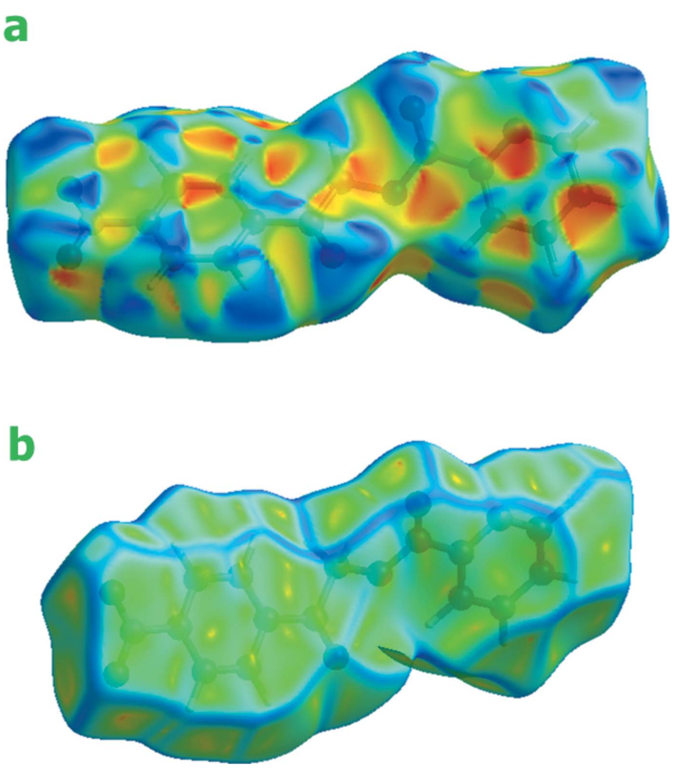


Figure 5
Hirshfeld surface of the title compound mapped with shape-index and curvedness.

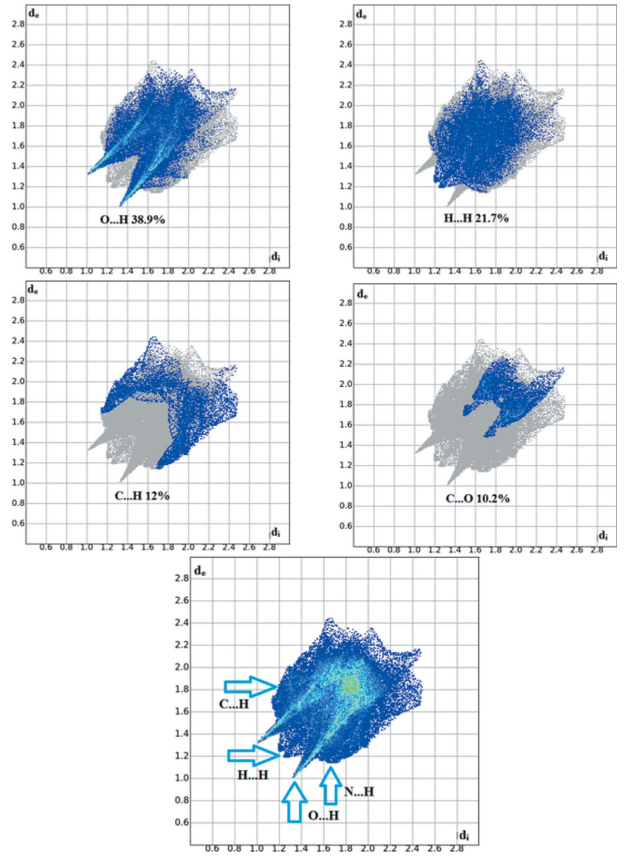


Figure 6
Two-dimensional fingerprint plots of the title compound, showing the percentage contributions of all interactions, and the individual types of interactions.

4. Hirshfeld surface analysis

Hirshfeld surfaces and fingerprint plots (McKinnon *et al.*, 2007) were generated for the title compound based on the crystallographic information file (CIF) using *CrystalExplorer* (Wolff *et al.*, 2012). Hirshfeld surfaces enable the visualization of intermolecular interactions by different colours and colour intensity, representing short or long contacts and indicating the relative strengths of the interactions. Figs. 4 and 5 show the Hirshfeld surfaces mapped over $d_{\rm norm}$ (−0.196 to 1.128 a.u.) and shape-index (−1.0 to 1.0 a.u.), respectively. The calculated volume inside the Hirshfeld surface is 311.97 Å^3 in the area of 305.78 Å^3.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{10}N_2O_5$
M_r	286.24
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	297
a, *b*, *c* (Å)	4.6292 (4), 10.6563 (9), 13.3592 (11)
α, β, γ (°)	99.136 (1), 93.426 (1), 100.556 (1)
V (Å^3)	636.95 (9)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.12
Crystal size (mm)	0.41 × 0.27 × 0.16
Data collection	
Diffractometer	Bruker APEXII DUO CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.953, 0.981
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21701, 3496, 2571
R_{int}	0.022
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.690
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.136, 1.07
No. of reflections	3496
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.19

Computer programs: *APEX2* (Bruker, 2012), *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXL2015* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

In Fig. 4, the dark spots near the C and O atoms result from C—H⋯O interactions, which play a significant role in the molecular packing of the title compound. The Hirshfeld surfaces illustrated in Fig. 4 also reflect the involvement of different atoms in the intermolecular interactions through the appearance of blue and red regions around the participating atoms, which correspond to positive and negative electrostatic potential, respectively. The shape-index surface clearly shows that the two sides of the molecules are involved in the same contacts with neighbouring molecules and the curvedness plots show flat surface patches characteristic of planar stacking.

The overall two-dimensional fingerprint plot for the title compound and those delineated into O⋯H/H⋯H, H⋯H, C⋯H/H⋯C, C⋯O/O⋯C and N⋯H/H⋯N contacts are illustrated in Fig. 6; the percentage contributions from the different interatomic contacts to the Hirshfeld surfaces are as follows: O—H 38.9%, H—H 21.7%, C—H12%, C—O 10.2% and N—H 8.2%, as shown in the two-dimensional fingerprint plots, respectively, in Fig. 6. The percentage contributions for the other intermolecular contacts are less than 5% in the Hirshfeld surface mapping.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.40, last update May 2019; Groom *et al.*, 2016) using 2-oxo-2-phenylethyl benzoate as the main skeleton revealed the presence of a number structures containing a moiety similar to the title compound, but with different substituents on the terminal phenyl rings. These include the following: 2-oxo-2-phenylethyl benzoate, 2-(4-bromophenyl)-2-oxoethyl 4-methoxybenzoate, 2-(4-bromophenyl)-2-oxoethyl 4-chlorobenzoate, 2-(4-bromophenyl)-2-oxoethyl 4-bromobenzoate, 2-(4-chlorophenyl)-2-oxoethyl 2-methoxybenzoate, 2-(4-bromophenyl)-2-oxoethyl 2-methoxybenzoate, 2-(4-chlorophenyl)-2-oxoethyl 2,4-difluoro-benzoate, 2-(4-chlorophenyl)-2-oxoethyl 2,4-difluorobenzoate, 2-(4-chlorophenyl)-2-oxoethyl benzoate, 2-(4-chlorophenyl)-2-oxoethyl 4-hydroxybenzoate, 2-(4-bromophenyl)-2-oxoethyl 2-methylbenzoate, 2-(4-chlorophenyl)-2-oxoethyl 4-methylbenzoate, 2-(4-bromophenyl)-2-oxoethyl 4-hydroxybenzoate, 2-(4-bromophenyl)-2-oxoethyl 4-methylbenzoate, 2-(2,4-dichlorophenyl)-2-oxoethyl 4-methoxybenzoate, 2-(4-fluorophenyl)-2-oxoethyl 4-methoxybenzoate and 2-(4-chlorophenyl)-2-oxoethyl 3,4-dimethoxybenzoate (Fun *et al.*, 2011*a*,*b*,*c*,*d*,*e*,*f*,*g*,*h*,*i*,*j*,*k*,*l*,*m*,*n*,*o*), 2-(4-fluorophenyl)-2-oxoethyl 2-methoxybenzoate (Isloor *et al.*, 2012), 1-(4-bromophenyl)-2-(2-chlorophenoxy)ethanone (Shenvi *et al.*, 2012) and 2,4-dichlorobenzyl 2-methoxybenzoate (Isloor *et al.*, 2013). In these 19 compounds, the dihedral angles between the phenyl rings are in the range 3.2 (2)–85.92 (10)°. The difference may arise from the weak intermolecular interactions between adjacent molecules (Fig. 7).

6. Synthesis and crystallization

The title compound was synthesized as per the procedure of Kumar *et al.* (2014). A mixture of 2-bromo-1-(4-nitrophenyl)ethanone (0.2 g, 0.5 mmol), potassium carbonate (0.087 g, 0.63 mmol) and nicotinic acid (0.079 g, 0.65 mmol) in dimethylformamide (5 ml) was stirred at room temperature for 5 h. After completion of the reaction, the reaction mixture was poured into ice-cold water. The solid product obtained was filtered off, washed with water and recrystallized from ethanol [m.p. 407–410 K, determined with a Stuart Scientific (UK) apparatus].

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms on C atoms were positioned geometrically (C—H = 0.95–0.99 Å) and refined using a riding model, with $U_{iso}(H)$ = 1.2 or $1.5U_{eq}(C)$.

Acknowledgements

CSCK extends his appreciation to Vidya Vikas Research & Development Centre for the facilities and encouragement. NS thanks Jain University for sanctioning research grants under minor project.

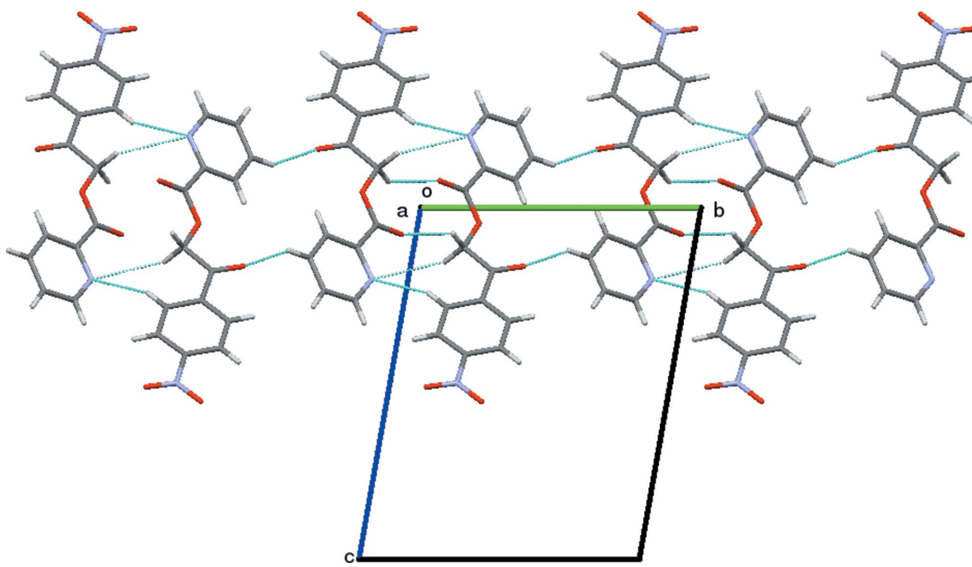


Figure 7
Packing of the molecules when viewed down along the *a* axis. The dashed lines represent C—H···O hydrogen bonds.

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supporting information

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Crystal structure and Hirshfeld surface analysis of 2-(4-nitrophenyl)-2-oxoethyl picolinate

T. N. Sanjeeva Murthy, C. S. Chidan Kumar, S. Naveen, M. K. Veeraiah, Kakarla Raghava Reddy and Ismail Warad

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXL2015* (Sheldrick, 2015) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2015* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

2-(4-Nitrophenyl)-2-oxoethyl picolinate

Crystal data

$C_{14}H_{10}N_2O_5$
M_r = 286.24
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 4.6292 (4) Å
b = 10.6563 (9) Å
c = 13.3592 (11) Å
α = 99.136 (1)°
β = 93.426 (1)°
γ = 100.556 (1)°
V = 636.95 (9) Å^3
Z = 2
F(000) = 296
D_x = 1.492 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2571 reflections
θ = 1.6–29.4°
μ = 0.12 mm^{-1}
T = 297 K
Rectangle, white
0.41 × 0.27 × 0.16 mm

Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
T_{min} = 0.953, T_{max} = 0.981
21701 measured reflections
3496 independent reflections
2571 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 29.4°, θ_{min} = 1.6°
h = −6→6
k = −14→14
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.136
S = 1.07
3496 reflections
190 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.1188P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of F^2 > 2sigma(F^2) is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5089 (2)	0.21852 (9)	0.04455 (7)	0.0528 (3)
O2	0.3481 (3)	0.40340 (11)	0.16679 (10)	0.0824 (5)
O3	0.2932 (2)	0.05168 (10)	−0.07629 (8)	0.0578 (3)
O4	−0.6315 (3)	0.13249 (15)	0.50999 (11)	0.0961 (6)
O5	−0.5484 (4)	0.33778 (16)	0.55148 (12)	0.1149 (7)
N1	−0.5128 (3)	0.23923 (15)	0.49895 (10)	0.0653 (5)
N2	0.7107 (3)	0.12934 (12)	−0.20395 (9)	0.0563 (4)
C1	−0.0180 (4)	0.38578 (14)	0.32225 (12)	0.0581 (5)
C2	−0.2018 (4)	0.37345 (15)	0.39938 (12)	0.0614 (5)
C3	−0.3152 (3)	0.25177 (14)	0.41686 (10)	0.0493 (4)
C4	−0.2565 (3)	0.14168 (14)	0.36073 (11)	0.0547 (4)
C5	−0.0737 (3)	0.15511 (13)	0.28293 (11)	0.0512 (4)
C6	0.0465 (3)	0.27660 (12)	0.26370 (9)	0.0426 (3)
C7	0.2433 (3)	0.29607 (13)	0.17993 (10)	0.0466 (4)
C8	0.2962 (3)	0.17779 (13)	0.11235 (10)	0.0491 (4)
C9	0.4795 (3)	0.14691 (12)	−0.04857 (10)	0.0435 (4)
C10	0.7087 (3)	0.20214 (12)	−0.11282 (10)	0.0442 (4)
C11	0.9099 (4)	0.17721 (17)	−0.26372 (13)	0.0659 (6)
C12	1.1060 (4)	0.29307 (18)	−0.23613 (14)	0.0707 (6)
C13	1.1009 (4)	0.36515 (16)	−0.14264 (14)	0.0675 (5)
C14	0.8961 (3)	0.31902 (13)	−0.07891 (12)	0.0536 (4)
H1A	0.06280	0.46770	0.30960	0.0700*
H2A	−0.24750	0.44630	0.43860	0.0740*
H4A	−0.33680	0.06020	0.37440	0.0660*
H5A	−0.03160	0.08170	0.24340	0.0610*
H8A	0.36960	0.12060	0.15300	0.0590*
H8B	0.11330	0.13120	0.07380	0.0590*
H11A	0.91590	0.12910	−0.32780	0.0790*
H12A	1.24020	0.32180	−0.28060	0.0850*
H13A	1.23200	0.44370	−0.12200	0.0810*

H14A	0.88590	0.36610	−0.01480	0.0640*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0520 (5)	0.0536 (5)	0.0472 (5)	−0.0055 (4)	0.0231 (4)	0.0038 (4)
O2	0.1022 (9)	0.0475 (6)	0.0962 (9)	−0.0035 (6)	0.0567 (8)	0.0123 (6)
O3	0.0560 (6)	0.0544 (6)	0.0562 (6)	−0.0052 (4)	0.0168 (4)	0.0034 (4)
O4	0.1105 (11)	0.0952 (10)	0.0910 (10)	0.0128 (8)	0.0615 (9)	0.0306 (8)
O5	0.1705 (16)	0.0994 (11)	0.0930 (10)	0.0483 (11)	0.0884 (11)	0.0174 (9)
N1	0.0719 (8)	0.0818 (10)	0.0506 (7)	0.0243 (7)	0.0280 (6)	0.0176 (7)
N2	0.0651 (7)	0.0588 (7)	0.0479 (6)	0.0142 (6)	0.0207 (5)	0.0096 (5)
C1	0.0717 (9)	0.0420 (7)	0.0613 (9)	0.0079 (6)	0.0242 (7)	0.0080 (6)
C2	0.0757 (10)	0.0527 (8)	0.0587 (9)	0.0193 (7)	0.0263 (7)	0.0035 (7)
C3	0.0501 (7)	0.0608 (8)	0.0394 (6)	0.0129 (6)	0.0150 (5)	0.0098 (6)
C4	0.0638 (8)	0.0489 (7)	0.0510 (7)	0.0032 (6)	0.0225 (6)	0.0102 (6)
C5	0.0617 (8)	0.0416 (7)	0.0489 (7)	0.0045 (6)	0.0223 (6)	0.0035 (5)
C6	0.0424 (6)	0.0427 (6)	0.0412 (6)	0.0037 (5)	0.0103 (5)	0.0057 (5)
C7	0.0451 (6)	0.0453 (7)	0.0479 (7)	0.0010 (5)	0.0143 (5)	0.0089 (5)
C8	0.0500 (7)	0.0483 (7)	0.0478 (7)	0.0002 (5)	0.0222 (5)	0.0087 (5)
C9	0.0437 (6)	0.0432 (6)	0.0456 (7)	0.0082 (5)	0.0143 (5)	0.0102 (5)
C10	0.0461 (6)	0.0452 (6)	0.0455 (7)	0.0116 (5)	0.0175 (5)	0.0126 (5)
C11	0.0812 (11)	0.0742 (10)	0.0521 (8)	0.0272 (9)	0.0313 (8)	0.0170 (7)
C12	0.0771 (10)	0.0764 (11)	0.0763 (11)	0.0270 (9)	0.0479 (9)	0.0368 (9)
C13	0.0670 (9)	0.0548 (8)	0.0852 (11)	0.0043 (7)	0.0367 (8)	0.0236 (8)
C14	0.0573 (8)	0.0468 (7)	0.0581 (8)	0.0057 (6)	0.0256 (6)	0.0107 (6)

Geometric parameters (Å, º)

O1—C8	1.4329 (17)	C7—C8	1.4973 (19)
O1—C9	1.3374 (16)	C9—C10	1.4998 (19)
O2—C7	1.2021 (18)	C10—C14	1.3737 (19)
O3—C9	1.1969 (17)	C11—C12	1.375 (3)
O4—N1	1.205 (2)	C12—C13	1.362 (3)
O5—N1	1.211 (2)	C13—C14	1.387 (2)
N1—C3	1.4761 (19)	C1—H1A	0.9300
N2—C10	1.3372 (18)	C2—H2A	0.9300
N2—C11	1.339 (2)	C4—H4A	0.9300
C1—C2	1.382 (2)	C5—H5A	0.9300
C1—C6	1.386 (2)	C8—H8A	0.9700
C2—C3	1.369 (2)	C8—H8B	0.9700
C3—C4	1.369 (2)	C11—H11A	0.9300
C4—C5	1.387 (2)	C12—H12A	0.9300
C5—C6	1.3822 (19)	C13—H13A	0.9300
C6—C7	1.5006 (19)	C14—H14A	0.9300
C8—O1—C9	116.39 (10)	N2—C11—C12	123.99 (16)
O4—N1—O5	123.38 (16)	C11—C12—C13	119.00 (17)

O4—N1—C3	118.83 (14)	C12—C13—C14	118.62 (16)
O5—N1—C3	117.79 (15)	C10—C14—C13	118.39 (14)
C10—N2—C11	115.93 (13)	C2—C1—H1A	120.00
C2—C1—C6	120.27 (14)	C6—C1—H1A	120.00
C1—C2—C3	118.56 (14)	C1—C2—H2A	121.00
N1—C3—C2	118.29 (14)	C3—C2—H2A	121.00
N1—C3—C4	118.83 (13)	C3—C4—H4A	121.00
C2—C3—C4	122.88 (14)	C5—C4—H4A	121.00
C3—C4—C5	118.09 (13)	C4—C5—H5A	120.00
C4—C5—C6	120.56 (13)	C6—C5—H5A	120.00
C1—C6—C5	119.64 (13)	O1—C8—H8A	110.00
C1—C6—C7	117.81 (12)	O1—C8—H8B	110.00
C5—C6—C7	122.54 (12)	C7—C8—H8A	110.00
O2—C7—C6	120.57 (13)	C7—C8—H8B	110.00
O2—C7—C8	121.71 (13)	H8A—C8—H8B	108.00
C6—C7—C8	117.70 (12)	N2—C11—H11A	118.00
O1—C8—C7	108.11 (11)	C12—C11—H11A	118.00
O1—C9—O3	123.96 (13)	C11—C12—H12A	120.00
O1—C9—C10	111.08 (11)	C13—C12—H12A	121.00
O3—C9—C10	124.96 (12)	C12—C13—H13A	121.00
N2—C10—C9	114.56 (12)	C14—C13—H13A	121.00
N2—C10—C14	124.07 (13)	C10—C14—H14A	121.00
C9—C10—C14	121.36 (12)	C13—C14—H14A	121.00

C9—O1—C8—C7	−147.02 (11)	C4—C5—C6—C1	−0.5 (2)
C8—O1—C9—O3	−1.63 (19)	C4—C5—C6—C7	−179.49 (13)
C8—O1—C9—C10	178.12 (11)	C1—C6—C7—O2	2.4 (2)
O4—N1—C3—C2	174.45 (15)	C1—C6—C7—C8	−175.97 (13)
O4—N1—C3—C4	−4.7 (2)	C5—C6—C7—O2	−178.60 (14)
O5—N1—C3—C2	−5.1 (2)	C5—C6—C7—C8	3.1 (2)
O5—N1—C3—C4	175.83 (15)	O2—C7—C8—O1	6.80 (19)
C11—N2—C10—C9	178.95 (13)	C6—C7—C8—O1	−174.90 (11)
C11—N2—C10—C14	−0.4 (2)	O1—C9—C10—N2	174.17 (12)
C10—N2—C11—C12	0.4 (3)	O1—C9—C10—C14	−6.46 (18)
C6—C1—C2—C3	0.6 (3)	O3—C9—C10—N2	−6.1 (2)
C2—C1—C6—C5	−0.1 (2)	O3—C9—C10—C14	173.28 (14)
C2—C1—C6—C7	178.99 (15)	N2—C10—C14—C13	0.0 (2)
C1—C2—C3—N1	−179.64 (15)	C9—C10—C14—C13	−179.32 (14)
C1—C2—C3—C4	−0.6 (2)	N2—C11—C12—C13	−0.1 (3)
N1—C3—C4—C5	179.10 (13)	C11—C12—C13—C14	−0.4 (3)
C2—C3—C4—C5	0.0 (2)	C12—C13—C14—C10	0.4 (2)
C3—C4—C5—C6	0.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···O3^{i}	0.93	2.55	3.2283 (18)	130
C8—H8*B*···O3^{i}	0.97	2.45	3.2681 (17)	141

C12—H12*A*···O5^{ii}	0.93	2.52	3.396 (3)	157
C13—H13*A*···O2^{iii}	0.93	2.47	3.277 (2)	146
C9—O3···*Cg*1		3.35 (1)	3.4735 (16)	86 (1)
C7—O2···*Cg*2		3.58 (1)	3.8788 (15)	67 (1)
N1—O4···*Cg*2		3.76 (1)	3.5479 (16)	71 (1)
N1—O5···*Cg*2		3.68 (1)	3.5479 (16)	74 (1)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*+2, *y*, *z*−1; (iii) −*x*+2, −*y*+1, −*z*.