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N′-[(*E*)-4-Bromobenzylidene]pyrazine-2-carbohydrazide

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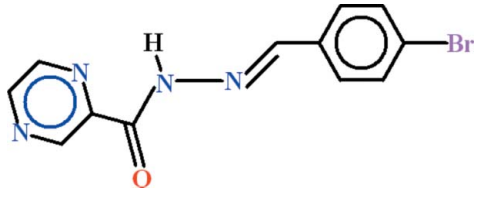
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.084; data-to-parameter ratio = 15.5.

In the title compound, $C_{12}H_9BrN_4O$, the *N*′-methylidenepyrazine-2-carbohydrazide and 4-bromobenzene groups are oriented at a dihedral angle of 10.57 (7)°. The hydrazide N—H group is involved in intramolecular N—H···N interaction, which generates an S(5) motif. A short C—H···O interaction is formed between the methylidene H atom and the carbonyl O atom. It connects molecules into chains extending along [100]. In addition, molecules are arranged into stacks extending along [010] *via* π–π interactions between pyrazine and benzene rings, with centroid–centroid distances of 3.837 (2) and 3.860 (2) Å.

Related literature

For a related crystal structure and related studies, see: Hearn & Cynamon (2004); Jin *et al.* (2006); Yuan *et al.* (2006). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{12}H_9BrN_4O$
M_r = 305.14
Triclinic, $P\overline{1}$
a = 5.8947 (9) Å
b = 7.6941 (12) Å
c = 14.029 (2) Å
α = 83.273 (7)°
β = 80.086 (7)°
γ = 72.440 (6)°
V = 596.11 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.44 mm^{-1}
T = 296 K
0.26 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.425, T_{max} = 0.503
7382 measured reflections
2529 independent reflections
1403 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.084
S = 0.94
2529 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.93	2.24	3.132 (4)	161
N3—H3A···N1	0.86	2.27	2.671 (3)	108

Symmetry code: (i) $x+1, y, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2580).

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supplementary materials

Acta Cryst. (2013). E**69**, o1141 [doi:10.1107/S1600536813016917]

N′-[(*E*)-4-Bromobenzylidene]pyrazine-2-carbohydrazide

Shahid Hameed, Mushtaq Ahmad, M. Nawaz Tahir, Muhammad Abdullah Shah and Hazoor Ahmad Shad

Comment

The title compound (Fig. 1) was prepared to study biological activities of hydrazone compounds (Hearn & Cynamon, 2004; Jin *et al.*, 2006).

Crystals of the earlier reported 4-chlorobenzaldehyde(pyrazine-2-carbonyl) hydrazone (Yuan *et al.*, 2006) are practically isostructural with the title compound.

In the title compound the N′-methylidenepyrazine-2-carbohydrazide (A) (C1–C6/N1–N4/O1) and 4-bromophenyl (B) (C7–C12/Br1) moieties are almost planar with r. m. s. deviations of 0.061 Å and 0.009 Å, respectively. The dihedral angle between A/B is 10.57 (7)°. There exists intramolecular N—H···.N hydrogen bond (Table 1, Fig. 2) forming *S*(5) motif (Bernstein *et al.*, 1995). The intermolecular hydrogen bonds of C—H···.O type (Table 1, Fig. 2) generate *C*(6) chains (Bernstein *et al.*, 1995) along the crystallographic *a*-axis. There exist *π*–*π* interactions with a distance of 3.838 (2) Å [*Cg*1—*Cg*2^{i} & *Cg*2— *Cg*1^{i}: i = -*x*, 2 - *y*, -*z*] and 3.860 (2) Å [*Cg*1—*Cg*2^{ii} & *Cg*2—*Cg*1^{ii}: ii = -*x*, 1 - *y*, -*z*], between the centroids of pyrazine (*Cg*1) and benzene (*Cg*2) rings.

Experimental

The title compound was prepared by the condensation of equimolar ratio of pyrazine-2-carbohydrazide (0.50 g, 3.6 mmol) and 4-bromobenzaldehyde (0.67 g, 3.6 mmol) in methanol by the reflux of 5 h. The resulting reaction mixture was allowed to cool over night. The precipitated solid was filtered, washed with petroleum ether and recrystalized from chloroform in petroleum ether and dried under reduced pressure over $CaCl_2$ to give white prisms. Rf: 0.40 (30% acetone in petroleum ether): Yield: 83%, soluble in chloroform; m.p. 546–547 K.

Refinement

The H atoms were positioned geometrically (N–H = 0.86 Å, C–H = 0.93 Å) and refined as riding on their carriers with U_{iso}(H) = xU_{eq}(C, N), where x = 1.2 for all H-atoms.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

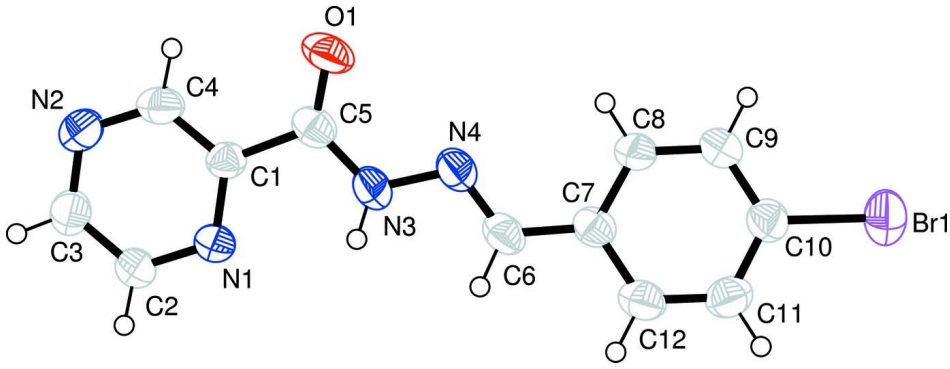

Figure 1

View of the title compound with the displacement ellipsoids drawn at the 50% probability level. H atoms are shown by small circles of arbitrary radii.

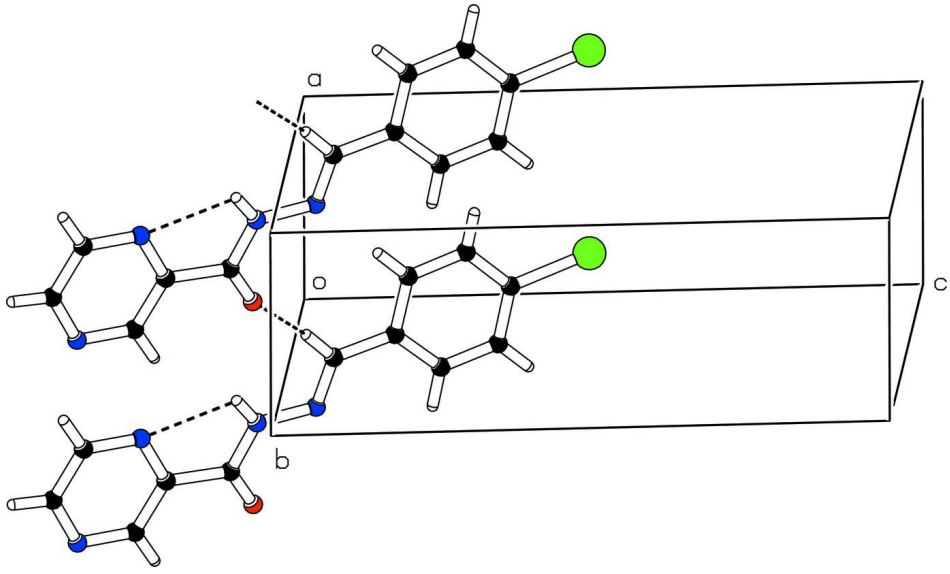

Figure 2

Packing diagram of the title compound showing *S*(5) motif and *C*(6) chains along [1 0 0].

N′-[(*E*)-4-Bromobenzylidene]pyrazine-2-carbohydrazide

Crystal data

$C_{12}H_9BrN_4O$
$M_r = 305.14$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.8947\ (9)$ Å
$b = 7.6941\ (12)$ Å
$c = 14.029\ (2)$ Å
$\alpha = 83.273\ (7)°$
$\beta = 80.086\ (7)°$
$\gamma = 72.440\ (6)°$
$V = 596.11\ (16)$ Å^3
$Z = 2$
$F(000) = 304$
$D_x = 1.700$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1403 reflections
$\theta = 2.1–25.5°$
$\mu = 3.44$ mm^{-1}
$T = 296$ K
Prism, white
0.26 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.425, T_{max} = 0.503
7382 measured reflections
2529 independent reflections
1403 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 27.1°, θ_{min} = 1.5°
h = −7→6
k = −9→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.084
S = 0.94
2529 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *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}
Br1	0.36405 (7)	0.25644 (5)	0.47485 (3)	0.07332 (19)
O1	−0.4594 (4)	0.8146 (3)	−0.03918 (16)	0.0633 (7)
N1	−0.0274 (4)	0.9547 (3)	−0.21291 (18)	0.0486 (7)
N2	−0.4307 (5)	1.1093 (4)	−0.3071 (2)	0.0599 (8)
N3	−0.0701 (5)	0.7949 (3)	−0.03380 (18)	0.0523 (7)
H3A	0.0565	0.8198	−0.0649	0.063*
N4	−0.0613 (5)	0.7038 (3)	0.05682 (19)	0.0508 (7)
C1	−0.2458 (5)	0.9456 (4)	−0.1727 (2)	0.0401 (8)
C2	−0.0148 (6)	1.0405 (4)	−0.3008 (2)	0.0538 (9)
H2	0.1337	1.0501	−0.3321	0.065*
C3	−0.2126 (6)	1.1151 (4)	−0.3467 (2)	0.0549 (9)
H3	−0.1927	1.1724	−0.4084	0.066*
C4	−0.4426 (6)	1.0230 (4)	−0.2191 (3)	0.0540 (9)
H4	−0.5918	1.0148	−0.1877	0.065*
C5	−0.2732 (6)	0.8455 (4)	−0.0745 (2)	0.0476 (8)
C6	0.1460 (6)	0.6511 (4)	0.0827 (2)	0.0496 (9)

H6	0.2748	0.6734	0.0398	0.060*
C7	0.1898 (6)	0.5575 (4)	0.1764 (2)	0.0449 (8)
C8	0.0083 (6)	0.5360 (4)	0.2494 (2)	0.0496 (8)
H8	−0.1509	0.5833	0.2386	0.060*
C9	0.0571 (6)	0.4466 (4)	0.3372 (2)	0.0524 (9)
H9	−0.0679	0.4339	0.3853	0.063*
C10	0.2919 (6)	0.3757 (4)	0.3537 (2)	0.0500 (8)
C11	0.4775 (6)	0.3941 (4)	0.2827 (2)	0.0555 (9)
H11	0.6361	0.3455	0.2939	0.067*
C12	0.4264 (6)	0.4854 (4)	0.1945 (2)	0.0543 (9)
H12	0.5516	0.4989	0.1467	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0815 (3)	0.0777 (3)	0.0601 (3)	−0.0224 (2)	−0.0225 (2)	0.01461 (19)
O1	0.0580 (15)	0.0762 (17)	0.0622 (15)	−0.0398 (13)	0.0071 (13)	0.0006 (12)
N1	0.0420 (16)	0.0576 (17)	0.0482 (17)	−0.0216 (13)	−0.0063 (13)	0.0069 (13)
N2	0.0479 (18)	0.070 (2)	0.064 (2)	−0.0208 (15)	−0.0186 (16)	0.0107 (15)
N3	0.0564 (19)	0.0604 (18)	0.0429 (16)	−0.0271 (14)	−0.0057 (15)	0.0106 (13)
N4	0.0555 (19)	0.0552 (17)	0.0433 (17)	−0.0238 (14)	−0.0035 (14)	0.0059 (13)
C1	0.0373 (19)	0.0392 (18)	0.0455 (19)	−0.0143 (15)	−0.0058 (16)	−0.0009 (14)
C2	0.048 (2)	0.066 (2)	0.050 (2)	−0.0259 (17)	−0.0076 (18)	0.0125 (17)
C3	0.057 (2)	0.061 (2)	0.051 (2)	−0.0225 (18)	−0.0159 (19)	0.0060 (17)
C4	0.041 (2)	0.062 (2)	0.062 (2)	−0.0221 (17)	−0.0034 (18)	−0.0014 (18)
C5	0.052 (2)	0.047 (2)	0.048 (2)	−0.0234 (17)	−0.0001 (18)	−0.0048 (16)
C6	0.055 (2)	0.053 (2)	0.045 (2)	−0.0293 (17)	−0.0008 (18)	0.0027 (16)
C7	0.048 (2)	0.0429 (18)	0.048 (2)	−0.0225 (15)	−0.0039 (17)	−0.0031 (15)
C8	0.0401 (19)	0.053 (2)	0.057 (2)	−0.0192 (16)	−0.0062 (17)	0.0068 (17)
C9	0.048 (2)	0.059 (2)	0.051 (2)	−0.0221 (17)	−0.0024 (18)	0.0051 (17)
C10	0.052 (2)	0.049 (2)	0.051 (2)	−0.0199 (16)	−0.0092 (18)	0.0019 (15)
C11	0.043 (2)	0.060 (2)	0.065 (2)	−0.0157 (17)	−0.0119 (19)	−0.0025 (18)
C12	0.048 (2)	0.064 (2)	0.054 (2)	−0.0247 (17)	0.0008 (18)	−0.0048 (18)

Geometric parameters (Å, º)

Br1—C10	1.886 (3)	C3—H3	0.9300
O1—C5	1.204 (3)	C4—H4	0.9300
N1—C2	1.329 (4)	C6—C7	1.447 (4)
N1—C1	1.332 (3)	C6—H6	0.9300
N2—C3	1.322 (4)	C7—C8	1.383 (4)
N2—C4	1.332 (4)	C7—C12	1.393 (4)
N3—C5	1.346 (4)	C8—C9	1.370 (4)
N3—N4	1.379 (3)	C8—H8	0.9300
N3—H3A	0.8600	C9—C10	1.376 (4)
N4—C6	1.268 (4)	C9—H9	0.9300
C1—C4	1.370 (4)	C10—C11	1.377 (4)
C1—C5	1.506 (4)	C11—C12	1.382 (4)
C2—C3	1.368 (4)	C11—H11	0.9300
C2—H2	0.9300	C12—H12	0.9300

C2—N1—C1	115.4 (3)	N4—C6—C7	122.5 (3)
C3—N2—C4	114.6 (3)	N4—C6—H6	118.7
C5—N3—N4	121.3 (3)	C7—C6—H6	118.7
C5—N3—H3A	119.4	C8—C7—C12	117.9 (3)
N4—N3—H3A	119.4	C8—C7—C6	123.3 (3)
C6—N4—N3	114.5 (3)	C12—C7—C6	118.7 (3)
N1—C1—C4	121.5 (3)	C9—C8—C7	121.6 (3)
N1—C1—C5	118.5 (3)	C9—C8—H8	119.2
C4—C1—C5	119.9 (3)	C7—C8—H8	119.2
N1—C2—C3	122.4 (3)	C8—C9—C10	119.7 (3)
N1—C2—H2	118.8	C8—C9—H9	120.2
C3—C2—H2	118.8	C10—C9—H9	120.2
N2—C3—C2	122.8 (3)	C9—C10—C11	120.4 (3)
N2—C3—H3	118.6	C9—C10—Br1	120.6 (3)
C2—C3—H3	118.6	C11—C10—Br1	119.0 (3)
N2—C4—C1	123.2 (3)	C10—C11—C12	119.5 (3)
N2—C4—H4	118.4	C10—C11—H11	120.2
C1—C4—H4	118.4	C12—C11—H11	120.2
O1—C5—N3	125.4 (3)	C11—C12—C7	120.9 (3)
O1—C5—C1	121.7 (3)	C11—C12—H12	119.6
N3—C5—C1	112.9 (3)	C7—C12—H12	119.6

C5—N3—N4—C6	174.4 (3)	C4—C1—C5—N3	−173.2 (3)
C2—N1—C1—C4	−1.1 (4)	N3—N4—C6—C7	178.3 (3)
C2—N1—C1—C5	178.2 (3)	N4—C6—C7—C8	−7.6 (5)
C1—N1—C2—C3	0.3 (5)	N4—C6—C7—C12	172.5 (3)
C4—N2—C3—C2	−0.7 (5)	C12—C7—C8—C9	−0.1 (5)
N1—C2—C3—N2	0.7 (5)	C6—C7—C8—C9	−180.0 (3)
C3—N2—C4—C1	−0.1 (5)	C7—C8—C9—C10	−0.1 (5)
N1—C1—C4—N2	1.0 (5)	C8—C9—C10—C11	0.0 (5)
C5—C1—C4—N2	−178.2 (3)	C8—C9—C10—Br1	178.7 (2)
N4—N3—C5—O1	−1.9 (5)	C9—C10—C11—C12	0.4 (5)
N4—N3—C5—C1	179.1 (2)	Br1—C10—C11—C12	−178.3 (2)
N1—C1—C5—O1	−171.5 (3)	C10—C11—C12—C7	−0.6 (5)
C4—C1—C5—O1	7.8 (5)	C8—C7—C12—C11	0.5 (5)
N1—C1—C5—N3	7.6 (4)	C6—C7—C12—C11	−179.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{i}	0.93	2.24	3.132 (4)	161
N3—H3*A*···N1	0.86	2.27	2.671 (3)	108

Symmetry code: (i) *x*+1, *y*, *z*.