# Crystal structure of 4-fluoro-*N*-(2-hydroxy-4-nitrophenyl)benzamide, $C_{13}H_9FN_2O_4$

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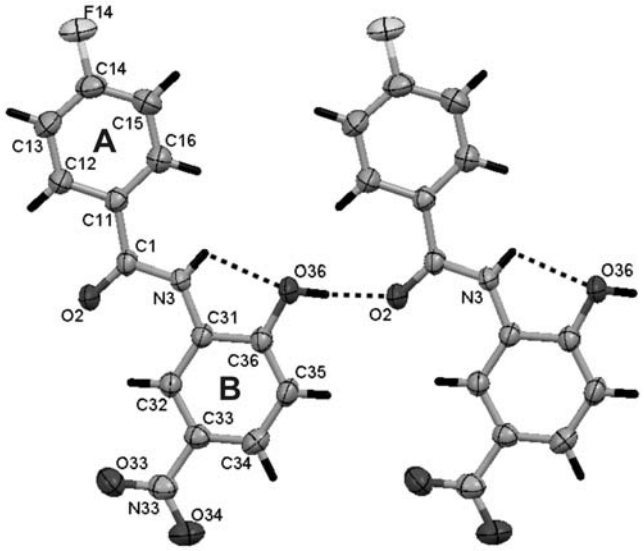


**Abstract**

$C_{13}H_9FN_2O_4$, monoclinic, $P12_1/c1$ (no. 14), $a$ = 7.3477(7) Å, $b$ = 7.7697(9) Å, $c$ = 21.295(3) Å, $\beta$ = 99.25(1)°, $V$ = 1199.9 Å$^3$, $Z$ = 4, $R_{gt}(F)$ = 0.031, $wR_{ref}(F^2)$ = 0.087, $T$ = 298 K.

**Source of material**

The title structure synthesis was described and published previously [1]. The crystals for X-ray studies were obtained from ethanol solution by slow solvent evaporation.

**Discussion**

The crystal structure studies of the title compound were conducted with the aim to obtain 3D structure which subsequently can be used as a starting point for molecular modeling of other (2-hydroxyphenyl)benzamides. The dihedral angle between two aromatic rings, describing whole molecule deviation from planarity, is the most important geometrical parameter in the studied structure. The CSD [2] search for (2-hydroxyphenyl)benzamide leading as the basic structure moiety gave three similar structures. Among them one is almost flat (angle close to 0°) [3], while remaining two molecules assume butterfly shape with the higher dihedral angle values exciding 8° and 14°, respectively [3,4]. In the title crystal structure, the dihedral angle between the aromatic rings is 14.1(2)°. The angles between the plane of the amide group and both aromatic rings are not equal. The 4-fluoro-substituted phenyl (ring A) is inclined at 20.9(2)°, while 2-hydroxy-4-nitrophenyl (ring B) - only at 6.8(2)°. This important flattening of the B ring and amide group is caused by stable five-membered ring constructed by intramolecular hydrogen bond of $d$(N3–H3···O36) = 2.573(1) Å. The crystal structure consists of infinite ribbons of 4-fluoro-*N*-(2-hydroxy-4-nitrophenyl)-benzamide molecules connected by intermolecular hydrogen bonds between the hydroxyl and carbonyl groups of adjacent molecules. The interaction O36–H36···O2 occurring over a distance of 2.591(1) Å and possessing angle of 174.9°, can be classified as a strong hydrogen bond.

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

| | |
|---|---|
| Crystal: | colourless prisma, size 0.15 × 0.35 × 0.40 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 1.25 cm$^{-1}$ |
| Diffractometer, scan mode: | Kuma KM-4 CCD, $\omega$ |
| $2\theta_{max}$: | 50° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 13469, 2118 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 1588 |
| $N(param)_{refined}$: | 182 |
| Programs: | SHELXTL [5], Mercury [6], PLATON [7] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(3) | 4*e* | 0.2196 | 0.6100 | 0.4076 | 0.045 |
| H(12) | 4*e* | –0.3537 | 0.5925 | 0.3497 | 0.058 |
| H(13) | 4*e* | –0.4599 | 0.4413 | 0.2578 | 0.069 |
| H(15) | 4*e* | 0.0452 | 0.2545 | 0.2564 | 0.062 |
| H(16) | 4*e* | 0.1519 | 0.4038 | 0.3489 | 0.052 |
| H(32) | 4*e* | 0.0327 | 0.8239 | 0.5279 | 0.044 |
| H(34) | 4*e* | 0.5290 | 0.9534 | 0.6242 | 0.052 |
| H(35) | 4*e* | 0.6704 | 0.8127 | 0.5488 | 0.052 |
| H(36) | 4*e* | 0.6257 | 0.6552 | 0.4520 | 0.070 |

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**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| C(1) | 4*e* | –0.0296(2) | 0.6125(2) | 0.41899(6) | 0.0256(6) | 0.0443(8) | 0.0342(7) | –0.0006(5) | 0.0056(5) | 0.0021(6) |
| O(2) | 4*e* | –0.1396(1) | 0.6627(1) | 0.45321(4) | 0.0253(5) | 0.0737(7) | 0.0458(6) | –0.0041(4) | 0.0098(4) | –0.0174(5) |
| N(3) | 4*e* | 0.1516(1) | 0.6467(1) | 0.43413(5) | 0.0243(6) | 0.0551(7) | 0.0342(6) | –0.0015(4) | 0.0078(5) | –0.0098(5) |
| C(11) | 4*e* | –0.0895(2) | 0.5145(2) | 0.35956(6) | 0.0308(7) | 0.0411(7) | 0.0327(7) | –0.0022(5) | 0.0055(5) | 0.0015(6) |
| C(12) | 4*e* | –0.2727(2) | 0.5242(2) | 0.33133(7) | 0.0341(7) | 0.0698(9) | 0.0411(8) | 0.0022(6) | 0.0037(6) | –0.0135(7) |
| C(13) | 4*e* | –0.3368(2) | 0.4343(2) | 0.27652(7) | 0.0394(8) | 0.086(1) | 0.0443(9) | –0.0002(7) | –0.0038(7) | –0.0148(8) |
| C(14) | 4*e* | –0.2163(2) | 0.3353(2) | 0.25046(7) | 0.0571(9) | 0.0610(9) | 0.0338(8) | –0.0062(7) | 0.0033(7) | –0.0107(7) |
| F(14) | 4*e* | –0.2809(1) | 0.2470(1) | 0.19644(4) | 0.0786(7) | 0.1041(8) | 0.0511(6) | –0.0027(5) | –0.0020(5) | –0.0371(5) |
| C(15) | 4*e* | –0.0344(2) | 0.3222(2) | 0.27576(7) | 0.0529(9) | 0.0548(9) | 0.0485(9) | 0.0031(7) | 0.0134(7) | –0.0122(8) |
| C(16) | 4*e* | 0.0284(2) | 0.4120(2) | 0.33075(7) | 0.0356(7) | 0.0501(8) | 0.0442(8) | 0.0000(6) | 0.0051(6) | –0.0046(7) |
| C(31) | 4*e* | 0.2443(2) | 0.7342(2) | 0.48749(6) | 0.0273(6) | 0.0405(7) | 0.0314(7) | –0.0014(5) | 0.0033(5) | 0.0015(6) |
| C(32) | 4*e* | 0.1606(2) | 0.8200(2) | 0.53186(6) | 0.0295(7) | 0.0449(8) | 0.0365(7) | 0.0020(5) | 0.0046(6) | 0.0000(6) |
| C(33) | 4*e* | 0.2696(2) | 0.8997(2) | 0.58219(6) | 0.0413(8) | 0.0380(7) | 0.0333(7) | 0.0019(5) | 0.0055(6) | 0.0002(6) |
| N(33) | 4*e* | 0.1770(2) | 0.9881(1) | 0.62859(6) | 0.0558(8) | 0.0490(7) | 0.0373(7) | 0.0055(6) | 0.0053(6) | –0.0030(6) |
| O(33) | 4*e* | 0.0083(2) | 0.9935(1) | 0.61987(5) | 0.0523(7) | 0.0749(7) | 0.0531(7) | 0.0139(5) | 0.0142(5) | –0.0079(6) |
| O(34) | 4*e* | 0.2721(2) | 1.0550(2) | 0.67453(6) | 0.0745(8) | 0.0897(8) | 0.0520(7) | 0.0027(6) | –0.0007(6) | –0.0316(6) |
| C(34) | 4*e* | 0.4588(2) | 0.8986(2) | 0.58972(7) | 0.0410(8) | 0.0480(8) | 0.0380(8) | –0.0052(6) | –0.0035(6) | –0.0021(6) |
| C(35) | 4*e* | 0.5425(2) | 0.8143(2) | 0.54477(6) | 0.0270(7) | 0.0543(9) | 0.0467(8) | –0.0038(6) | 0.0004(6) | –0.0005(7) |
| C(36) | 4*e* | 0.4375(2) | 0.7327(2) | 0.49411(6) | 0.0281(7) | 0.0421(7) | 0.0368(7) | 0.0000(5) | 0.0075(6) | 0.0020(6) |
| O(36) | 4*e* | 0.5059(1) | 0.6493(1) | 0.44779(4) | 0.0239(5) | 0.0709(6) | 0.0473(6) | –0.0014(4) | 0.0092(4) | –0.0121(5) |

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