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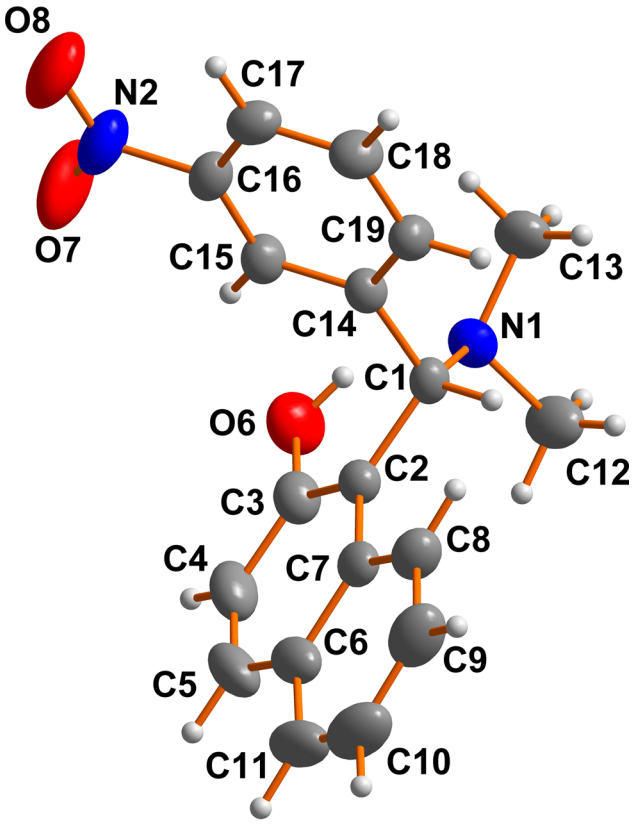
# The crystal structure of 1-((dimethylamino)(3-nitrophenyl)methyl) naphthalen-2-ol, $C_{19}H_{18}N_2O_3$

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**Abstract**

$C_{19}H_{18}N_2O_3$, orthorhombic, $P2_12_12_1$ (no. 19), $a$ = 9.5079(19) Å, $b$ = 18.423(4) Å, $c$ = 19.018(4) Å, $V$ = 3331.4(12) Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.0555, $wR_{ref}(F^2)$ = 0.1275, $T$ = 293 K.

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

| | |
|---|---|
| Crystal: | Colorless prism |
| Size: | 0.38 × 0.18 × 0.16 mm |
| Wavelength: | Mo $K\alpha$ radiation (0.71073 Å) |
| $\mu$: | 0.09 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker P4, $\omega$ |
| $\theta_{max}$, completeness: | 27.5°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 34,778, 4266, 0.090 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 2709 |
| $N(param)_{refined}$: | 439 |
| Programs: | CrystalClear [1], OLEX2 [2], SHELX [3, 4], Diamond [5] |

The molecular structure is shown in the Figure (only one of the two crystallographically independent molecules is shown). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

## Source of material

A dry 50 ml flask was charged with 3-nitrobenzaldehyde (10 mmol), naphthalen-2-ol (10 mmol), dimethylamine (10 mmol) (33% aq). The mixture was stirred at 100 °C for 10 h and then added ethanol (15 ml). After heated under reflux for 30 min, the precipitate was filtrated out and washed with ethanol for two to three times and purified by recrystallization from dichloromethane to give the target material. Crystals of the 1-((dimethylamino)(3-nitrophenyl) methyl)naphthalen-2-ol were obtained by slow evaporation from mixture of methanol and DMF.

## Experimental details

All hydrogen atoms were calculated geometrically and added with C–H distances ranging from 0.93 to 0.98 Å. $C_{aryl}$–H = 0.93 Å, with $U_{iso}$(H) = 1.2 $U_{eq}$(C). $C_{methyl}$–H = 0.96 Å, with $U_{iso}$(H) = 1.5 $U_{eq}$(C). O–H = 0.82 Å with $U_{iso}$(H) = 1.5 $U_{eq}$(O). The absolute structure cannot be established as no atom in the structure is heavier than silicon [6].

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1234 (3) | 0.42450 (17) | 0.52846 (17) | 0.0439 (8) |
| H1 | 0.1489 | 0.4722 | 0.5473 | 0.053* |
| C2 | −0.0195 (3) | 0.40450 (17) | 0.55787 (16) | 0.0452 (8) |
| C3 | −0.0580 (4) | 0.3330 (2) | 0.56804 (19) | 0.0579 (10) |
| C4 | −0.1884 (5) | 0.3145 (3) | 0.5957 (2) | 0.0717 (12) |
| H4 | −0.2126 | 0.2659 | 0.6010 | 0.086* |
| C5 | −0.2800 (4) | 0.3667 (3) | 0.6149 (2) | 0.0783 (13) |
| H5 | −0.3662 | 0.3534 | 0.6341 | 0.094* |
| C6 | −0.2483 (4) | 0.4414 (3) | 0.60663 (19) | 0.0662 (11) |
| C7 | −0.1171 (4) | 0.4602 (2) | 0.57655 (17) | 0.0512 (9) |
| C8 | −0.0900 (4) | 0.5352 (2) | 0.56584 (19) | 0.0612 (10) |
| H8 | −0.0067 | 0.5492 | 0.5441 | 0.073* |
| C9 | −0.1826 (6) | 0.5870 (3) | 0.5866 (2) | 0.0837 (14) |
| H9 | −0.1611 | 0.6357 | 0.5795 | 0.100* |
| C10 | −0.3083 (6) | 0.5683 (4) | 0.6182 (3) | 0.0979 (17) |
| H10 | −0.3703 | 0.6043 | 0.6327 | 0.117* |
| C11 | −0.3416 (5) | 0.4973 (4) | 0.6279 (2) | 0.0898 (16) |
| H11 | −0.4268 | 0.4852 | 0.6489 | 0.108* |
| C12 | 0.2565 (4) | 0.3815 (2) | 0.62771 (19) | 0.0739 (12) |
| H12A | 0.3242 | 0.3464 | 0.6434 | 0.111* |
| H12B | 0.1698 | 0.3747 | 0.6527 | 0.111* |
| H12C | 0.2915 | 0.4295 | 0.6364 | 0.111* |
| C13 | 0.3654 (4) | 0.3800 (2) | 0.5146 (2) | 0.0667 (11) |
| H13A | 0.3513 | 0.3716 | 0.4653 | 0.100* |
| H13B | 0.4317 | 0.3453 | 0.5325 | 0.100* |
| H13C | 0.4011 | 0.4282 | 0.5216 | 0.100* |
| C14 | 0.1182 (3) | 0.43062 (16) | 0.44872 (16) | 0.0436 (7) |
| C15 | 0.0611 (3) | 0.37630 (18) | 0.40759 (18) | 0.0506 (8) |
| H15 | 0.0230 | 0.3350 | 0.4282 | 0.061* |
| C16 | 0.0614 (4) | 0.38425 (19) | 0.33584 (18) | 0.0516 (9) |
| C17 | 0.1144 (4) | 0.4440 (2) | 0.30205 (19) | 0.0578 (9) |
| H17 | 0.1122 | 0.4477 | 0.2533 | 0.069* |
| C18 | 0.1710 (4) | 0.4981 (2) | 0.34301 (19) | 0.0589 (10) |
| H18 | 0.2083 | 0.5393 | 0.3219 | 0.071* |
| C19 | 0.1725 (4) | 0.49141 (18) | 0.41560 (18) | 0.0516 (9) |
| H19 | 0.2108 | 0.5285 | 0.4426 | 0.062* |
| C20 | 0.6305 (4) | 0.60171 (17) | 0.37120 (17) | 0.0481 (8) |
| H20 | 0.6670 | 0.6079 | 0.4190 | 0.058* |
| C21 | 0.4918 (4) | 0.64329 (16) | 0.36575 (16) | 0.0443 (8) |
| C22 | 0.4487 (4) | 0.67272 (16) | 0.30293 (17) | 0.0472 (8) |
| C23 | 0.3197 (4) | 0.70905 (18) | 0.2974 (2) | 0.0550 (9) |
| H23 | 0.2935 | 0.7292 | 0.2544 | 0.066* |
| C24 | 0.2329 (4) | 0.71538 (18) | 0.3530 (2) | 0.0579 (10) |
| H24 | 0.1478 | 0.7397 | 0.3480 | 0.069* |
| C25 | 0.2696 (4) | 0.68554 (17) | 0.41874 (18) | 0.0499 (8) |
| C26 | 0.4008 (4) | 0.64986 (16) | 0.42539 (16) | 0.0440 (8) |
| C27 | 0.4343 (4) | 0.61931 (19) | 0.49207 (17) | 0.0582 (10) |
| H27 | 0.5193 | 0.5952 | 0.4985 | 0.070* |
| C28 | 0.3412 (5) | 0.6254 (2) | 0.5467 (2) | 0.0720 (12) |
| H28 | 0.3657 | 0.6060 | 0.5901 | 0.086* |
| C29 | 0.2125 (5) | 0.6592 (2) | 0.5399 (2) | 0.0706 (12) |
| H29 | 0.1504 | 0.6611 | 0.5776 | 0.085* |
| C30 | 0.1779 (4) | 0.6898 (2) | 0.4772 (2) | 0.0645 (10) |
| H30 | 0.0925 | 0.7138 | 0.4726 | 0.077* |
| C31 | 0.7813 (5) | 0.7032 (2) | 0.3446 (3) | 0.0850 (14) |
| H31A | 0.7006 | 0.7342 | 0.3488 | 0.127* |
| H31B | 0.8454 | 0.7232 | 0.3108 | 0.127* |
| H31C | 0.8273 | 0.6994 | 0.3894 | 0.127* |
| C32 | 0.8609 (4) | 0.5847 (2) | 0.3165 (2) | 0.0775 (13) |
| H32A | 0.8995 | 0.5774 | 0.3626 | 0.116* |
| H32B | 0.9297 | 0.6078 | 0.2871 | 0.116* |
| H32C | 0.8354 | 0.5387 | 0.2966 | 0.116* |
| C33 | 0.6060 (4) | 0.52116 (17) | 0.35897 (16) | 0.0462 (8) |
| C34 | 0.5319 (4) | 0.49743 (16) | 0.30064 (17) | 0.0487 (8) |
| H34 | 0.4960 | 0.5308 | 0.2686 | 0.058* |
| C35 | 0.5119 (4) | 0.42447 (18) | 0.29041 (18) | 0.0546 (9) |
| C36 | 0.5626 (4) | 0.3729 (2) | 0.3360 (2) | 0.0690 (11) |
| H36 | 0.5478 | 0.3237 | 0.3278 | 0.083* |
| C37 | 0.6353 (5) | 0.3960 (2) | 0.3938 (2) | 0.0718 (12) |
| H37 | 0.6710 | 0.3621 | 0.4254 | 0.086* |
| C38 | 0.6565 (4) | 0.4697 (2) | 0.4058 (2) | 0.0610 (10) |
| H38 | 0.7051 | 0.4846 | 0.4457 | 0.073* |
| N1 | 0.2317 (3) | 0.37204 (15) | 0.55165 (15) | 0.0530 (7) |
| N2 | 0.0031 (4) | 0.3257 (2) | 0.29293 (19) | 0.0773 (10) |
| N3 | 0.7363 (3) | 0.63079 (15) | 0.32145 (15) | 0.0557 (8) |
| N4 | 0.4300 (4) | 0.4022 (2) | 0.2285 (2) | 0.0790 (11) |
| O6 | 0.0308 (3) | 0.27718 (13) | 0.55245 (16) | 0.0752 (8) |
| H6 | 0.1088 | 0.2934 | 0.5429 | 0.113* |
| O7 | −0.0380 (5) | 0.2713 (2) | 0.32155 (18) | 0.1305 (16) |
| O8 | 0.0007 (4) | 0.33316 (17) | 0.22952 (17) | 0.1061 (12) |
| O9 | 0.5235 (3) | 0.66837 (15) | 0.24250 (11) | 0.0608 (7) |
| H9A | 0.6050 | 0.6572 | 0.2515 | 0.091* |
| O10 | 0.3732 (3) | 0.44732 (17) | 0.19253 (15) | 0.0796 (8) |
| O11 | 0.4201 (6) | 0.33836 (19) | 0.2165 (2) | 0.166 (2) |

# Comment

We are interested in the dielectric-ferroelectric materials, including organic ones [7], metal-organic coordination compounds and organic–inorganic hybrids [8]. Because of their wide distribution in bioactive molecules [9] and pharmaceuticals [10], there is considerable interest in the development of effective methods for the synthesis of compounds derived from naphthalen-2-ol. Recent studies have revealed that BETTI-base organic compounds crystallized in noncentrosymmetric space groups.

There are two crystallographically independent molecules in the asymmetric unit, all bond lengths are in normal ranges [11–15]. The dihedral angle between the naphthyl ring and phenyl ring are 72.00(10)° (between C2 to C11 naphthyl ring and C14 to C19 phenyl ring) and 78.73(10)° (between C21 to C30 naphthyl ring and C33 to C38 phenyl ring). Strong intramolecular O–H···N hydrogen bonds [O6–H6 = 0.82 Å, H1A···N1 = 1.869(3) Å, O6···N1 = 2.589(4) Å, O6–H6···N1 = 72.0(1)°; O9–H9A = 0.82 Å, H9A···N3 = 1.888(3) Å, O9···N3 = 2.613(4) Å,

O9–H9A···N3 = 78.7(1)°] together with van der Waals interactions stabilize the molecular conformation.

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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