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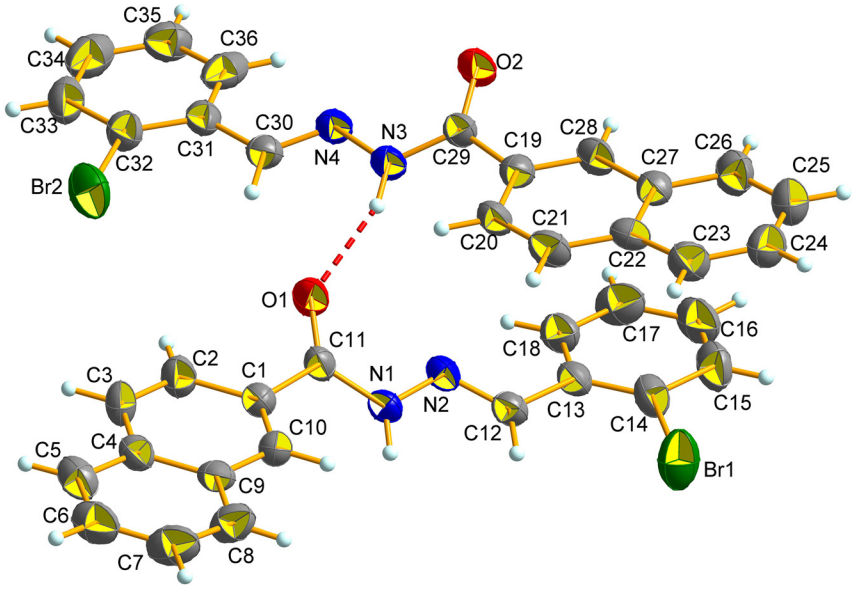
# The crystal structure of (*E*)-*N*′-(2-bromobenzylidene)-2-naphthohydrazide, $C_{36}H_{26}Br_2N_4O_2$

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**Abstract**

$C_{36}H_{26}Br_2N_4O_2$, triclinic, $P\bar{1}$ (no. 1), $a$ = 8.700(5) Å, $b$ = 9.188(5) Å, $c$ = 9.722(6) Å, $\alpha$ = 91.610(6)°, $\beta$ = 91.436(6)°, $\gamma$ = 100.925(6)°, $V$ = 762.4(8) Å$^3$, $Z$ = 1, $R_{gt}(F)$ = 0.0381, $wR_{ref}(F^2)$ = 0.1016, T = 296(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | block |
| Size: | 0.45 × 0.42 × 0.38 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 2.70 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 25.0°, 99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 7133, 5181, 0.021 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs}$ > 2 σ($I_{obs}$), 4577 |
| $N(param)_{refined}$: | 397 |
| Programs: | Bruker [1], SHELX [2, 3] |

## 1 Source of material

2-Naphthohydrazide (1.86 g, 10 mmol) and 2-bromobenzaldehyde (1.85 g, 10 mmol) were dissolved in ethanol (25 mL) and the mixture was refluxed for 6 h. The target compound (3.2 g, yield 91 %) was collected by filtration and washed with ethanol. The crystals of the product can be obtained by recrystallization in ethanol.

## 2 Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The $U_{iso}$ values of all hydrogen atoms were set to 1.2 $U_{eq}$(C).

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**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | −0.79202 (8) | −1.54403 (7) | 0.77589 (6) | 0.0770 (3) |
| Br2 | −0.18486 (7) | −0.84277 (7) | −0.03225 (7) | 0.0745 (3) |
| C1 | −0.6556 (6) | −0.9566 (6) | 0.2845 (5) | 0.0378 (11) |
| C2 | −0.5987 (7) | −0.8701 (7) | 0.1693 (6) | 0.0495 (13) |
| H2 | −0.517986 | −0.895443 | 0.118396 | 0.059* |
| C3 | −0.6616 (7) | −0.7522 (6) | 0.1343 (6) | 0.0484 (13) |
| H3A | −0.624865 | −0.699254 | 0.057831 | 0.058* |
| C4 | −0.7811 (6) | −0.7072 (6) | 0.2103 (6) | 0.0432 (12) |
| C5 | −0.8429 (8) | −0.5799 (7) | 0.1798 (7) | 0.0560 (15) |
| H5 | −0.807376 | −0.525094 | 0.104095 | 0.067* |
| C6 | −0.9528 (8) | −0.5363 (7) | 0.2587 (8) | 0.0634 (17) |
| H6 | −0.990912 | −0.451264 | 0.237722 | 0.076* |
| C7 | −1.0090 (8) | −0.6185 (9) | 0.3713 (10) | 0.068 (2) |
| H7 | −1.084797 | −0.587861 | 0.424926 | 0.081* |
| C8 | −0.9538 (7) | −0.7444 (8) | 0.4042 (8) | 0.0566 (17) |
| H8 | −0.993355 | −0.798479 | 0.479220 | 0.068* |
| C9 | −0.8383 (6) | −0.7919 (6) | 0.3256 (6) | 0.0409 (12) |
| C10 | −0.7725 (6) | −0.9160 (6) | 0.3587 (5) | 0.0400 (11) |
| H10 | −0.810048 | −0.971780 | 0.433307 | 0.048* |
| C11 | −0.5731 (6) | −1.0778 (6) | 0.3225 (5) | 0.0400 (11) |
| C12 | −0.6592 (6) | −1.4017 (6) | 0.5025 (6) | 0.0429 (12) |
| H12 | −0.757257 | −1.390810 | 0.532367 | 0.051* |
| C13 | −0.5897 (6) | −1.5263 (6) | 0.5472 (6) | 0.0440 (12) |
| C14 | −0.6355 (7) | −1.6003 (6) | 0.6648 (6) | 0.0484 (13) |
| C15 | −0.5680 (9) | −1.7179 (7) | 0.7099 (7) | 0.0646 (18) |
| H15 | −0.599391 | −1.764427 | 0.791012 | 0.078* |
| C16 | −0.4567 (9) | −1.7628 (7) | 0.6339 (9) | 0.070 (2) |
| H16 | −0.409836 | −1.839501 | 0.664276 | 0.084* |
| C17 | −0.4106 (8) | −1.6955 (7) | 0.5099 (9) | 0.0656 (18) |
| H17 | −0.336689 | −1.729448 | 0.456480 | 0.079* |
| C18 | −0.4764 (7) | −1.5787 (7) | 0.4687 (7) | 0.0541 (14) |
| H18 | −0.445407 | −1.533158 | 0.386994 | 0.065* |
| C19 | −0.2020 (6) | −1.2446 (6) | 0.6102 (5) | 0.0385 (11) |
| C20 | −0.3133 (6) | −1.1548 (6) | 0.6348 (6) | 0.0425 (12) |
| H20 | −0.331801 | −1.087876 | 0.569180 | 0.051* |
| C21 | −0.3947 (7) | −1.1643 (7) | 0.7538 (6) | 0.0497 (13) |
| H21 | −0.467896 | −1.103943 | 0.767701 | 0.060* |
| C22 | −0.3695 (6) | −1.2636 (6) | 0.8552 (5) | 0.0413 (12) |
| C23 | −0.4453 (7) | −1.2737 (8) | 0.9821 (6) | 0.0547 (15) |
| H23 | −0.515830 | −1.211885 | 1.000800 | 0.066* |
| C24 | −0.4176 (8) | −1.3719 (8) | 1.0779 (7) | 0.0611 (16) |
| H24 | −0.469143 | −1.376376 | 1.160709 | 0.073* |
| C25 | −0.3116 (8) | −1.4661 (8) | 1.0519 (7) | 0.0610 (16) |
| H25 | −0.294568 | −1.534530 | 1.116569 | 0.073* |
| C26 | −0.2334 (8) | −1.4573 (7) | 0.9314 (7) | 0.0569 (15) |
| H26 | −0.161094 | −1.518319 | 0.916208 | 0.068* |
| C27 | −0.2597 (6) | −1.3585 (6) | 0.8305 (5) | 0.0413 (12) |
| C28 | −0.1765 (6) | −1.3431 (6) | 0.7077 (6) | 0.0443 (12) |
| H28 | −0.101912 | −1.401611 | 0.692272 | 0.053* |
| C29 | −0.0993 (6) | −1.2299 (6) | 0.4889 (5) | 0.0385 (11) |
| C30 | −0.1080 (6) | −1.0898 (6) | 0.1637 (6) | 0.0438 (12) |
| H30 | −0.197078 | −1.048472 | 0.172455 | 0.053* |
| C31 | −0.0188 (6) | −1.0723 (6) | 0.0367 (5) | 0.0432 (12) |
| C32 | −0.0419 (7) | −0.9716 (6) | −0.0601 (6) | 0.0492 (13) |
| C33 | 0.0404 (9) | −0.9580 (8) | −0.1836 (7) | 0.0640 (18) |
| H33 | 0.023829 | −0.889162 | −0.247933 | 0.077* |
| C34 | 0.1452 (9) | −1.0492 (9) | −0.2057 (7) | 0.071 (2) |
| H34 | 0.200485 | −1.041208 | −0.286692 | 0.085* |
| C35 | 0.1717 (7) | −1.1517 (8) | −0.1130 (7) | 0.0600 (16) |
| H35 | 0.242625 | −1.213069 | −0.132250 | 0.072* |
| C36 | 0.0936 (7) | −1.1642 (8) | 0.0083 (6) | 0.0587 (16) |
| H36 | 0.113572 | −1.232229 | 0.072192 | 0.070* |
| N1 | −0.6579 (5) | −1.1953 (5) | 0.3830 (5) | 0.0428 (10) |
| H1 | −0.755881 | −1.199970 | 0.396825 | 0.051* |
| N2 | −0.5836 (5) | −1.3079 (5) | 0.4220 (5) | 0.0420 (11) |
| N3 | −0.1548 (5) | −1.1771 (5) | 0.3743 (5) | 0.0442 (10) |
| H3 | −0.245893 | −1.153536 | 0.371955 | 0.053* |
| N4 | −0.0626 (5) | −1.1616 (6) | 0.2605 (5) | 0.0417 (10) |
| O1 | −0.4329 (5) | −1.0680 (5) | 0.3012 (5) | 0.0556 (11) |
| O2 | 0.0330 (5) | −1.2610 (5) | 0.4952 (4) | 0.0511 (11) |

# 3 Comment

Hydrazones are important Schiff base ligands with a wide range of biological and pharmaceutical activities. Hydrazone compounds have been screened for antibacterial, anti-tuberculosis, anti-cancer and antioxidant behavior [4, 5]. The structure of hydrazone compounds has received the attention of scientists [6–8].

In the crystal, the two crystallographically independent molecules adopt an (*E*) configuration across the C=N bond, joining the hydrazide group and the benzene ring (see the figure). The dihedral angle between rings C1–C10 and C13–C18 is 5.015(17)° and between rings C19–C28 and C31–C36 is 1.858(12)°. The two crystallographically independent adjacent molecules are connected by hydrogen bonds, and the hydrogen bond length of O(1)···N(3)–H(1) is 2.05 Å and the hydrogen bond to the next dimer is 2.08 Å to form a chain structure. The bond lengths of C(1)–C(11), C(11)–O(1), C(11)–N(1), N(1)–N(2), N(2)–C(12), C(12)–C(13) and C(14)–Br(1) are 1.485(7), 1.228(7), 1.346(7), 1.377(6), 1.280(7), 1.463(7) and 1.897(6) respectively. The bond angles of C(11)–N(1)–N(2) and C(12)–N(2)–N(1) are 118.3(4)° and 115.8(4)°. The bond angles of C(1)–C(11)–N(1), C(1)–C(11)–O(1) and O(1)–C(11)–N(1) are 122.4(5)°, 120.6(5)° and 122.4(5)°. The geometric parameters in the second molecule are very similar and fit with the literature [9–11].

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