# Crystal structure of diiodo-bis[(4*R*,5*R*)-*trans*-4,5-bis[(diphenylphosphino-methyl)-2,2-dimethyl-1,3-dioxalane]dicopper(I), $Cu_2I_2(C_{31}H_{32}O_2P_2)_2$

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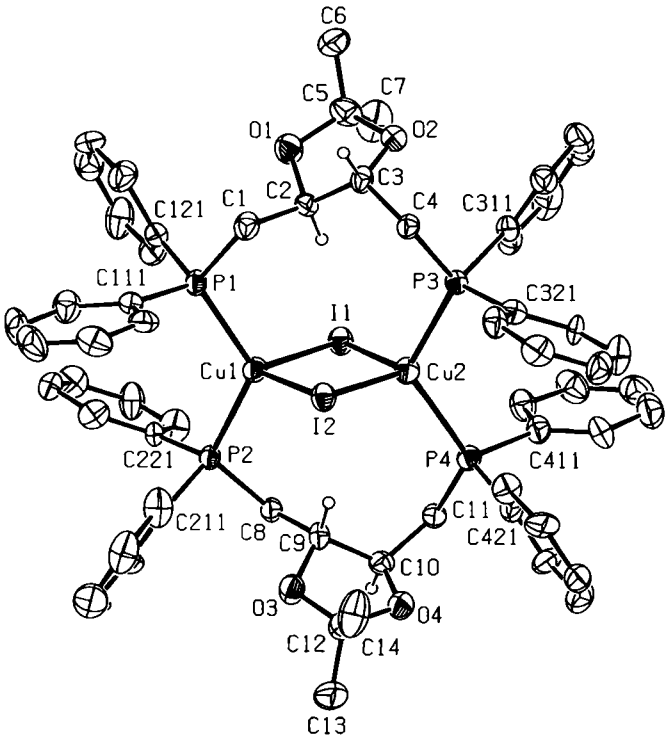


**Abstract**

$C_{62}H_{64}Cu_2I_2O_4P_4$, triclinic, *P*1 (no. 1), $a$ = 10.0989(2) Å, $b$ = 12.8084(1) Å, $c$ = 12.8423(2) Å, $\alpha$ = 65.074(1)°, $\beta$ = 84.31°, $\gamma$ = 87.854(1)°, $V$ = 1499.0 Å$^3$, $Z$ = 1, $R_{gt}(F)$ = 0.036, $wR_{ref}(F^2)$ = 0.098, $T$ = 293 K.

**Source of material**

The title compound was synthesized following a published procedure for the silver(I) analogs [1]. To a solution of optically pure DIOP (50.0 mg, 0.10 mmol; DIOP = (4*R*,5*R*)-*trans*-4,5-bis[(diphenylphosphino)methyl]-2,2-dimethyl-1,3-dioxalane) in $CH_2Cl_2$ (5 mL) was added an excess of CuI (40.0 mg, 0.21 mmol). After refluxing the mixture for 0.5 h, a precipitate was removed by filtration and the filtrate treated with dried diethyl ether (10 mL) to give a white powder (yield 76 %). Colorless crystals suitable for X-ray studies were obtained by slow evaporation of its solution in $CH_2Cl_2$/*n*-heptane (1:1).
Elemental analysis – found: C, 53.58 %; H, 4.82% (VarioEL); calc. for $C_{62}H_{64}Cu_2I_2O_4P_4$: C, 54.04 %; H, 4.68%.

**Experimental details**

The absolute configuration of the chiral complex was confirmed by a value of the Flack parameter of 0.02(3) [2].

**Discussion**

The chiral diphosphine DIOP is an important bidentate ligand for transition metal complexes that can be used for asymmetric catalytic reactions [3-5]. In the search for such complexes we have obtained a dimeric Cu(I) compound, $[CuI(R,R\text{-DIOP})]_2$, which features a novel $Cu_2$ core quadruply bridged by all the four ligands. Each copper atom resides at a slightly distorted tetrahedral environment composed of two iodine atoms and two phosphorous atoms each from a DIOP ligand. The four bridging ligands and the two copper atoms form a rhombic four-membered $Cu_2I_2$ ring (I–Cu–I, 109.11(6) and 110.42(6)°; Cu–I–Cu, 70.22(5)° and 70.24(5)°, respectively) and an outer 14-membered ring, Cu-DIOP-Cu-DIOP. Both of the Cu1-I1-Cu2-I2 and Cu1-P1-P3-Cu2-P4-P2 cores are coplanar (largest deviation 0.0069 Å and 0.0317 Å, respectively), intersecting at Cu1···Cu2 with a dihedral angle of 97.4(6)°. The coordination parameters around the two Cu(I) centers are slightly different. The Cu1—P1 and Cu1—P2 distances (2.252(4) Å and 2.254(4) Å) are shorter than the Cu2—P3 and Cu2—P4 distances (2.305(4) Å and 2.320(4) Å), while the P1–Cu1–P2 angle (122.5(2)°) is slightly wider than P3–Cu2–P4 (120.2(2)°). The bond angles about the two bridging iodine atoms are nearly identical (∠Cu2–I1–Cu1 = 70.22(5)°; ∠Cu2–I2–Cu1 = 70.24(5)°). The Cu···Cu separation of 3.141 Å indicates no significant interaction of the metals (the sum of the covalent radii is 2.76 Å). Similar coordination mode has been reported for some Ag(I)-DIOP compounds [1] and ((4*R*,5*R*)-*trans*-4,5-bis(((3-methylpheny1)phosphino)-methyl)-2,2-dimeth:y1-1,3-dioxalane)copper(I) chloride [5].

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

| | |
|---|---|
| Crystal: | colorless block, size 0.25 × 0.30 × 0.33 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 18.91 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART CCD, $\varphi/\omega$ |
| $2\theta_{max}$: | 49.94° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 7502, 6122 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 5213 |
| $N(param)_{refined}$: | 667 |
| Programs: | SHELXS-97 [6], SHELXL-97 [7] |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(1A) | 1*a* | 0.3841 | 0.1906 | 0.1975 | 0.066 |
| H(1B) | 1*a* | 0.3117 | 0.2000 | 0.3070 | 0.066 |
| H(2A) | 1*a* | 0.1583 | 0.0512 | 0.3038 | 0.052 |
| H(3A) | 1*a* | 0.4121 | −0.0057 | 0.3871 | 0.055 |
| H(4A) | 1*a* | 0.2709 | 0.0386 | 0.5128 | 0.050 |
| H(4B) | 1*a* | 0.3152 | −0.0895 | 0.5684 | 0.050 |
| H(6A) | 1*a* | 0.4605 | −0.1313 | 0.1524 | 0.148 |
| H(6B) | 1*a* | 0.4664 | −0.2249 | 0.2791 | 0.148 |
| H(6C) | 1*a* | 0.5209 | −0.1005 | 0.2438 | 0.148 |
| H(7A) | 1*a* | 0.1223 | −0.1501 | 0.2795 | 0.144 |
| H(7B) | 1*a* | 0.2169 | −0.2556 | 0.3008 | 0.144 |
| H(7C) | 1*a* | 0.2042 | −0.1622 | 0.1750 | 0.144 |
| H(8A) | 1*a* | −0.4245 | 0.3747 | 0.2353 | 0.049 |
| H(8B) | 1*a* | −0.3682 | 0.2501 | 0.2661 | 0.049 |
| H(9A) | 1*a* | −0.2658 | 0.2752 | 0.4232 | 0.051 |
| H(10A) | 1*a* | −0.5429 | 0.2407 | 0.4416 | 0.052 |
| H(11F) | 1*a* | −0.4350 | 0.0788 | 0.4531 | 0.051 |
| H(11G) | 1*a* | −0.5142 | 0.0574 | 0.5705 | 0.051 |
| H(13A) | 1*a* | −0.6191 | 0.4369 | 0.4728 | 0.157 |
| H(13B) | 1*a* | −0.5323 | 0.5288 | 0.4861 | 0.157 |
| H(13C) | 1*a* | −0.5974 | 0.4268 | 0.5960 | 0.157 |
| H(14A) | 1*a* | −0.2577 | 0.3347 | 0.5952 | 0.157 |
| H(14B) | 1*a* | −0.3693 | 0.3672 | 0.6702 | 0.157 |
| H(14C) | 1*a* | −0.2966 | 0.4640 | 0.5602 | 0.157 |
| H(11A) | 1*a* | 0.2214 | 0.4925 | −0.0542 | 0.081 |
| H(11B) | 1*a* | 0.2915 | 0.6771 | −0.1030 | 0.104 |
| H(11C) | 1*a* | 0.3761 | 0.7190 | 0.0375 | 0.109 |
| H(11D) | 1*a* | 0.3756 | 0.5822 | 0.2241 | 0.091 |
| H(11E) | 1*a* | 0.2951 | 0.3988 | 0.2715 | 0.074 |
| H(12A) | 1*a* | 0.0040 | 0.2451 | 0.0022 | 0.080 |
| H(12B) | 1*a* | 0.0243 | 0.2458 | −0.1709 | 0.100 |
| H(12C) | 1*a* | 0.2300 | 0.2475 | −0.2632 | 0.098 |

**Table 2.** Continued.

| Atom | Site | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|
| H(12D) | 1*a* | 0.4174 | 0.2669 | −0.1850 | 0.101 |
| H(12E) | 1*a* | 0.4016 | 0.2786 | −0.0110 | 0.094 |
| H(21A) | 1*a* | −0.3523 | 0.5900 | 0.1005 | 0.075 |
| H(21B) | 1*a* | −0.3489 | 0.7686 | 0.0917 | 0.122 |
| H(21C) | 1*a* | −0.1989 | 0.8232 | 0.1826 | 0.117 |
| H(21D) | 1*a* | −0.0390 | 0.6925 | 0.2729 | 0.101 |
| H(21E) | 1*a* | −0.0263 | 0.5149 | 0.2704 | 0.083 |
| H(22A) | 1*a* | −0.3447 | 0.2860 | 0.0666 | 0.078 |
| H(22B) | 1*a* | −0.3362 | 0.3170 | −0.1207 | 0.081 |
| H(22C) | 1*a* | −0.2020 | 0.4466 | −0.2589 | 0.080 |
| H(22D) | 1*a* | −0.0577 | 0.5577 | −0.2157 | 0.080 |
| H(22E) | 1*a* | −0.0705 | 0.5368 | −0.0216 | 0.073 |
| H(31A) | 1*a* | 0.2375 | −0.2917 | 0.6678 | 0.076 |
| H(31B) | 1*a* | 0.2385 | −0.4716 | 0.6650 | 0.095 |
| H(31C) | 1*a* | 0.0701 | −0.5150 | 0.5803 | 0.113 |
| H(31D) | 1*a* | −0.0976 | −0.3861 | 0.4999 | 0.117 |
| H(31E) | 1*a* | −0.0821 | −0.1987 | 0.4908 | 0.070 |
| H(32A) | 1*a* | −0.0447 | −0.2349 | 0.7813 | 0.056 |
| H(32B) | 1*a* | −0.0491 | −0.2652 | 0.9683 | 0.086 |
| H(32C) | 1*a* | 0.0619 | −0.1445 | 1.0208 | 0.083 |
| H(32D) | 1*a* | 0.2054 | −0.0056 | 0.8836 | 0.079 |
| H(32E) | 1*a* | 0.2175 | 0.0181 | 0.6917 | 0.067 |
| H(41A) | 1*a* | −0.3697 | −0.1086 | 0.4772 | 0.073 |
| H(41B) | 1*a* | −0.4488 | −0.2913 | 0.5287 | 0.095 |
| H(41C) | 1*a* | −0.4743 | −0.4217 | 0.7190 | 0.098 |
| H(41D) | 1*a* | −0.4078 | −0.3756 | 0.8551 | 0.100 |
| H(41E) | 1*a* | −0.3310 | −0.1893 | 0.8138 | 0.080 |
| H(42A) | 1*a* | −0.1166 | 0.0668 | 0.7308 | 0.070 |
| H(42B) | 1*a* | −0.1363 | 0.0768 | 0.9134 | 0.081 |
| H(42C) | 1*a* | −0.3414 | 0.0541 | 1.0165 | 0.089 |
| H(42D) | 1*a* | −0.5296 | 0.0250 | 0.9415 | 0.090 |
| H(42E) | 1*a* | −0.5068 | 0.0110 | 0.7676 | 0.073 |

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

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| I(1) | 1*a* | −0.14501(5) | 0.06170(5) | 0.28491(5) | 0.0491(6) | 0.0502(5) | 0.0463(5) | −0.0026(4) | −0.0089(4) | −0.0146(4) |
| I(2) | 1*a* | 0.04143(5) | 0.24304(5) | 0.46430(5) | 0.0494(6) | 0.0503(5) | 0.0460(5) | −0.0058(4) | −0.0085(4) | −0.0133(4) |
| Cu(1) | 1*a* | −0.0213(2) | 0.2610(2) | 0.2550(1) | 0.035(1) | 0.053(1) | 0.046(1) | 0.0020(8) | −0.0018(8) | −0.0098(9) |
| Cu(2) | 1*a* | −0.0839(2) | 0.0473(1) | 0.4916(1) | 0.039(1) | 0.050(1) | 0.045(1) | −0.0016(8) | −0.0083(8) | −0.0129(9) |
| P(1) | 1*a* | 0.1781(4) | 0.2823(3) | 0.1527(3) | 0.036(2) | 0.045(2) | 0.037(2) | −0.001(2) | −0.004(2) | −0.003(2) |
| P(2) | 1*a* | −0.1901(4) | 0.3851(3) | 0.1907(3) | 0.035(2) | 0.042(2) | 0.033(2) | −0.002(2) | −0.003(2) | −0.007(2) |
| P(3) | 1*a* | 0.0856(4) | −0.0808(3) | 0.5649(3) | 0.035(2) | 0.038(2) | 0.039(2) | −0.001(2) | −0.008(2) | −0.013(2) |
| P(4) | 1*a* | −0.2901(4) | 0.0221(3) | 0.5965(4) | 0.033(2) | 0.046(2) | 0.048(2) | −0.004(2) | −0.002(2) | −0.013(2) |
| O(1) | 1*a* | 0.3015(8) | 0.0124(8) | 0.2055(7) | 0.078(6) | 0.062(5) | 0.051(5) | 0.006(4) | −0.010(4) | −0.021(4) |
| O(2) | 1*a* | 0.3095(8) | −0.1323(7) | 0.3873(7) | 0.061(4) | 0.049(4) | 0.052(5) | 0.005(3) | 0.000(3) | −0.018(4) |
| O(3) | 1*a* | −0.3826(9) | 0.4061(6) | 0.4070(7) | 0.089(6) | 0.043(4) | 0.052(5) | −0.012(4) | 0.011(4) | −0.024(4) |
| O(4) | 1*a* | −0.4730(7) | 0.2579(6) | 0.5688(6) | 0.066(5) | 0.055(4) | 0.048(4) | 0.000(3) | 0.000(3) | −0.020(3) |
| C(1) | 1*a* | 0.299(1) | 0.181(1) | 0.243(1) | 0.044(7) | 0.058(8) | 0.052(7) | −0.005(5) | −0.003(5) | −0.013(6) |
| C(2) | 1*a* | 0.2555(9) | 0.0566(7) | 0.2899(9) | 0.038(5) | 0.038(5) | 0.047(6) | 0.005(4) | −0.004(4) | −0.012(4) |
| C(3) | 1*a* | 0.3178(9) | −0.0261(7) | 0.3960(7) | 0.041(5) | 0.052(5) | 0.034(5) | −0.003(4) | −0.007(4) | −0.007(4) |
| C(4) | 1*a* | 0.260(1) | −0.036(1) | 0.512(1) | 0.037(5) | 0.043(6) | 0.037(6) | −0.001(4) | −0.004(4) | −0.009(5) |
| C(5) | 1*a* | 0.317(2) | −0.108(1) | 0.265(1) | 0.084(9) | 0.059(8) | 0.068(9) | 0.010(6) | −0.016(7) | −0.040(8) |
| C(6) | 1*a* | 0.454(2) | −0.145(2) | 0.232(2) | 0.10(2) | 0.11(2) | 0.06(1) | 0.04(1) | 0.02(1) | −0.01(1) |
| C(7) | 1*a* | 0.205(1) | −0.175(1) | 0.254(1) | 0.12(1) | 0.11(1) | 0.079(9) | −0.025(8) | −0.016(8) | −0.050(8) |
| C(8) | 1*a* | −0.353(1) | 0.323(1) | 0.2703(9) | 0.039(5) | 0.039(5) | 0.037(6) | 0.000(4) | −0.003(4) | −0.009(5) |
| C(9) | 1*a* | −0.3534(9) | 0.3028(8) | 0.3964(9) | 0.042(5) | 0.039(5) | 0.036(5) | −0.006(4) | −0.007(4) | −0.005(4) |
| C(10) | 1*a* | −0.4597(9) | 0.2227(7) | 0.4789(7) | 0.038(5) | 0.049(5) | 0.042(5) | 0.006(4) | −0.008(4) | −0.018(4) |
| C(11) | 1*a* | −0.436(1) | 0.096(1) | 0.520(1) | 0.033(5) | 0.046(6) | 0.044(6) | 0.002(4) | −0.006(4) | −0.012(5) |
| C(12) | 1*a* | −0.433(2) | 0.376(1) | 0.521(1) | 0.075(9) | 0.07(1) | 0.069(9) | −0.007(8) | 0.010(7) | −0.033(8) |
| C(13) | 1*a* | −0.557(2) | 0.449(2) | 0.519(2) | 0.13(2) | 0.07(1) | 0.11(2) | 0.01(1) | 0.04(1) | −0.04(1) |
| C(14) | 1*a* | −0.330(2) | 0.386(1) | 0.593(1) | 0.13(1) | 0.12(1) | 0.055(8) | −0.046(9) | −0.010(7) | −0.027(8) |
| C(111) | 1*a* | 0.252(1) | 0.425(1) | 0.115(1) | 0.037(7) | 0.043(7) | 0.045(7) | 0.006(5) | −0.003(5) | −0.015(6) |
| C(112) | 1*a* | 0.252(2) | 0.511(2) | 0.002(2) | 0.06(1) | 0.07(1) | 0.06(1) | −0.009(9) | −0.008(8) | −0.017(9) |
| C(113) | 1*a* | 0.295(2) | 0.621(2) | −0.028(2) | 0.09(2) | 0.04(1) | 0.10(2) | −0.020(9) | −0.01(1) | 0.00(1) |
| C(114) | 1*a* | 0.343(2) | 0.646(2) | 0.057(2) | 0.08(1) | 0.04(1) | 0.13(2) | −0.012(9) | −0.01(1) | −0.02(1) |
| C(115) | 1*a* | 0.344(2) | 0.564(2) | 0.168(2) | 0.071(9) | 0.07(1) | 0.10(1) | 0.008(8) | −0.022(8) | −0.05(1) |

**Table 3.** Continued.

| Atom | Site | x | y | z | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| C(116) | 1*a* | 0.297(2) | 0.454(1) | 0.196(2) | 0.048(7) | 0.055(8) | 0.08(1) | 0.009(6) | 0.006(6) | −0.030(7) |
| C(121) | 1*a* | 0.198(2) | 0.267(1) | 0.021(1) | 0.048(9) | 0.037(7) | 0.053(9) | 0.002(6) | 0.004(7) | −0.012(7) |
| C(122) | 1*a* | 0.089(2) | 0.253(2) | −0.036(2) | 0.042(9) | 0.06(1) | 0.08(1) | −0.008(7) | 0.007(8) | −0.015(9) |
| C(123) | 1*a* | 0.100(2) | 0.250(2) | −0.137(2) | 0.09(1) | 0.09(1) | 0.05(1) | −0.03(1) | −0.017(9) | −0.013(9) |
| C(124) | 1*a* | 0.222(2) | 0.253(2) | −0.193(2) | 0.12(2) | 0.06(1) | 0.06(1) | −0.01(1) | 0.00(1) | −0.03(1) |
| C(125) | 1*a* | 0.334(2) | 0.264(2) | −0.146(2) | 0.09(1) | 0.08(1) | 0.07(1) | 0.03(1) | 0.03(1) | −0.02(1) |
| C(126) | 1*a* | 0.325(2) | 0.271(2) | −0.041(2) | 0.05(1) | 0.10(1) | 0.06(1) | 0.007(9) | 0.000(8) | −0.01(1) |
| C(211) | 1*a* | −0.190(2) | 0.526(1) | 0.185(1) | 0.051(9) | 0.063(9) | 0.036(7) | −0.001(7) | 0.009(6) | −0.009(6) |
| C(212) | 1*a* | −0.285(2) | 0.609(1) | 0.134(2) | 0.06(1) | 0.049(9) | 0.09(1) | 0.001(7) | 0.010(7) | −0.039(8) |
| C(213) | 1*a* | −0.285(2) | 0.716(2) | 0.131(2) | 0.12(2) | 0.06(1) | 0.13(2) | 0.02(1) | 0.04(1) | −0.05(1) |
| C(214) | 1*a* | −0.196(3) | 0.750(2) | 0.183(2) | 0.14(2) | 0.07(1) | 0.09(1) | −0.01(1) | 0.02(1) | −0.05(1) |
| C(215) | 1*a* | −0.101(2) | 0.672(2) | 0.236(2) | 0.12(1) | 0.08(1) | 0.060(9) | −0.05(1) | 0.006(9) | −0.040(8) |
| C(216) | 1*a* | −0.095(2) | 0.564(2) | 0.236(1) | 0.09(1) | 0.08(1) | 0.043(7) | −0.021(9) | −0.029(7) | −0.023(7) |
| C(221) | 1*a* | −0.210(1) | 0.412(1) | 0.040(1) | 0.045(7) | 0.031(6) | 0.032(6) | 0.000(5) | 0.002(5) | −0.003(5) |
| C(222) | 1*a* | −0.289(2) | 0.343(2) | 0.011(2) | 0.07(1) | 0.066(9) | 0.064(9) | −0.020(7) | −0.011(7) | −0.034(8) |
| C(223) | 1*a* | −0.282(2) | 0.361(2) | −0.100(1) | 0.08(1) | 0.063(9) | 0.051(9) | −0.027(7) | −0.014(7) | −0.011(7) |
| C(224) | 1*a* | −0.201(2) | 0.438(2) | −0.183(1) | 0.08(1) | 0.08(1) | 0.047(8) | 0.003(8) | −0.021(7) | −0.034(8) |
| C(225) | 1*a* | −0.117(2) | 0.506(1) | −0.159(1) | 0.08(1) | 0.06(1) | 0.05(1) | −0.001(8) | 0.017(8) | −0.012(8) |
| C(226) | 1*a* | −0.124(2) | 0.492(2) | −0.042(1) | 0.06(1) | 0.07(1) | 0.058(9) | −0.004(8) | −0.007(7) | −0.037(9) |
| C(311) | 1*a* | 0.079(1) | −0.230(1) | 0.574(1) | 0.044(8) | 0.030(6) | 0.051(7) | −0.011(5) | −0.002(6) | −0.018(6) |
| C(312) | 1*a* | 0.174(2) | −0.311(1) | 0.631(2) | 0.052(9) | 0.06(1) | 0.062(8) | 0.003(7) | −0.005(7) | −0.011(7) |
| C(313) | 1*a* | 0.173(2) | −0.418(2) | 0.632(2) | 0.07(1) | 0.049(9) | 0.10(1) | 0.000(8) | 0.003(9) | −0.017(9) |
| C(314) | 1*a* | 0.072(3) | −0.443(2) | 0.581(2) | 0.14(2) | 0.05(1) | 0.09(1) | −0.02(1) | 0.04(1) | −0.04(1) |
| C(315) | 1*a* | −0.028(3) | −0.365(2) | 0.530(2) | 0.14(2) | 0.08(1) | 0.07(1) | −0.04(1) | 0.03(1) | −0.04(1) |
| C(316) | 1*a* | −0.019(2) | −0.254(1) | 0.526(1) | 0.08(1) | 0.046(8) | 0.052(8) | −0.016(7) | 0.006(7) | −0.020(7) |
| C(321) | 1*a* | 0.087(1) | −0.107(1) | 0.714(1) | 0.039(7) | 0.050(8) | 0.044(8) | 0.005(6) | −0.016(5) | −0.022(6) |
| C(322) | 1*a* | 0.008(2) | −0.189(1) | 0.800(1) | 0.058(9) | 0.040(7) | 0.026(6) | −0.018(6) | 0.007(6) | −0.001(5) |
| C(323) | 1*a* | 0.002(2) | −0.205(2) | 0.913(1) | 0.10(1) | 0.07(1) | 0.044(9) | −0.033(9) | −0.007(8) | −0.014(8) |
| C(324) | 1*a* | 0.071(2) | −0.136(2) | 0.945(1) | 0.09(1) | 0.08(1) | 0.037(7) | −0.003(8) | 0.000(6) | −0.016(7) |
| C(325) | 1*a* | 0.155(2) | −0.052(2) | 0.863(1) | 0.08(1) | 0.08(1) | 0.056(9) | 0.006(8) | −0.021(7) | −0.041(8) |
| C(326) | 1*a* | 0.162(2) | −0.038(1) | 0.747(1) | 0.045(7) | 0.058(8) | 0.050(8) | −0.005(6) | −0.018(5) | −0.006(6) |
| C(411) | 1*a* | −0.345(2) | −0.129(1) | 0.643(2) | 0.031(6) | 0.049(8) | 0.060(9) | −0.005(5) | −0.004(6) | −0.004(7) |
| C(412) | 1*a* | −0.379(2) | −0.161(1) | 0.554(2) | 0.061(9) | 0.054(8) | 0.058(8) | −0.007(6) | −0.017(6) | −0.012(7) |
| C(413) | 1*a* | −0.426(2) | −0.270(1) | 0.586(2) | 0.08(1) | 0.053(9) | 0.11(1) | −0.010(7) | −0.014(9) | −0.032(9) |
| C(414) | 1*a* | −0.439(2) | −0.349(2) | 0.699(2) | 0.07(1) | 0.06(1) | 0.11(2) | −0.002(9) | −0.00(1) | −0.04(1) |
| C(415) | 1*a* | −0.402(2) | −0.320(2) | 0.779(2) | 0.09(2) | 0.06(1) | 0.07(1) | 0.00(1) | −0.01(1) | −0.00(1) |
| C(416) | 1*a* | −0.354(2) | −0.208(1) | 0.755(2) | 0.08(1) | 0.038(9) | 0.06(1) | 0.007(8) | −0.015(8) | −0.005(8) |
| C(421) | 1*a* | −0.311(2) | 0.037(1) | 0.735(1) | 0.05(1) | 0.053(9) | 0.042(8) | 0.003(7) | −0.005(7) | −0.005(7) |
| C(422) | 1*a* | −0.199(2) | 0.057(1) | 0.774(1) | 0.08(1) | 0.07(1) | 0.046(8) | −0.001(8) | −0.015(7) | −0.031(8) |
| C(423) | 1*a* | −0.211(2) | 0.064(1) | 0.884(1) | 0.08(1) | 0.07(1) | 0.07(1) | 0.011(8) | −0.003(9) | −0.056(9) |
| C(424) | 1*a* | −0.334(2) | 0.051(2) | 0.945(2) | 0.11(2) | 0.06(1) | 0.05(1) | 0.01(1) | 0.01(1) | −0.018(9) |
| C(425) | 1*a* | −0.446(2) | 0.032(2) | 0.901(2) | 0.07(1) | 0.09(1) | 0.046(9) | 0.005(9) | 0.002(8) | −0.012(9) |
| C(426) | 1*a* | −0.432(2) | 0.025(2) | 0.797(1) | 0.047(9) | 0.09(1) | 0.043(8) | 0.012(8) | 0.003(7) | −0.023(8) |

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