Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$C_{14}H_{10}N_2O$
M_r	222.24
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	8.099 (6), 6.847 (5), 19.748 (15)
β (°)	93.91 (3)
V (Å^3)	1092.6 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.14 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker *APEX3* CCD
Absorption correction	Multi-scan Bruker
T_{min}, T_{max}	0.661, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25043, 2033, 1214
R_{int}	0.094
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.118, 1.04
No. of reflections	2033
No. of parameters	155
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.14

Computer programs: *APEX3* (Bruker, 2013), *SAINT*(Bruker, 2013), Bruker *SAINT*, *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *Mercury* (Macrae, 2020), *WinGX* (Farrugia, 2012).

Acknowledgements

Funding information

References

Figure 1

supporting information

Title

Computing details

Data collection: *APEX3* (Bruker, 2013); cell refinement: *SAINT*(Bruker, 2013); data reduction: Bruker *SAINT*; program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *Mercury* (Macrae, 2020); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

(shelx)

Crystal data

$C_{14}H_{10}N_2O$
$M_r = 222.24$
Monoclinic, $P2_1/n$
$a = 8.099$ (6) Å
$b = 6.847$ (5) Å
$c = 19.748$ (15) Å
$\beta = 93.91$ (3)°
$V = 1092.6$ (14) Å^3
$Z = 4$
$F(000) = 464$
$D_x = 1.351$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2983 reflections
$\theta = 2.8$–19.8°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.14 × 0.11 × 0.10 mm

Data collection

Bruker APEX-3 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan Bruker
$T_{min} = 0.661$, $T_{max} = 0.745$
25043 measured reflections
2033 independent reflections
1214 reflections with $I > 2\sigma(I)$
$R_{int} = 0.094$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.8°$
$h = -9\rightarrow9$
$k = -8\rightarrow8$
$l = -23\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.118$
$S = 1.04$
2033 reflections
155 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.1539P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.034 (4)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6807 (3)	0.5124 (3)	0.41091 (10)	0.0512 (6)
C2	0.8423 (3)	0.4494 (4)	0.42817 (12)	0.0661 (7)
H2	0.9315	0.5300	0.4204	0.079*
C3	0.8688 (3)	0.2693 (4)	0.45640 (12)	0.0703 (7)
H3	0.9763	0.2281	0.4683	0.084*
C4	0.7365 (3)	0.1466 (4)	0.46761 (12)	0.0675 (7)
H4	0.7558	0.0242	0.4870	0.081*
C5	0.5763 (3)	0.2064 (3)	0.45006 (11)	0.0583 (6)
H5	0.4880	0.1241	0.4575	0.070*
C6	0.5469 (2)	0.3897 (3)	0.42117 (9)	0.0454 (5)
C7	0.3781 (3)	0.4511 (3)	0.39992 (10)	0.0469 (5)
C8	0.6424 (3)	0.6977 (4)	0.38067 (12)	0.0651 (7)
H8	0.7300	0.7835	0.3762	0.078*
C9	0.2122 (3)	0.7008 (3)	0.33438 (10)	0.0487 (6)
C10	0.1616 (3)	0.8906 (3)	0.34662 (11)	0.0600 (6)
H10	0.2211	0.9676	0.3785	0.072*
C11	0.0223 (3)	0.9642 (4)	0.31115 (13)	0.0692 (7)
H11	−0.0125	1.0910	0.3192	0.083*
C12	−0.0652 (3)	0.8498 (4)	0.26383 (13)	0.0702 (7)
H12	−0.1582	0.9001	0.2397	0.084*
C13	−0.0152 (3)	0.6610 (4)	0.25215 (11)	0.0661 (7)
H13	−0.0749	0.5843	0.2202	0.079*
C14	0.1232 (3)	0.5853 (3)	0.28764 (11)	0.0556 (6)
H14	0.1561	0.4575	0.2801	0.067*
N1	0.3660 (2)	0.6302 (2)	0.36662 (8)	0.0493 (5)
N2	0.4962 (3)	0.7574 (3)	0.35879 (10)	0.0638 (6)
O1	0.25364 (17)	0.3537 (2)	0.40891 (8)	0.0605 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0474 (14)	0.0591 (15)	0.0474 (13)	−0.0121 (12)	0.0068 (10)	−0.0084 (11)
C2	0.0456 (15)	0.093 (2)	0.0598 (16)	−0.0174 (14)	0.0046 (11)	−0.0128 (14)
C3	0.0496 (16)	0.096 (2)	0.0640 (17)	0.0057 (15)	−0.0047 (12)	−0.0123 (15)
C4	0.0604 (17)	0.0729 (17)	0.0681 (17)	0.0031 (14)	−0.0049 (13)	−0.0025 (13)
C5	0.0495 (15)	0.0619 (16)	0.0633 (15)	−0.0050 (12)	0.0010 (11)	0.0044 (12)
C6	0.0439 (13)	0.0527 (14)	0.0401 (12)	−0.0060 (11)	0.0069 (9)	−0.0058 (10)
C7	0.0474 (14)	0.0468 (14)	0.0474 (13)	−0.0055 (11)	0.0091 (10)	−0.0028 (10)
C8	0.0547 (17)	0.0679 (18)	0.0735 (17)	−0.0258 (13)	0.0092 (13)	−0.0046 (13)
C9	0.0512 (14)	0.0474 (14)	0.0484 (13)	−0.0034 (11)	0.0109 (11)	0.0016 (11)
C10	0.0709 (16)	0.0513 (16)	0.0588 (15)	−0.0003 (13)	0.0115 (12)	−0.0015 (11)
C11	0.0830 (19)	0.0564 (16)	0.0703 (17)	0.0162 (14)	0.0214 (15)	0.0063 (14)
C12	0.0688 (17)	0.082 (2)	0.0613 (17)	0.0136 (15)	0.0137 (13)	0.0124 (14)
C13	0.0647 (17)	0.0779 (18)	0.0554 (15)	−0.0023 (14)	0.0007 (13)	−0.0020 (13)
C14	0.0564 (15)	0.0544 (14)	0.0563 (14)	−0.0032 (12)	0.0063 (12)	−0.0031 (12)
N1	0.0469 (11)	0.0461 (11)	0.0553 (11)	−0.0104 (9)	0.0051 (9)	0.0022 (9)
N2	0.0626 (14)	0.0543 (12)	0.0751 (14)	−0.0207 (11)	0.0104 (11)	0.0030 (10)
O1	0.0422 (9)	0.0590 (10)	0.0809 (11)	−0.0118 (7)	0.0083 (8)	0.0125 (8)

Geometric parameters (Å, º)

C1—C6	1.397 (3)	C8—H8	0.9300
C1—C2	1.398 (3)	C9—C14	1.381 (3)
C1—C8	1.428 (3)	C9—C10	1.388 (3)
C2—C3	1.365 (3)	C9—N1	1.443 (3)
C2—H2	0.9300	C10—C11	1.382 (3)
C3—C4	1.391 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.378 (3)
C4—C5	1.382 (3)	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.379 (3)
C5—C6	1.393 (3)	C12—H12	0.9300
C5—H5	0.9300	C13—C14	1.381 (3)
C6—C7	1.464 (3)	C13—H13	0.9300
C7—O1	1.232 (2)	C14—H14	0.9300
C7—N1	1.392 (3)	N1—N2	1.384 (2)
C8—N2	1.298 (3)		
C6—C1—C2	120.1 (2)	C1—C8—H8	117.1
C6—C1—C8	116.5 (2)	C14—C9—C10	120.4 (2)
C2—C1—C8	123.3 (2)	C14—C9—N1	119.92 (19)
C3—C2—C1	119.8 (2)	C10—C9—N1	119.5 (2)
C3—C2—H2	120.1	C11—C10—C9	119.6 (2)
C1—C2—H2	120.1	C11—C10—H10	120.2
C2—C3—C4	120.6 (2)	C9—C10—H10	120.2
C2—C3—H3	119.7	C12—C11—C10	120.0 (2)
C4—C3—H3	119.7	C12—C11—H11	120.0
C5—C4—C3	120.1 (2)	C10—C11—H11	120.0
C5—C4—H4	119.9	C11—C12—C13	120.2 (2)
C3—C4—H4	119.9	C11—C12—H12	119.9
C4—C5—C6	120.1 (2)	C13—C12—H12	119.9
C4—C5—H5	120.0	C12—C13—C14	120.3 (2)
C6—C5—H5	120.0	C12—C13—H13	119.9
C5—C6—C1	119.3 (2)	C14—C13—H13	119.9
C5—C6—C7	120.42 (19)	C9—C14—C13	119.5 (2)
C1—C6—C7	120.3 (2)	C9—C14—H14	120.2
O1—C7—N1	120.88 (19)	C13—C14—H14	120.2
O1—C7—C6	124.1 (2)	N2—N1—C7	125.27 (18)
N1—C7—C6	115.01 (18)	N2—N1—C9	112.39 (17)
N2—C8—C1	125.9 (2)	C7—N1—C9	122.32 (17)
N2—C8—H8	117.1	C8—N2—N1	116.68 (19)
C6—C1—C2—C3	−1.4 (3)	N1—C9—C10—C11	174.20 (18)
C8—C1—C2—C3	−179.4 (2)	C9—C10—C11—C12	−0.2 (3)
C1—C2—C3—C4	0.6 (3)	C10—C11—C12—C13	0.7 (4)
C2—C3—C4—C5	0.1 (3)	C11—C12—C13—C14	−0.2 (3)
C3—C4—C5—C6	−0.1 (3)	C10—C9—C14—C13	1.1 (3)
C4—C5—C6—C1	−0.7 (3)	N1—C9—C14—C13	−173.71 (18)
C4—C5—C6—C7	177.55 (19)	C12—C13—C14—C9	−0.7 (3)
C2—C1—C6—C5	1.4 (3)	O1—C7—N1—N2	174.56 (18)
C8—C1—C6—C5	179.57 (19)	C6—C7—N1—N2	−6.7 (3)
C2—C1—C6—C7	−176.82 (18)	O1—C7—N1—C9	−7.2 (3)
C8—C1—C6—C7	1.4 (3)	C6—C7—N1—C9	171.59 (16)

C5—C6—C7—O1	3.9 (3)	C14—C9—N1—N2	125.3 (2)
C1—C6—C7—O1	−177.91 (19)	C10—C9—N1—N2	−49.6 (2)
C5—C6—C7—N1	−174.82 (18)	C14—C9—N1—C7	−53.2 (3)
C1—C6—C7—N1	3.4 (3)	C10—C9—N1—C7	131.9 (2)
C6—C1—C8—N2	−3.9 (3)	C1—C8—N2—N1	1.1 (3)
C2—C1—C8—N2	174.2 (2)	C7—N1—N2—C8	4.6 (3)
C14—C9—C10—C11	−0.7 (3)	C9—N1—N2—C8	−173.79 (18)