IUCrData

ISSN 2414-3146

Received 1 August 2024
Accepted 2 September 2024

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

**Keywords:** crystal structure; hydrogen bonding; C—H···Br interaction; acetamide; carbamoyl group; carboxamide dimer.

**CCDC reference:** 2381424

**Structural data:** full structural data are available from iucrdata.iucr.org

# 2-Bromoacetamide

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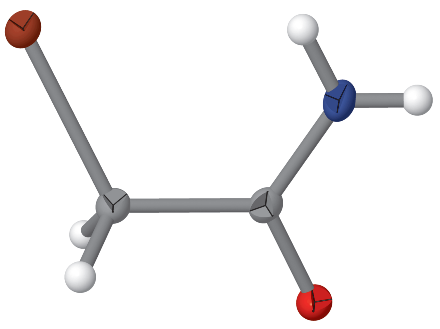
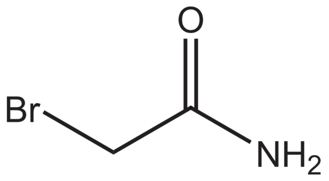
The title compound, $C_2H_4BrNO$, crystallizes in the monoclinic space group $P2_1/c$ with one molecule in the asymmetric unit. The almost planar molecules are organized *via* N—H···O hydrogen bonds into a ladder-type network, which can be characterized by the graph sets $R_2^2(8)$ and $R_4^2(8)$. In addition, the molecules are connected by C—H···O and C—H···Br contacts.



3D view



Chemical scheme

## Structure description

2-Bromoacetamide described here is isostructural to 2-chloroacetamide (Kalyanaraman *et al.*, 1978; Rheingold, 2021), but not to 2-fluoroacetamide (Hughes & Small, 1962; Jeffrey *et al.*, 1981).

The molecular structure of the title compound is almost planar, with the bromine atom lying only slightly out of the amide plane [distance = 0.374 (3) Å] and orientated in the opposite direction to the carbonyl oxygen atom (Fig. 1). This is reflected in the torsion angles (O1/N1)—C1—C2—Br1 with values of −166.7 (2) and 14.4 (4)°, respectively. Furthermore, an intramolecular N—H···Br contact of 2.69 (4) Å is observed. The crystal structure consists of layers that extend parallel to the (102) plane and are composed of centrosymmetric dimers of the title compound as the smallest supramolecular unit (Fig. 2). Within these dimers, the molecules are held together by N—H···O hydrogen bonds [N1—H2*N*···O1, 2.17 (5) Å; Table 1]. The resulting hydrogen-bonding motif, which can be described by the graph set $R_2^2(8)$ (Etter, 1990, 1991; Bernstein *et al.*, 1995), is characteristic of primary carboxamides (Leiserowitz & Schmidt, 1969; Leiserowitz & Hagler, 1983; Aakeröy *et al.*, 2007) and has been observed by us previously, *e.g.*, for formamide molecules contained in the crystal structure of a solvate of 1-{[2,6-bis(hydroxymethyl)-4-methylphenoxy]methyl}-3,5-bis{[(4,6-dimethylpyridin-2-yl)amino]methyl}-2,4,6-triethylbenzene (Stapf *et al.*, 2023). This motif is also found for isomorphous 2-chloroacetamide and in the structure of 2-fluoroacetamide. As in these, the dimers in the present structure are connected by N—H···O bonds to form a ladder-type network. Here, the carbonyl oxygen atom additionally interacts with the H1*N* atom of a neighbouring molecule [N1—H1*N*···O1, 2.29 (4) Å] and acts as a double acceptor for strong

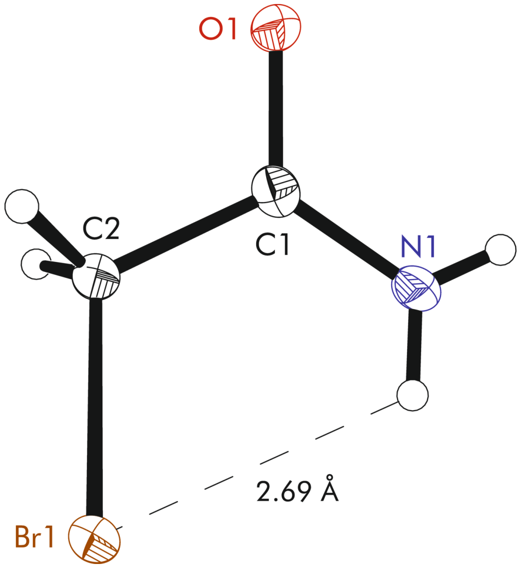


**Figure 1**
Molecular structure of the title compound including the numbering scheme. Atoms are drawn with displacement ellipsoids at the 50% probability level. The intramolecular N—H···Br contact is shown as dashed line.

hydrogen bonds. This forms a further motif of the graph set $R_4^2(8)$, as depicted in Fig. 2. The association of the dimers is supported by C—H···Br contacts [$d$(H···Br) = 2.98 Å], whereas the layers are only linked to each other *via* C—H···O interactions [$d$(H···O) = 2.55 Å, see Table 1].

## Synthesis and crystallization

2-Bromoacetamide was used as purchased from Fluka. Single crystals suitable for X-ray analysis were obtained by crystallization from petroleum ether (boiling range 313–333 K) according to a literature known procedure for purification of the title compound (Halpern & Maher, 1965). $^1$H NMR (500 MHz, DMSO-$d_6$, 298 K), δ: 3.81 (*s*, 2H, CH$_2$), 7.29 (*br*, 1H, NH), 7.66 (*br*, 1H, NH) p.p.m. $^{13}$C NMR (125 MHz, DMSO-$d_6$, 298 K), δ: 29.63 (CH$_2$), 167.92 (C═O) p.p.m. MS (ESI): *m*/*z* calcd. for $C_2H_4BrNONa$: 159.94 [$M$ + Na]$^+$, found 159.94.

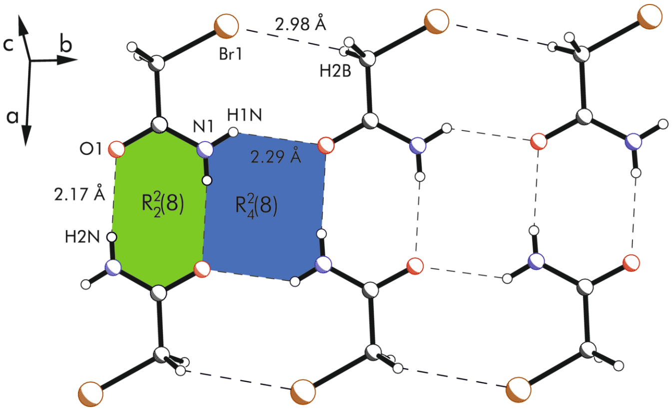


**Figure 2**
Excerpt of the crystal packing showing the $R_2^2(8)$ and $R_4^2(8)$ motifs of the N—H···O═C interactions, as well as the C—H···Br contact within one layer of amide molecules. These interactions are drawn as dashed lines.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···Br1 | 0.82 (4) | 2.69 (4) | 3.120 (3) | 115 (3) |
| N1—H1*N*···O1$^{i}$ | 0.82 (4) | 2.29 (4) | 2.955 (4) | 140 (4) |
| N1—H2*N*···O1$^{ii}$ | 0.75 (5) | 2.17 (5) | 2.915 (5) | 172 (5) |
| C2—H2*B*···Br1$^{iii}$ | 0.99 | 2.98 | 3.610 (3) | 122 |
| C2—H2*A*···O1$^{iv}$ | 0.99 | 2.55 | 3.462 (4) | 153 |

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $x, y-1, z$; (iv) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_2H_4BrNO$ |
| $M_r$ | 137.97 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 93 |
| *a*, *b*, *c* (Å) | 10.373 (4), 5.1899 (14), 7.557 (3) |
| β (°) | 99.94 (3) |
| *V* (Å$^3$) | 400.7 (3) |
| *Z* | 4 |
| Radiation type | Mo *K*α |
| μ (mm$^{-1}$) | 10.06 |
| Crystal size (mm) | 0.11 × 0.09 × 0.04 |
| | |
| Data collection | |
| Diffractometer | Stoe Stadivari |
| Absorption correction | Multi-scan [*X-RED32* (Stoe & Cie, 2023; Koziskova *et al.*, 2016)] |
| $T_{min}$, $T_{max}$ | 0.330, 0.668 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 4506, 879, 731 |
| $R_{int}$ | 0.036 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.638 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.028, 0.068, 1.04 |
| No. of reflections | 879 |
| No. of parameters | 52 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.58, −0.51 |

Computer programs: *X-AREA* (Stoe & Cie, 2023), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *XP* (Sheldrick, 2008), *WinGX* (Farrugia, 2012), *publCIF* (Westrip, 2010) and *ShelXle* (Hübschle *et al.*, 2011).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

The authors would like to thank Professor Dr Monika Mazik (Technische Universität Bergakademie Freiberg) for her general support.

## Funding information

Funding for this research was provided by: Open Access Funding by the Publication Fund of the TU Bergakademie Freiberg.

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# full crystallographic data

*IUCrData* (2024). **9**, x240863 [https://doi.org/10.1107/S2414314624008630]

## 2-Bromoacetamide

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### 2-Bromoacetamide

*Crystal data*

$C_2H_4BrNO$
$M_r = 137.97$
Monoclinic, $P2_1/c$
$a = 10.373$ (4) Å
$b = 5.1899$ (14) Å
$c = 7.557$ (3) Å
$\beta = 99.94$ (3)°
$V = 400.7$ (3) Å$^3$
$Z = 4$

$F(000) = 264$
$D_x = 2.287$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1778 reflections
$\theta = 1.7$–22.5°
$\mu = 10.06$ mm$^{-1}$
$T = 93$ K
Plate, colorless
0.11 × 0.09 × 0.04 mm

*Data collection*

Stoe Stadivari diffractometer
Radiation source: Primux 50 Mo
Graded multilayer mirror monochromator
Detector resolution: 5.81 pixels mm$^{-1}$
rotation method, $\omega$ scans
Absorption correction: multi-scan [X-Red32 (Stoe & Cie, 2023; Koziskova *et al.*, 2016]

$T_{\min} = 0.330$, $T_{\max} = 0.668$
4506 measured reflections
879 independent reflections
731 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 27.0°$, $\theta_{\min} = 2.0°$
$h = -13 \rightarrow 13$
$k = -6 \rightarrow 6$
$l = -9 \rightarrow 9$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.068$
$S = 1.04$
879 reflections
52 parameters
0 restraints
Primary atom site location: dual

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.0569P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.58$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.51$ e Å$^{-3}$

*Special details*

**Refinement**. The hydrogen atoms at N1 were located in a difference Fourier map and refined with free coordinates, and with the $U_{\rm iso}$(H) values fixed at 1.5 times the equivalent $U_{\rm eq}$ value of the parent nitrogen atom (N1). The H atoms at the methylene carbon atom (C2) were included using a riding model with C—H = 0.99 Å, and the $U_{\rm iso}$(H) values were fixed at 1.2 times the equivalent $U_{\rm eq}$ value of C2.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.61180 (3) | 0.82582 (6) | 0.68653 (4) | 0.01566 (15) |
| O1 | 0.8681 (3) | 0.2945 (4) | 0.5541 (3) | 0.0181 (6) |
| N1 | 0.8855 (3) | 0.7271 (6) | 0.5813 (4) | 0.0174 (7) |
| H1N | 0.854 (4) | 0.863 (7) | 0.608 (6) | 0.026* |
| H2N | 0.950 (5) | 0.735 (8) | 0.550 (6) | 0.026* |
| C1 | 0.8257 (3) | 0.5060 (7) | 0.5962 (4) | 0.0140 (7) |
| C2 | 0.6997 (3) | 0.4974 (6) | 0.6709 (5) | 0.0160 (7) |
| H2A | 0.718682 | 0.421332 | 0.792727 | 0.019* |
| H2B | 0.638276 | 0.380045 | 0.594915 | 0.019* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0141 (2) | 0.0146 (2) | 0.0191 (2) | 0.00213 (14) | 0.00526 (14) | 0.00064 (14) |
| O1 | 0.0169 (14) | 0.0129 (12) | 0.0260 (15) | 0.0002 (10) | 0.0078 (12) | −0.0005 (10) |
| N1 | 0.0135 (16) | 0.0153 (14) | 0.0251 (18) | 0.0008 (13) | 0.0081 (14) | −0.0024 (13) |
| C1 | 0.0114 (18) | 0.0167 (16) | 0.0135 (16) | 0.0029 (14) | 0.0013 (13) | 0.0034 (14) |
| C2 | 0.0147 (19) | 0.0128 (15) | 0.0216 (17) | 0.0012 (15) | 0.0063 (14) | 0.0006 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C2 | 1.946 (3) | N1—H2N | 0.75 (5) |
| O1—C1 | 1.244 (4) | C1—C2 | 1.512 (5) |
| N1—C1 | 1.318 (5) | C2—H2A | 0.9900 |
| N1—H1N | 0.82 (4) | C2—H2B | 0.9900 |
| | | | |
| C1—N1—H1N | 121 (3) | C1—C2—Br1 | 116.2 (2) |
| C1—N1—H2N | 122 (3) | C1—C2—H2A | 108.2 |
| H1N—N1—H2N | 117 (5) | Br1—C2—H2A | 108.2 |
| O1—C1—N1 | 123.7 (3) | C1—C2—H2B | 108.2 |
| O1—C1—C2 | 115.8 (3) | Br1—C2—H2B | 108.2 |
| N1—C1—C2 | 120.5 (3) | H2A—C2—H2B | 107.4 |
| | | | |
| O1—C1—C2—Br1 | −166.7 (2) | N1—C1—C2—Br1 | 14.4 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···Br1 | 0.82 (4) | 2.69 (4) | 3.120 (3) | 115 (3) |
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| C2—H2*A*···O1$^{iv}$ | 0.99 | 2.55 | 3.462 (4) | 153 |

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