# Crystal structure of tetrakis[μ-(4-chlorobenzoato-*O*,*O*′)-μ$_3$-(2-dimethylaminoethanolato)copper(II)]) dimethanol, $C_{46}H_{64}Cl_4Cu_4N_4O_{14}$

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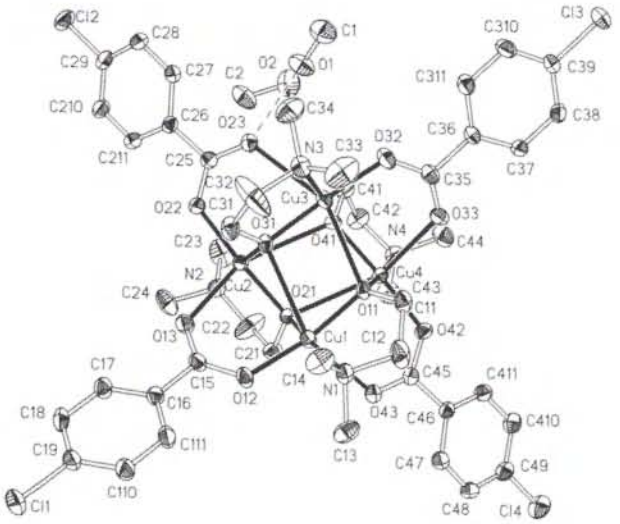


**Abstract**

$C_{46}H_{64}Cl_4Cu_4N_4O_{14}$, triclinic, $P\bar{1}$ (No. 2), $a$ = 14.056(4) Å, $b$ = 14.704(4) Å, $c$ = 15.335(3) Å, α = 106.27(2)°, β = 105.76(2)°, γ = 102.24(2)°, $V$ = 2782.2 Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.035, $wR_{ref}(F^2)$ = 0.081, $T$ = 293 K.

**Source of material**

The compound was obtained with treatment of 2-dimethylaminoethanol and Cu(II) 4-chlorobenzoate (1:1 ratio) in methanol solution according to the method described in [1].

**Discussion**

Each complex molecule is constructed around an eight-membered $Cu_4O_4$ ring of cubane-type structure. Within the $Cu_4O_4$ core, the four short Cu—Cu distances vary between 3.095 Å and 3.192 Å and the two long distances are 3.664 Å and 3.797 Å. Each Cu atom is surrounded by two ethanolato oxygen atoms, a carboxyl oxygen atom and an amino nitrogen atom in a nearly square-planar arrangement with average Cu—O and Cu—N distances of 1.936 Å and 2.054 Å. The axial sites of each Cu atom are occupied by an ethanolato oxygen and an oxygen atom of the carboxylate group with Cu—O distances of 2.407 Å – 2.816 Å. The methanol oxygen atom O1 is hydrogen bonded to the other methanol O2 atom and to the carboxylic O23 atom with the distances O1—O2 of 2.765 Å and O1—O23 of 2.775 Å. Owing to the disorder of the 2-dimethylaminoethanol C32 atom, the C31—C32 bond length differs from normal C—C bond.

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

| | |
|---|---|
| Crystal: | blue, irregular, size 0.25 × 0.30 × 0.35 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| μ: | 17.64 cm$^{-1}$ |
| Diffractometer, scan mode: | Nicolet P3, ω/2θ |
| $2\theta_{max}$: | 46° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 5563, 5563 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 5563 |
| $N(param)_{refined}$: | 651 |
| Programs: | SHELXS-97 [2], SHELXL-97 [3], SHELXTL [4] |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(11A) | 2*i* | 0.0404 | 0.4394 | 0.0688 | 0.077 |
| H(11B) | 2*i* | 0.0973 | 0.5015 | 0.1800 | 0.077 |
| H(12A) | 2*i* | 0.0960 | 0.6154 | 0.1206 | 0.123 |
| H(12B) | 2*i* | 0.1110 | 0.5539 | 0.0266 | 0.123 |
| H(13A) | 2*i* | 0.2364 | 0.7355 | 0.0870 | 0.105 |
| H(13B) | 2*i* | 0.2422 | 0.6405 | 0.0129 | 0.105 |
| H(13C) | 2*i* | 0.3428 | 0.7137 | 0.0997 | 0.105 |
| H(14A) | 2*i* | 0.2451 | 0.7472 | 0.2382 | 0.110 |
| H(14B) | 2*i* | 0.3530 | 0.7277 | 0.2628 | 0.110 |
| H(14C) | 2*i* | 0.2600 | 0.6622 | 0.2784 | 0.110 |
| H(17A) | 2*i* | 0.7347 | 0.6589 | 0.3315 | 0.076 |
| H(18A) | 2*i* | 0.8682 | 0.8084 | 0.4001 | 0.082 |
| H(11C) | 2*i* | 0.6691 | 0.9481 | 0.3131 | 0.090 |
| H(11D) | 2*i* | 0.5364 | 0.7989 | 0.2400 | 0.089 |
| H(21A) | 2*i* | 0.4675 | 0.4601 | 0.0449 | 0.078 |
| H(21B) | 2*i* | 0.3674 | 0.3841 | –0.0411 | 0.078 |
| H(22A) | 2*i* | 0.5142 | 0.3286 | –0.0068 | 0.168 |
| H(22B) | 2*i* | 0.4083 | 0.2553 | –0.0202 | 0.168 |
| H(23A) | 2*i* | 0.5326 | 0.1834 | 0.0618 | 0.127 |
| H(23B) | 2*i* | 0.4210 | 0.1697 | 0.0675 | 0.127 |
| H(23C) | 2*i* | 0.5174 | 0.1987 | 0.1619 | 0.127 |
| H(24A) | 2*i* | 0.6522 | 0.3330 | 0.1206 | 0.119 |
| H(24B) | 2*i* | 0.6427 | 0.3568 | 0.2236 | 0.119 |
| H(24C) | 2*i* | 0.6315 | 0.4321 | 0.1695 | 0.119 |
| H(27A) | 2*i* | 0.4139 | 0.1958 | 0.4691 | 0.068 |
| H(28A) | 2*i* | 0.5113 | 0.1229 | 0.5584 | 0.076 |
| H(21C) | 2*i* | 0.7226 | 0.1671 | 0.4330 | 0.075 |
| H(21D) | 2*i* | 0.6281 | 0.2463 | 0.3489 | 0.068 |
| H(31A) | 2*i* | 0.4544 | 0.4768 | 0.4024 | 0.084 |
| H(31D) | 2*i* | 0.4392 | 0.5685 | 0.3741 | 0.084 |
| H(32A) | 2*i* | 0.3256 | 0.5763 | 0.4249 | 0.246 |
| H(32B) | 2*i* | 0.3745 | 0.5181 | 0.4858 | 0.246 |
| H(33A) | 2*i* | 0.1714 | 0.5275 | 0.4556 | 0.151 |
| H(33B) | 2*i* | 0.0911 | 0.4396 | 0.3624 | 0.151 |
| H(33C) | 2*i* | 0.1616 | 0.5314 | 0.3525 | 0.151 |
| H(34A) | 2*i* | 0.2431 | 0.4232 | 0.5110 | 0.121 |
| H(34B) | 2*i* | 0.2896 | 0.3514 | 0.4513 | 0.121 |
| H(34C) | 2*i* | 0.1688 | 0.3292 | 0.4203 | 0.121 |

**Table 2.** Continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(37A) | 2*i* | –0.1840 | 0.1643 | 0.0097 | 0.064 |
| H(38A) | 2*i* | –0.3405 | 0.0722 | 0.0058 | 0.067 |
| H(31B) | 2*i* | –0.2104 | 0.1068 | 0.2835 | 0.078 |
| H(31C) | 2*i* | –0.0540 | 0.2008 | 0.2881 | 0.075 |
| H(41A) | 2*i* | 0.1224 | 0.1348 | 0.1109 | 0.073 |
| H(41B) | 2*i* | 0.2390 | 0.1361 | 0.1445 | 0.073 |
| H(42A) | 2*i* | 0.2473 | 0.1213 | –0.0038 | 0.093 |
| H(42B) | 2*i* | 0.1449 | 0.0394 | –0.0217 | 0.093 |
| H(43A) | 2*i* | 0.1349 | 0.0738 | –0.1837 | 0.101 |
| H(43B) | 2*i* | 0.2259 | 0.1741 | –0.1237 | 0.101 |
| H(43C) | 2*i* | 0.1175 | 0.1752 | –0.1858 | 0.101 |
| H(44A) | 2*i* | –0.0083 | 0.0338 | –0.1391 | 0.100 |
| H(44B) | 2*i* | –0.0305 | 0.1345 | –0.1360 | 0.100 |

**Table 2.** Continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(44C) | 2*i* | –0.0174 | 0.1027 | –0.0452 | 0.100 |
| H(47A) | 2*i* | 0.1731 | 0.5057 | –0.2173 | 0.076 |
| H(48A) | 2*i* | 0.0977 | 0.4831 | –0.3785 | 0.084 |
| H(41C) | 2*i* | –0.1043 | 0.2260 | –0.4210 | 0.082 |
| H(41D) | 2*i* | –0.0304 | 0.2507 | –0.2581 | 0.071 |
| H(1) | 2*i* | 0.2507 | 0.1304 | 0.3166 | 0.116 |
| H(1C) | 2*i* | 0.1904 | 0.1180 | 0.4270 | 0.127 |
| H(1A) | 2*i* | 0.1063 | 0.0200 | 0.3484 | 0.127 |
| H(1B) | 2*i* | 0.1077 | 0.1233 | 0.3380 | 0.127 |
| H(2) | 2*i* | 0.2437 | –0.0257 | 0.2139 | 0.135 |
| H(2C) | 2*i* | 0.3986 | –0.0253 | 0.2845 | 0.127 |
| H(2A) | 2*i* | 0.3950 | –0.0804 | 0.1795 | 0.127 |
| H(2B) | 2*i* | 0.3947 | 0.0298 | 0.2102 | 0.127 |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Cu(1) | 2*i* | 0.31377(4) | 0.51659(4) | 0.12943(5) | 0.0388(3) | 0.0368(3) | 0.0782(5) | 0.0151(3) | 0.0180(3) | 0.0229(3) |
| Cu(2) | 2*i* | 0.42732(4) | 0.37328(4) | 0.19961(4) | 0.0415(3) | 0.0482(4) | 0.0537(4) | 0.0209(3) | 0.0203(3) | 0.0248(3) |
| Cu(3) | 2*i* | 0.21865(4) | 0.35152(4) | 0.24825(4) | 0.0425(3) | 0.0501(4) | 0.0403(3) | 0.0045(3) | 0.0163(3) | 0.0057(3) |
| Cu(4) | 2*i* | 0.15006(4) | 0.30008(4) | 0.02598(4) | 0.0463(3) | 0.0375(3) | 0.0381(3) | 0.0100(3) | 0.0098(3) | 0.0108(3) |
| Cl(1) | 2*i* | 0.8807(1) | 1.0045(1) | 0.4168(1) | 0.068(1) | 0.084(1) | 0.093(1) | –0.0173(9) | 0.0010(9) | 0.019(1) |
| Cl(2) | 2*i* | 0.6955(1) | 0.0772(1) | 0.5658(1) | 0.095(1) | 0.087(1) | 0.078(1) | 0.038(1) | 0.0122(9) | 0.0485(9) |
| Cl(3) | 2*i* | –0.4073(1) | 0.0118(1) | 0.1418(1) | 0.0522(9) | 0.087(1) | 0.099(1) | 0.0039(8) | 0.0301(8) | 0.039(1) |
| Cl(4) | 2*i* | –0.0651(2) | 0.3338(2) | –0.5362(1) | 0.111(1) | 0.137(2) | 0.0459(9) | 0.048(1) | 0.0278(9) | 0.034(1) |
| O(11) | 2*i* | 0.1822(2) | 0.4344(2) | 0.1198(2) | 0.034(2) | 0.038(2) | 0.051(2) | 0.014(1) | 0.010(2) | 0.010(2) |
| O(12) | 2*i* | 0.4491(3) | 0.6162(2) | 0.1788(3) | 0.040(2) | 0.045(2) | 0.118(3) | 0.010(2) | 0.012(2) | 0.037(2) |
| O(13) | 2*i* | 0.5516(3) | 0.5432(3) | 0.2543(3) | 0.054(2) | 0.052(2) | 0.093(3) | 0.017(2) | 0.020(2) | 0.033(2) |
| O(21) | 2*i* | 0.3577(2) | 0.4012(2) | 0.0875(2) | 0.047(2) | 0.049(2) | 0.054(2) | 0.024(2) | 0.026(2) | 0.025(2) |
| O(22) | 2*i* | 0.4900(3) | 0.3215(3) | 0.2971(3) | 0.047(2) | 0.074(2) | 0.071(2) | 0.025(2) | 0.023(2) | 0.044(2) |
| O(23) | 2*i* | 0.3502(3) | 0.2524(3) | 0.3272(3) | 0.046(2) | 0.064(2) | 0.070(2) | 0.015(2) | 0.016(2) | 0.031(2) |
| O(31) | 2*i* | 0.3532(2) | 0.4401(2) | 0.2725(2) | 0.037(2) | 0.048(2) | 0.038(2) | 0.010(2) | 0.010(1) | 0.005(2) |
| O(32) | 2*i* | 0.0770(3) | 0.2804(3) | 0.2286(3) | 0.049(2) | 0.089(3) | 0.050(2) | –0.004(2) | 0.020(2) | 0.009(2) |
| O(33) | 2*i* | 0.0012(3) | 0.2639(3) | 0.0742(3) | 0.054(2) | 0.076(3) | 0.062(2) | 0.008(2) | 0.023(2) | 0.030(2) |
| O(41) | 2*i* | 0.2225(2) | 0.2619(2) | 0.1300(2) | 0.054(2) | 0.035(2) | 0.038(2) | 0.014(2) | 0.017(2) | 0.012(1) |
| O(42) | 2*i* | 0.0887(3) | 0.3278(3) | –0.0886(2) | 0.059(2) | 0.054(2) | 0.046(2) | 0.005(2) | 0.004(2) | 0.022(2) |
| O(43) | 2*i* | 0.2185(3) | 0.4582(3) | –0.0701(3) | 0.050(2) | 0.066(2) | 0.059(2) | 0.008(2) | 0.009(2) | 0.023(2) |
| N(1) | 2*i* | 0.2469(3) | 0.6269(3) | 0.1398(3) | 0.047(3) | 0.039(2) | 0.078(3) | 0.020(2) | 0.014(2) | 0.019(2) |
| N(2) | 2*i* | 0.5077(3) | 0.3131(3) | 0.1170(3) | 0.057(3) | 0.074(3) | 0.073(3) | 0.043(2) | 0.036(2) | 0.038(3) |
| N(3) | 2*i* | 0.2378(3) | 0.4385(3) | 0.3861(3) | 0.059(3) | 0.069(3) | 0.042(2) | 0.013(2) | 0.022(2) | 0.003(2) |
| N(4) | 2*i* | 0.1177(3) | 0.1534(3) | –0.0619(3) | 0.068(3) | 0.040(2) | 0.040(2) | 0.011(2) | 0.009(2) | 0.007(2) |
| C(11) | 2*i* | 0.1063(4) | 0.4842(4) | 0.1175(5) | 0.048(3) | 0.053(3) | 0.093(4) | 0.026(3) | 0.022(3) | 0.023(3) |
| C(12) | 2*i* | 0.1333(5) | 0.5717(5) | 0.0965(6) | 0.056(4) | 0.076(5) | 0.181(8) | 0.038(4) | 0.033(5) | 0.050(5) |
| C(13) | 2*i* | 0.2690(6) | 0.6840(5) | 0.0797(5) | 0.123(6) | 0.063(4) | 0.087(5) | 0.049(4) | 0.028(4) | 0.035(4) |
| C(14) | 2*i* | 0.2790(6) | 0.6969(5) | 0.2381(5) | 0.123(6) | 0.079(5) | 0.083(5) | 0.053(4) | 0.039(4) | 0.024(4) |
| C(15) | 2*i* | 0.5349(4) | 0.6156(4) | 0.2345(4) | 0.047(3) | 0.047(3) | 0.080(4) | 0.014(3) | 0.023(3) | 0.026(3) |
| C(16) | 2*i* | 0.6212(4) | 0.7127(4) | 0.2788(4) | 0.044(3) | 0.055(3) | 0.059(3) | 0.018(3) | 0.021(3) | 0.022(3) |
| C(17) | 2*i* | 0.7209(4) | 0.7169(4) | 0.3269(4) | 0.049(3) | 0.061(4) | 0.079(4) | 0.022(3) | 0.018(3) | 0.025(3) |
| C(18) | 2*i* | 0.8008(4) | 0.8063(5) | 0.3685(4) | 0.039(3) | 0.087(5) | 0.065(4) | 0.015(3) | 0.008(3) | 0.021(3) |
| C(19) | 2*i* | 0.7801(4) | 0.8915(4) | 0.3628(4) | 0.051(3) | 0.063(4) | 0.057(3) | 0.000(3) | 0.011(3) | 0.018(3) |
| C(110) | 2*i* | 0.6825(4) | 0.8895(4) | 0.3161(5) | 0.058(4) | 0.052(4) | 0.098(5) | 0.008(3) | 0.005(3) | 0.029(3) |
| C(111) | 2*i* | 0.6031(4) | 0.8003(4) | 0.2732(5) | 0.045(3) | 0.059(4) | 0.101(5) | 0.007(3) | 0.003(3) | 0.032(4) |
| C(21) | 2*i* | 0.4139(4) | 0.3967(4) | 0.0237(4) | 0.066(4) | 0.085(4) | 0.074(4) | 0.038(3) | 0.042(3) | 0.047(3) |
| C(22) | 2*i* | 0.4609(7) | 0.3186(8) | 0.0216(6) | 0.181(9) | 0.26(1) | 0.116(6) | 0.178(9) | 0.108(7) | 0.123(8) |
| C(23) | 2*i* | 0.4934(6) | 0.2070(5) | 0.1006(6) | 0.090(5) | 0.080(5) | 0.139(7) | 0.039(4) | 0.049(5) | 0.008(5) |
| C(24) | 2*i* | 0.6176(5) | 0.3629(5) | 0.1613(6) | 0.061(4) | 0.092(5) | 0.150(7) | 0.024(4) | 0.061(5) | 0.029(5) |
| C(25) | 2*i* | 0.4430(4) | 0.2697(4) | 0.3360(4) | 0.054(3) | 0.044(3) | 0.050(3) | 0.014(3) | 0.015(3) | 0.015(3) |
| C(26) | 2*i* | 0.5101(4) | 0.2274(4) | 0.3981(3) | 0.049(3) | 0.043(3) | 0.041(3) | 0.010(2) | 0.007(2) | 0.012(2) |
| C(27) | 2*i* | 0.4764(4) | 0.1906(4) | 0.4618(4) | 0.048(3) | 0.062(3) | 0.052(3) | 0.007(3) | 0.013(3) | 0.020(3) |
| C(28) | 2*i* | 0.5339(4) | 0.1464(4) | 0.5148(4) | 0.066(4) | 0.071(4) | 0.050(3) | 0.012(3) | 0.012(3) | 0.031(3) |
| C(29) | 2*i* | 0.6245(4) | 0.1377(4) | 0.5025(4) | 0.066(4) | 0.049(3) | 0.047(3) | 0.018(3) | 0.001(3) | 0.016(3) |
| C(210) | 2*i* | 0.6607(4) | 0.1736(4) | 0.4407(4) | 0.057(3) | 0.082(4) | 0.057(3) | 0.030(3) | 0.019(3) | 0.033(3) |
| C(211) | 2*i* | 0.6032(4) | 0.2198(4) | 0.3897(4) | 0.059(3) | 0.065(4) | 0.051(3) | 0.021(3) | 0.017(3) | 0.028(3) |
| C(31) | 2*i* | 0.4028(4) | 0.5031(5) | 0.3709(4) | 0.057(4) | 0.077(4) | 0.046(3) | 0.008(3) | 0.008(3) | –0.001(3) |
| C(32) | 2*i* | 0.3379(7) | 0.5129(8) | 0.4202(6) | 0.147(8) | 0.22(1) | 0.091(6) | –0.113(8) | 0.077(6) | –0.086(7) |
| C(33) | 2*i* | 0.1587(7) | 0.4886(6) | 0.3894(5) | 0.193(9) | 0.137(7) | 0.081(5) | 0.107(7) | 0.068(6) | 0.028(5) |

**Table 3.** Continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| C(34) | 2*i* | 0.2346(6) | 0.3808(6) | 0.4472(5) | 0.136(7) | 0.116(6) | 0.058(4) | 0.056(5) | 0.037(4) | 0.026(4) |
| C(35) | 2*i* | –0.0004(4) | 0.2512(4) | 0.1493(4) | 0.050(3) | 0.053(3) | 0.055(4) | 0.011(3) | 0.024(3) | 0.009(3) |
| C(36) | 2*i* | –0.1020(4) | 0.1928(4) | 0.1497(4) | 0.043(3) | 0.046(3) | 0.053(3) | 0.012(2) | 0.022(3) | 0.012(2) |
| C(37) | 2*i* | –0.1891(4) | 0.1534(4) | 0.0653(4) | 0.051(3) | 0.061(3) | 0.058(3) | 0.021(3) | 0.024(3) | 0.029(3) |
| C(38) | 2*i* | –0.2827(4) | 0.0984(4) | 0.0628(4) | 0.041(3) | 0.060(3) | 0.057(3) | 0.013(3) | 0.008(3) | 0.020(3) |
| C(39) | 2*i* | –0.2901(4) | 0.0826(4) | 0.1445(4) | 0.041(3) | 0.052(3) | 0.063(4) | 0.012(2) | 0.023(3) | 0.018(3) |
| C(310) | 2*i* | –0.2050(4) | 0.1193(4) | 0.2285(4) | 0.058(4) | 0.077(4) | 0.055(3) | 0.004(3) | 0.028(3) | 0.021(3) |
| C(311) | 2*i* | –0.1115(4) | 0.1750(4) | 0.2309(4) | 0.051(3) | 0.075(4) | 0.048(3) | 0.009(3) | 0.017(3) | 0.010(3) |
| C(41) | 2*i* | 0.1888(5) | 0.1564(4) | 0.1032(4) | 0.082(4) | 0.039(3) | 0.055(3) | 0.017(3) | 0.018(3) | 0.016(3) |
| C(42) | 2*i* | 0.1786(5) | 0.1108(4) | 0.0008(4) | 0.108(5) | 0.048(3) | 0.062(4) | 0.027(3) | 0.017(4) | 0.008(3) |
| C(43) | 2*i* | 0.1520(5) | 0.1432(5) | –0.1462(4) | 0.099(5) | 0.079(4) | 0.065(4) | 0.028(4) | 0.035(4) | 0.003(3) |
| C(44) | 2*i* | 0.0057(5) | 0.1017(5) | –0.0987(5) | 0.075(4) | 0.062(4) | 0.080(4) | –0.005(3) | 0.018(4) | 0.007(3) |
| C(45) | 2*i* | 0.1361(4) | 0.3915(4) | –0.1176(4) | 0.047(3) | 0.051(3) | 0.049(3) | 0.018(3) | 0.014(3) | 0.016(3) |
| C(46) | 2*i* | 0.0809(4) | 0.3787(4) | –0.2215(3) | 0.047(3) | 0.054(3) | 0.046(3) | 0.022(3) | 0.017(2) | 0.020(3) |
| C(47) | 2*i* | 0.1175(4) | 0.4489(4) | –0.2580(4) | 0.053(3) | 0.075(4) | 0.061(4) | 0.014(3) | 0.018(3) | 0.030(3) |
| C(48) | 2*i* | 0.0724(5) | 0.4357(5) | –0.3542(4) | 0.070(4) | 0.085(4) | 0.066(4) | 0.021(4) | 0.028(3) | 0.043(4) |
| C(49) | 2*i* | –0.0087(5) | 0.3532(5) | –0.4130(4) | 0.069(4) | 0.091(5) | 0.044(3) | 0.039(4) | 0.027(3) | 0.029(3) |
| C(410) | 2*i* | –0.0484(5) | 0.2824(5) | –0.3797(4) | 0.066(4) | 0.073(4) | 0.046(3) | 0.014(3) | 0.005(3) | 0.011(3) |
| C(411) | 2*i* | –0.0031(4) | 0.2972(4) | –0.2826(4) | 0.062(3) | 0.057(3) | 0.053(3) | 0.013(3) | 0.016(3) | 0.022(3) |
| O(1) | 2*i* | 0.2143(4) | 0.0751(3) | 0.3085(4) | 0.101(4) | 0.074(3) | 0.114(4) | 0.009(3) | 0.054(3) | 0.029(3) |
| C(1) | 2*i* | 0.1501(6) | 0.0848(6) | 0.3591(5) | 0.114(6) | 0.100(6) | 0.103(6) | 0.022(5) | 0.055(5) | 0.030(5) |
| O(2) | 2*i* | 0.2659(4) | –0.0682(4) | 0.1863(4) | 0.107(4) | 0.094(4) | 0.104(4) | 0.027(3) | 0.025(3) | 0.003(3) |
| C(2) | 2*i* | 0.3708(6) | –0.0329(5) | 0.2174(6) | 0.099(6) | 0.083(5) | 0.109(6) | –0.008(4) | 0.052(5) | 0.006(4) |

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