# Crystal structure of 2-hydroxy-2-(4-phenoxyphenyl)propanamide, with $Z'$ = 4, $C_{15}H_{15}NO_3$

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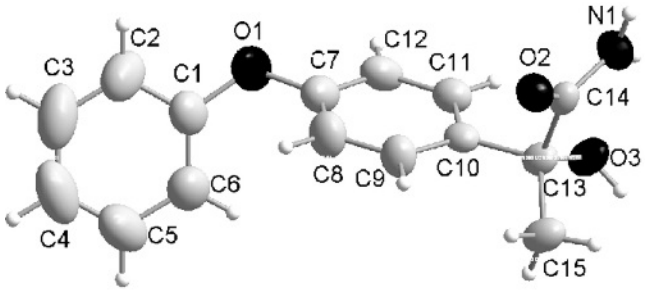


**Abstract**

$C_{15}H_{15}NO_3$, triclinic, $P\bar{1}$ (no. 2), $a$ = 10.428(1) Å, $b$ = 11.996(1) Å, $c$ = 22.421(2) Å, $\alpha$ = 82.167(2)°, $\beta$ = 81.538(2)°, $\gamma$ = 74.196(2)°, $V$ = 2655.7 Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.0640, $wR_{ref}(F^2)$ = 0.1529, $T$ = 298 K.

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

| | |
|---|---|
| Crystal: | colourless blocks, size 0.10×0.12×0.16 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 0.90 cm$^{-1}$ |
| Diffractometer, scan mode: | CCD area detector, $\varphi$ and $\omega$ |
| $2\theta_{max}$: | 51° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 16649, 9797 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 6208 |
| $N(param)_{refined}$: | 693 |
| Programs: | SHELX [14] |

## Source of material

The synthesis process of famoxadone is carried out using 5-methyl-5-(4-phenoxyphenyl)-1,3-dioxolane-2,4-dione and phenylhydrazine hydrochloride as starting material, using a modified Zheng reaction [1]. 2-Hydroxy-2-(4-phenoxyphenyl)-propanamide was the key intermediate for synthesizing famoxadone. 2-Hydroxy-2-(4-phenoxyphenyl)propanamide was prepared in high yields through a two-step procedure by using 1-(4-phenoxyphenyl)ethan-1-one as the starting material, according to modified Schenck reactions [2, 3]. 1-(4-phenoxyphenyl)-ethan-1-one (0.5 mol) was dissolved in dry $CH_2Cl_2$, then trimethylsilyl cyanide (1.1 mol) and $ZnI_2$ (0.5 mol) were added. The mixture was stirred at room temperature for 4 h. The reaction progress was monitered by the disappearance of the carbonyl stretching peak (1770 cm$^{-1}$), and by the appearance of the nitrile stretching peak (2200 cm$^{-1}$) in the IR spectrum. The $CH_2Cl_2$ layer was concentrated in vacuo, and a minimal amount of dry THF was added. The mixture was cooled to 0°C, and 15% HCl (5 mL) was added and then stirred at room temperature for 2 h. The solution was diluted with $H_2O$ and extracted with $Et_2O$ (3×25 mL), dried over $MgSO_4$, filtered, and concentrated to yield the 2-hydroxy-2-(4-phenoxyphenyl)propanamide. Crystals suitable for X-ray analysis were obtained by slow concentration of an ethanol/water solution. **m.p.**: 108-110 °C. **Elemental Analysis** calcd. for $C_{15}H_{15}NO_3$: C, 70.02; H, 5.88; N, 5.44%; found: C, 69.96; H, 5.92; N, 5.40 %.

## Experimental details

All H atoms were included in calculated positions and refined as riding atoms, with C–H = 0.93-0.96 Å, N–H = 0.86 Å and O–H = 0.82 Å, with $U_{iso}$(H) = 1.5 $U_{eq}$(C) for methyl H atoms and 1.2 $U_{eq}$(C) for all other H atoms.

## Discussion

5-Methyl-5-(4-phenoxyphenyl)-3-(phenylamino)oxazolidine-2,4-dione, was a new generation super efficient oxazolidinone fungicide devoloped by DuPont Company in 1990 [4]. Famoxadone is an excellent representative of cyt $bc_1$inhibitor with many advantages [5]. Its binds in the Qo domain of the cyt $bc_1$ complex and blocks the function of ubiquinol : cytochrome c-oxidoreductase ($bc_1$ , complex III) mitochondrial electron transport [6, 7]. It has been reported to exhibit excellent efficacy against plant pathogens in the Ascomycete, Basidiomycete and Oomycete classes that infect grapes, cereals, tomatoes, potatoes and other crops [8, 9]. Because of its wild fungicidal activity and its wild applications, the synthesis and biological activity of famoxadone and its intermediates have attracted much attention [10–13]. There are four crystallographic independant molecules in the asymmtric unit (only on of them is shown in the figure). In the molecule of the title compound (Fig.), bond lengths and angles within the pyridine ring, the pyrazole ring and the benzene ring are very similar to those given in the literature for benzene derivatives [12]. In the molecules of the title structure, show the benzene ring to be approximately planar, but the whole molecule is not. Intermolecular N–H···O hydrogen bonds and O–H···O hydrogen bonds link the molecules into chains along $a$ axis.

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(2) | 2*i* | 1.0337 | 0.4015 | 0.3716 | 0.093 |
| H(3) | 2*i* | 1.0764 | 0.2259 | 0.4307 | 0.112 |
| H(4) | 2*i* | 0.9192 | 0.1206 | 0.4515 | 0.115 |
| H(5) | 2*i* | 0.7146 | 0.1930 | 0.4157 | 0.104 |
| H(6) | 2*i* | 0.6666 | 0.3719 | 0.3591 | 0.085 |
| H(8) | 2*i* | 0.8248 | 0.3841 | 0.2423 | 0.074 |
| H(9) | 2*i* | 0.7074 | 0.4369 | 0.1586 | 0.061 |
| H(11) | 2*i* | 0.5463 | 0.7526 | 0.2133 | 0.055 |
| H(12) | 2*i* | 0.6643 | 0.7005 | 0.2962 | 0.063 |
| H(15A) | 2*i* | 0.4291 | 0.5154 | 0.1326 | 0.081 |
| H(15B) | 2*i* | 0.5661 | 0.4771 | 0.0919 | 0.081 |
| H(15C) | 2*i* | 0.4456 | 0.5703 | 0.0653 | 0.081 |
| H(17) | 2*i* | 1.0196 | –0.0950 | 0.3554 | 0.104 |
| H(18) | 2*i* | 1.0726 | –0.2683 | 0.4168 | 0.121 |
| H(19) | 2*i* | 0.9127 | –0.3669 | 0.4516 | 0.111 |
| H(20) | 2*i* | 0.6967 | –0.2893 | 0.4300 | 0.099 |
| H(21) | 2*i* | 0.6410 | –0.1137 | 0.3708 | 0.085 |
| H(23) | 2*i* | 0.6850 | 0.2111 | 0.2772 | 0.075 |
| H(24) | 2*i* | 0.5706 | 0.2621 | 0.1936 | 0.063 |
| H(26) | 2*i* | 0.6433 | –0.0727 | 0.1679 | 0.058 |
| H(27) | 2*i* | 0.7574 | –0.1241 | 0.2521 | 0.070 |
| H(30A) | 2*i* | 0.3602 | 0.2562 | 0.0829 | 0.081 |
| H(30B) | 2*i* | 0.4194 | 0.3007 | 0.1327 | 0.081 |
| H(30C) | 2*i* | 0.3331 | 0.2103 | 0.1512 | 0.081 |
| H(32) | 2*i* | 0.4191 | 0.5825 | 0.3117 | 0.103 |
| H(33) | 2*i* | 0.4747 | 0.6781 | 0.3826 | 0.114 |
| H(34) | 2*i* | 0.3997 | 0.6456 | 0.4833 | 0.101 |
| H(35) | 2*i* | 0.2683 | 0.5178 | 0.5126 | 0.103 |
| H(36) | 2*i* | 0.2103 | 0.4241 | 0.4420 | 0.088 |
| H(38) | 2*i* | 0.2398 | 0.3371 | 0.2447 | 0.067 |
| H(39) | 2*i* | 0.1365 | 0.4138 | 0.1595 | 0.058 |
| H(41) | 2*i* | 0.0747 | 0.7320 | 0.2083 | 0.071 |
| H(42) | 2*i* | 0.1720 | 0.6551 | 0.2957 | 0.080 |
| H(45A) | 2*i* | –0.1191 | 0.7662 | 0.0845 | 0.072 |
| H(45B) | 2*i* | –0.0563 | 0.7992 | 0.1369 | 0.072 |
| H(45C) | 2*i* | –0.1534 | 0.7172 | 0.1517 | 0.072 |
| H(47) | 2*i* | 0.3974 | 0.1029 | 0.3001 | 0.084 |
| H(48) | 2*i* | 0.4559 | 0.2001 | 0.3692 | 0.097 |
| H(49) | 2*i* | 0.4115 | 0.1512 | 0.4717 | 0.107 |
| H(50) | 2*i* | 0.3064 | 0.0044 | 0.5049 | 0.111 |
| H(51) | 2*i* | 0.2442 | –0.0920 | 0.4361 | 0.091 |
| H(53) | 2*i* | 0.1183 | 0.1413 | 0.3041 | 0.072 |
| H(54) | 2*i* | 0.0113 | 0.2194 | 0.2194 | 0.062 |
| H(56) | 2*i* | 0.1909 | –0.0691 | 0.1400 | 0.059 |
| H(57) | 2*i* | 0.2982 | –0.1471 | 0.2242 | 0.066 |
| H(60A) | 2*i* | –0.0954 | 0.0235 | 0.1138 | 0.079 |
| H(60B) | 2*i* | 0.0434 | –0.0120 | 0.0741 | 0.079 |
| H(60C) | 2*i* | –0.0719 | 0.0904 | 0.0497 | 0.079 |
| H(1A) | 2*i* | 0.6645 | 0.8197 | 0.0290 | 0.061 |
| H(1B) | 2*i* | 0.5413 | 0.8380 | 0.0734 | 0.061 |
| H(2A) | 2*i* | 0.7246 | 0.1396 | –0.0108 | 0.057 |
| H(2B) | 2*i* | 0.6379 | 0.0598 | 0.0139 | 0.057 |
| H(3A) | 2*i* | 0.2493 | 0.6346 | –0.0046 | 0.056 |
| H(3B) | 2*i* | 0.1556 | 0.5595 | 0.0165 | 0.056 |
| H(4A) | 2*i* | 0.1532 | 0.3248 | 0.0281 | 0.058 |
| H(4B) | 2*i* | 0.0263 | 0.3406 | 0.0702 | 0.058 |
| H(3C) | 2*i* | 0.3625 | 0.7307 | 0.1181 | 0.076 |
| H(6A) | 2*i* | 0.4160 | 0.0550 | 0.0871 | 0.072 |
| H(9A) | 2*i* | –0.0819 | 0.5676 | 0.0835 | 0.065 |
| H(12A) | 2*i* | –0.1550 | 0.2339 | 0.1148 | 0.074 |

**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) | 2*i* | 0.8460(3) | 0.4026(2) | 0.3598(1) | 0.079(2) | 0.065(2) | 0.040(2) | –0.021(2) | –0.014(2) | 0.001(1) |
| C(2) | 2*i* | 0.9687(3) | 0.3599(3) | 0.3808(1) | 0.072(2) | 0.115(3) | 0.047(2) | –0.028(2) | –0.010(2) | 0.001(2) |
| C(3) | 2*i* | 0.9940(4) | 0.2549(4) | 0.4156(2) | 0.087(3) | 0.117(3) | 0.058(2) | 0.008(2) | –0.018(2) | –0.003(2) |
| C(4) | 2*i* | 0.9002(5) | 0.1924(3) | 0.4284(2) | 0.144(4) | 0.075(2) | 0.054(2) | –0.007(3) | –0.018(2) | 0.005(2) |
| C(5) | 2*i* | 0.7786(4) | 0.2356(3) | 0.4071(1) | 0.129(3) | 0.081(2) | 0.059(2) | –0.047(2) | –0.015(2) | 0.006(2) |
| C(6) | 2*i* | 0.7501(3) | 0.3417(3) | 0.3730(1) | 0.083(2) | 0.075(2) | 0.061(2) | –0.028(2) | –0.020(2) | –0.003(2) |
| C(7) | 2*i* | 0.7525(3) | 0.5367(2) | 0.2781(1) | 0.069(2) | 0.063(2) | 0.048(2) | –0.030(2) | –0.015(1) | 0.005(2) |
| C(8) | 2*i* | 0.7676(3) | 0.4582(2) | 0.2367(1) | 0.066(2) | 0.052(2) | 0.062(2) | –0.002(1) | –0.014(2) | –0.004(2) |
| C(9) | 2*i* | 0.6972(2) | 0.4903(2) | 0.1865(1) | 0.056(2) | 0.044(2) | 0.047(2) | –0.003(1) | –0.009(1) | –0.008(1) |
| C(10) | 2*i* | 0.6122(2) | 0.6000(2) | 0.1772(1) | 0.033(1) | 0.037(1) | 0.040(1) | –0.012(1) | 0.004(1) | –0.004(1) |
| C(11) | 2*i* | 0.6017(2) | 0.6778(2) | 0.2190(1) | 0.046(1) | 0.043(1) | 0.047(2) | –0.014(1) | 0.001(1) | –0.007(1) |
| C(12) | 2*i* | 0.6720(3) | 0.6466(2) | 0.2689(1) | 0.072(2) | 0.053(2) | 0.042(2) | –0.030(1) | –0.002(1) | –0.007(1) |
| C(13) | 2*i* | 0.5377(2) | 0.6376(2) | 0.1214(1) | 0.030(1) | 0.035(1) | 0.048(2) | –0.005(1) | –0.001(1) | –0.011(1) |
| C(14) | 2*i* | 0.6352(2) | 0.6780(2) | 0.0711(1) | 0.036(1) | 0.034(1) | 0.040(1) | –0.005(1) | –0.011(1) | –0.007(1) |
| C(15) | 2*i* | 0.4902(2) | 0.5412(2) | 0.1009(1) | 0.041(1) | 0.049(2) | 0.076(2) | –0.012(1) | –0.008(1) | –0.016(1) |
| C(16) | 2*i* | 0.8256(3) | –0.0904(3) | 0.3571(1) | 0.092(2) | 0.067(2) | 0.043(2) | –0.028(2) | –0.023(2) | 0.003(2) |
| C(17) | 2*i* | 0.9543(3) | –0.1343(3) | 0.3705(1) | 0.087(3) | 0.111(3) | 0.064(2) | –0.038(2) | –0.005(2) | 0.008(2) |
| C(18) | 2*i* | 0.9855(4) | –0.2378(3) | 0.4068(2) | 0.088(3) | 0.115(3) | 0.082(3) | –0.005(2) | –0.015(2) | 0.010(2) |
| C(19) | 2*i* | 0.8902(4) | –0.2959(3) | 0.4281(2) | 0.127(3) | 0.081(2) | 0.060(2) | –0.017(2) | –0.016(2) | 0.014(2) |
| C(20) | 2*i* | 0.7621(4) | –0.2501(3) | 0.4149(1) | 0.112(3) | 0.090(3) | 0.052(2) | –0.042(2) | –0.009(2) | 0.002(2) |
| C(21) | 2*i* | 0.7289(3) | –0.1459(3) | 0.3794(1) | 0.081(2) | 0.079(2) | 0.059(2) | –0.025(2) | –0.021(2) | –0.004(2) |
| C(22) | 2*i* | 0.7305(3) | 0.0384(2) | 0.2734(1) | 0.087(2) | 0.064(2) | 0.049(2) | –0.042(2) | –0.023(2) | 0.008(2) |
| C(23) | 2*i* | 0.6759(3) | 0.1536(2) | 0.2554(1) | 0.101(2) | 0.053(2) | 0.048(2) | –0.041(2) | –0.019(2) | –0.000(1) |
| C(24) | 2*i* | 0.6078(3) | 0.1838(2) | 0.2052(1) | 0.071(2) | 0.040(1) | 0.051(2) | –0.023(1) | –0.007(1) | –0.001(1) |
| C(25) | 2*i* | 0.5932(2) | 0.1003(2) | 0.1711(1) | 0.042(1) | 0.039(1) | 0.038(1) | –0.017(1) | 0.005(1) | –0.002(1) |
| C(26) | 2*i* | 0.6507(2) | –0.0148(2) | 0.1898(1) | 0.062(2) | 0.043(2) | 0.044(2) | –0.020(1) | –0.003(1) | –0.007(1) |
| C(27) | 2*i* | 0.7192(3) | –0.0461(2) | 0.2405(1) | 0.081(2) | 0.047(2) | 0.050(2) | –0.022(1) | –0.015(2) | 0.007(1) |
| C(28) | 2*i* | 0.5240(2) | 0.1356(2) | 0.1136(1) | 0.036(1) | 0.037(1) | 0.044(2) | –0.011(1) | –0.000(1) | –0.012(1) |
| C(29) | 2*i* | 0.6233(2) | 0.1784(2) | 0.0645(1) | 0.036(1) | 0.038(1) | 0.038(1) | –0.005(1) | –0.005(1) | –0.005(1) |
| C(30) | 2*i* | 0.3975(2) | 0.2349(2) | 0.1208(1) | 0.035(1) | 0.059(2) | 0.069(2) | –0.010(1) | –0.002(1) | –0.019(1) |
| C(31) | 2*i* | 0.3080(3) | 0.4953(2) | 0.3702(1) | 0.063(2) | 0.068(2) | 0.038(2) | –0.017(2) | –0.014(1) | 0.002(1) |
| C(32) | 2*i* | 0.3876(3) | 0.5699(3) | 0.3524(1) | 0.089(2) | 0.134(3) | 0.047(2) | –0.054(2) | –0.002(2) | –0.010(2) |
| C(33) | 2*i* | 0.4213(3) | 0.6265(3) | 0.3948(2) | 0.091(2) | 0.140(3) | 0.075(3) | –0.062(2) | –0.005(2) | –0.018(2) |
| C(34) | 2*i* | 0.3769(3) | 0.6074(3) | 0.4546(2) | 0.093(2) | 0.110(3) | 0.056(2) | –0.023(2) | –0.025(2) | –0.020(2) |
| C(35) | 2*i* | 0.2985(3) | 0.5316(3) | 0.4719(1) | 0.109(3) | 0.110(3) | 0.038(2) | –0.033(2) | –0.010(2) | 0.005(2) |
| C(36) | 2*i* | 0.2638(3) | 0.4755(3) | 0.4298(1) | 0.094(2) | 0.090(2) | 0.041(2) | –0.035(2) | –0.013(2) | 0.008(2) |

**Table 3.** continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| C(37) | 2*i* | 0.2164(3) | 0.4880(2) | 0.2783(1) | 0.063(2) | 0.058(2) | 0.034(2) | –0.022(1) | –0.006(1) | 0.006(1) |
| C(38) | 2*i* | 0.2056(3) | 0.4172(2) | 0.2377(1) | 0.071(2) | 0.042(1) | 0.051(2) | –0.006(1) | –0.013(1) | –0.005(1) |
| C(39) | 2*i* | 0.1447(2) | 0.4634(2) | 0.1864(1) | 0.058(2) | 0.045(2) | 0.043(2) | –0.009(1) | –0.012(1) | –0.010(1) |
| C(40) | 2*i* | 0.0954(2) | 0.5815(2) | 0.1739(1) | 0.035(1) | 0.041(1) | 0.034(1) | –0.012(1) | 0.002(1) | –0.005(1) |
| C(41) | 2*i* | 0.1073(3) | 0.6517(2) | 0.2156(1) | 0.086(2) | 0.044(2) | 0.049(2) | –0.016(1) | –0.018(2) | –0.005(1) |
| C(42) | 2*i* | 0.1663(3) | 0.6063(2) | 0.2679(1) | 0.109(2) | 0.058(2) | 0.042(2) | –0.028(2) | –0.024(2) | –0.006(1) |
| C(43) | 2*i* | 0.0347(2) | 0.6328(2) | 0.1149(1) | 0.033(1) | 0.035(1) | 0.040(1) | –0.011(1) | –0.003(1) | –0.007(1) |
| C(44) | 2*i* | 0.1441(2) | 0.6724(2) | 0.0699(1) | 0.031(1) | 0.035(1) | 0.033(1) | –0.002(1) | –0.008(1) | –0.003(1) |
| C(45) | 2*i* | –0.0846(2) | 0.7387(2) | 0.1227(1) | 0.033(1) | 0.048(1) | 0.061(2) | –0.006(1) | 0.001(1) | –0.015(1) |
| C(46) | 2*i* | 0.3146(3) | –0.0026(2) | 0.3616(1) | 0.063(2) | 0.063(2) | 0.043(2) | –0.001(2) | –0.015(1) | –0.002(2) |
| C(47) | 2*i* | 0.3782(3) | 0.0835(3) | 0.3415(1) | 0.074(2) | 0.085(2) | 0.049(2) | –0.019(2) | –0.012(2) | 0.000(2) |
| C(48) | 2*i* | 0.4136(3) | 0.1409(3) | 0.3827(2) | 0.078(2) | 0.084(2) | 0.083(3) | –0.020(2) | –0.024(2) | –0.006(2) |
| C(49) | 2*i* | 0.3871(3) | 0.1121(3) | 0.4439(2) | 0.096(3) | 0.104(3) | 0.071(3) | –0.013(2) | –0.035(2) | –0.020(2) |
| C(50) | 2*i* | 0.3242(4) | 0.0247(3) | 0.4635(2) | 0.115(3) | 0.116(3) | 0.043(2) | –0.020(2) | –0.023(2) | –0.003(2) |
| C(51) | 2*i* | 0.2872(3) | –0.0331(3) | 0.4227(1) | 0.094(2) | 0.082(2) | 0.049(2) | –0.019(2) | –0.017(2) | 0.010(2) |
| C(52) | 2*i* | 0.2186(3) | –0.0109(2) | 0.2723(1) | 0.060(2) | 0.053(2) | 0.040(2) | –0.014(1) | –0.009(1) | 0.002(1) |
| C(53) | 2*i* | 0.1331(3) | 0.0986(2) | 0.2710(1) | 0.078(2) | 0.058(2) | 0.040(2) | –0.006(2) | –0.006(1) | –0.015(1) |
| C(54) | 2*i* | 0.0690(2) | 0.1451(2) | 0.2201(1) | 0.056(2) | 0.043(1) | 0.049(2) | 0.001(1) | –0.004(1) | –0.013(1) |
| C(55) | 2*i* | 0.0884(2) | 0.0841(2) | 0.1703(1) | 0.034(1) | 0.040(1) | 0.037(1) | –0.009(1) | 0.002(1) | –0.007(1) |
| C(56) | 2*i* | 0.1756(2) | –0.0260(2) | 0.1730(1) | 0.051(2) | 0.048(2) | 0.044(2) | –0.000(1) | –0.007(1) | –0.014(1) |
| C(57) | 2*i* | 0.2400(2) | –0.0729(2) | 0.2234(1) | 0.059(2) | 0.043(2) | 0.055(2) | 0.005(1) | –0.013(1) | –0.009(1) |
| C(58) | 2*i* | 0.0196(2) | 0.1382(2) | 0.1138(1) | 0.032(1) | 0.040(1) | 0.047(2) | –0.006(1) | –0.004(1) | –0.009(1) |
| C(59) | 2*i* | 0.1222(2) | 0.1820(2) | 0.0669(1) | 0.041(1) | 0.036(1) | 0.037(1) | –0.007(1) | –0.011(1) | –0.006(1) |
| C(60) | 2*i* | –0.0307(2) | 0.0520(2) | 0.0852(1) | 0.043(1) | 0.052(2) | 0.067(2) | –0.012(1) | –0.013(1) | –0.014(1) |
| N(1) | 2*i* | 0.6108(2) | 0.7919(2) | 0.05608(9) | 0.048(1) | 0.040(1) | 0.057(1) | –0.0048(9) | –0.002(1) | –0.001(1) |
| N(2) | 2*i* | 0.6670(2) | 0.1191(2) | 0.01703(8) | 0.049(1) | 0.059(1) | 0.039(1) | –0.019(1) | 0.0012(9) | –0.013(1) |
| N(3) | 2*i* | 0.1881(2) | 0.6156(2) | 0.02169(8) | 0.050(1) | 0.055(1) | 0.041(1) | –0.020(1) | 0.004(1) | –0.016(1) |
| N(4) | 2*i* | 0.0977(2) | 0.2956(2) | 0.05351(9) | 0.048(1) | 0.040(1) | 0.053(1) | –0.0080(9) | –0.002(1) | 0.000(1) |
| O(1) | 2*i* | 0.8223(2) | 0.5126(2) | 0.3285(1) | 0.136(2) | 0.078(1) | 0.080(2) | –0.050(1) | –0.063(2) | 0.016(1) |
| O(2) | 2*i* | 0.7343(2) | 0.6078(1) | 0.04735(7) | 0.0447(9) | 0.0428(9) | 0.043(1) | –0.0060(8) | 0.0030(8) | –0.0089(8) |
| O(3) | 2*i* | 0.4260(1) | 0.7341(1) | 0.13475(8) | 0.0319(9) | 0.048(1) | 0.070(1) | –0.0008(7) | –0.0057(8) | –0.0207(9) |
| O(4) | 2*i* | 0.7986(3) | 0.0181(2) | 0.3237(1) | 0.171(2) | 0.075(1) | 0.084(2) | –0.060(2) | –0.076(2) | 0.022(1) |
| O(5) | 2*i* | 0.6619(2) | 0.2644(1) | 0.07124(7) | 0.066(1) | 0.049(1) | 0.050(1) | –0.0255(9) | 0.0107(9) | –0.0116(9) |
| O(6) | 2*i* | 0.4937(2) | 0.0369(1) | 0.09519(8) | 0.0445(9) | 0.0450(9) | 0.059(1) | –0.0151(7) | –0.0068(9) | –0.0140(8) |
| O(7) | 2*i* | 0.2750(2) | 0.4323(2) | 0.32975(8) | 0.108(2) | 0.070(1) | 0.045(1) | –0.028(1) | –0.030(1) | 0.009(1) |
| O(8) | 2*i* | 0.1865(1) | 0.7540(1) | 0.08027(7) | 0.0455(9) | 0.0428(9) | 0.041(1) | –0.0179(8) | 0.0009(7) | –0.0095(8) |
| O(9) | 2*i* | –0.0032(1) | 0.5442(1) | 0.09014(7) | 0.0376(9) | 0.0403(9) | 0.055(1) | –0.0115(7) | –0.0095(8) | –0.0093(8) |
| O(10) | 2*i* | 0.2808(2) | –0.0678(2) | 0.32258(8) | 0.107(2) | 0.060(1) | 0.052(1) | –0.011(1) | –0.031(1) | 0.003(1) |
| O(11) | 2*i* | 0.2236(2) | 0.1128(1) | 0.04429(7) | 0.051(1) | 0.0428(9) | 0.053(1) | –0.0092(8) | 0.0091(8) | –0.0084(8) |
| O(12) | 2*i* | –0.0882(1) | 0.2359(1) | 0.12941(8) | 0.0356(9) | 0.049(1) | 0.060(1) | 0.0014(8) | –0.0081(8) | –0.0138(9) |

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