SUPLEMENTARY INFORMATION

# Mother structures related to the hexagonal and cubic close packing in $Cu_{24}$ clusters: solvent-influenced derivatives

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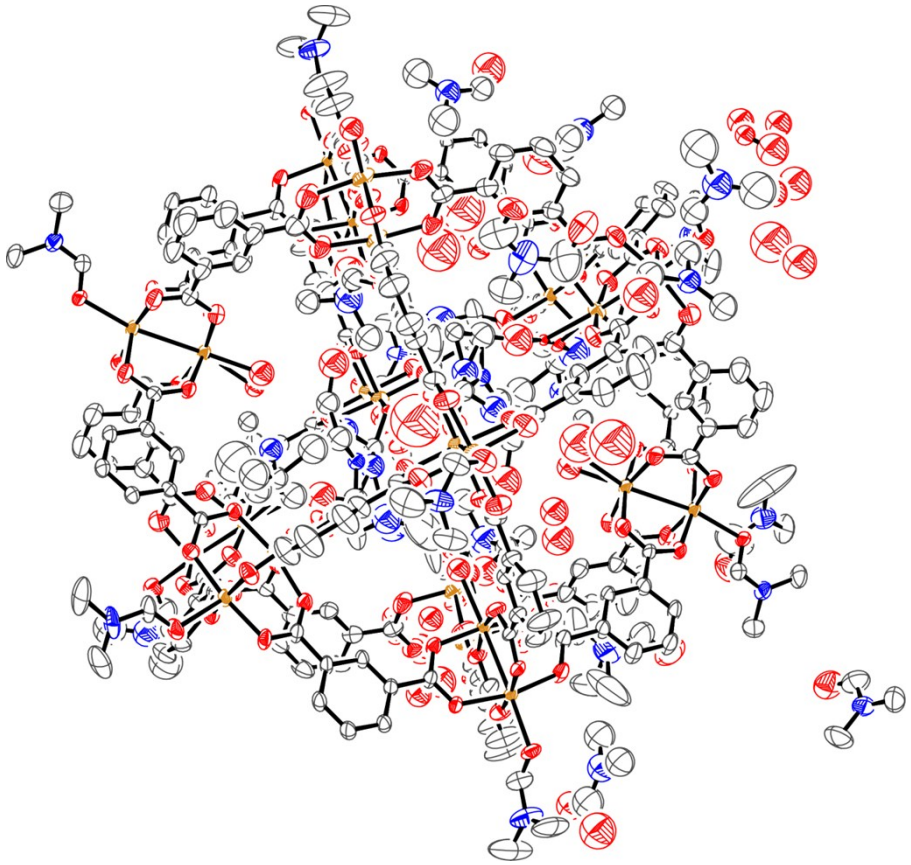

**Fig. S1** ORTEP[1] detail for compound **1**. The thermal ellipsoids correspond to 50% probability. Color codes: Cu= orange; C= grey; O= red; N= blue.

[1] Farrugia, L. J., *J. Appl. Crystallogr.* **1997,** *30*, 565.

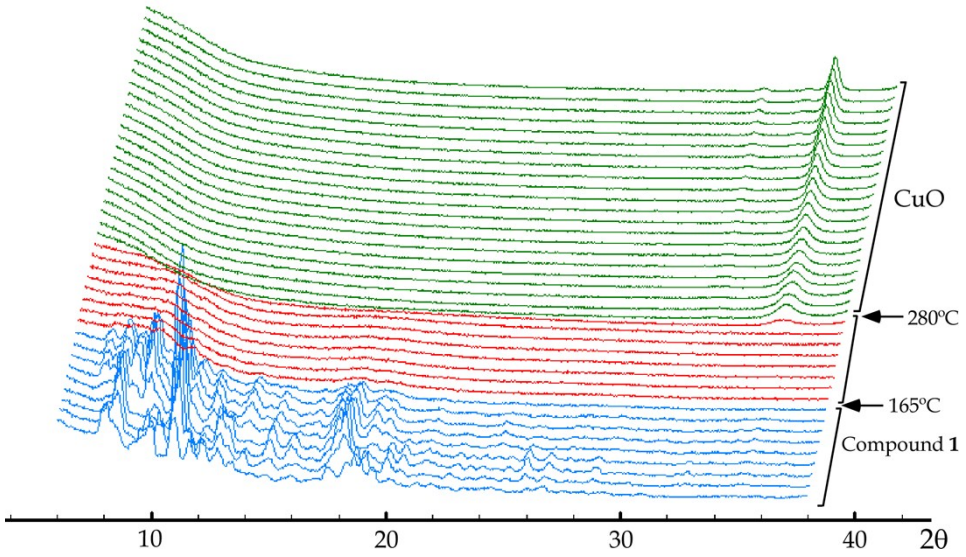


**Fig. S2** Thermodiffractogram for compound **1**.

**Table S1** Crystallographic parameters for the eight compared compounds.

| | **1** | **2**[18] | **3**[16] | **4**[17] |
|---|---|---|---|---|
| **structural formula** | $[Cu_{24}(m\text{-}BDC)_{24}(DMF)_{20}(H_2O)_4]\cdot 24DMF\cdot 40H_2O$ | $[Cu_{24}(m\text{-}BDC)_{24}(MeOH)_{24}]\cdot xS$ | $[Cu_{24}(m\text{-}BDC)_{24}(DMF)_{14}(H_2O)_{10}]\cdot 50(H_2O)6(DMF)6(C_2H_5OH)$ | $[Cu_{24}(m\text{-}BDC)_{24}(S)_{24}]\cdot xS$ |
| **empirical formula** | $C_{297.58}H_{466}Cu_{24}N_{35.6}O_{172.7}$ | $C_{308}H_{96}Cu_{24}O_{120}$ | $C_{264}H_{392}Cu_{24}N_{20}O_{182}$ | $C_{192}H_{96}Cu_{24}O_{120}$ |
| **$F_w$, g mol$^{-1}$** | 8830.49 | 7241.05 | 8282.94 | 5847.65 |
| **cryst system** | Triclinic | Hexagonal | Triclinic | Triclinic |
| **space group** | $P\bar{1}$ | $P6_3/m$ | $P\bar{1}$ | $P\bar{1}$ |
| ***a*, Å** | 24.4797(3) | 28.6458(19) | 23.5283(15) | 24.3386(18) |
| ***b*, Å** | 24.5938(3) | | 24.3224 (16) | 24.4267(18) |
| ***c*, Å** | 25.2374(3) | 28.165(3) | 25.0401 (16) | 25.442(3) |
| **$\alpha$, deg** | 118.4357(13) | | 61.479 (1) | 112.1900(10) |
| **$\beta$, deg** | 111.9694(11) | | 82.864 (1) | 115.5470(10) |
| **$\gamma$, deg** | 94.2287(10) | | 75.298 (1) | 98.0710(10) |
| ***V*, Å$^3$** | 11784.9 (2) | 20015(3) | 12178.1(14) | 11774.0(19) |
| ***Z*** | 1 | 2 | 1 | 1 |
| **$\rho_{obs}$, $\rho_{cal}$, g·cm$^{-3}$** | 1.346(5), 1.072 | none, 1.222 | none, 1.129 | none, 0.825 |
| **$\mu$, mm$^{-1}$** | 1.737 | 1.318 | 1.100 | 1.108 |
| **absorption correction** | Analytical | ---- | SADABS | Multi-scan |
| **radiation, λ, Å** | 1.54184 | 0.71073 | 0.71073 | 0.71073 |
| **temperature, K** | 100.0(2) | 173(2) | 158(2) | 110(2) |
| **reflns collected, unique** | 155317, 41318 | 8931, 4003 | 76620, 25727 | 44979, 21948 |
| **final *R* indices [I > 2σ(I)]** | R1=0.0859, wR2=0.2564 | *R*1=0.1116, *wR2*=0.3083 | *R*1=0.1710, *wR2*=0.4103 | *R*1=0.0638, *wR2*=0.1315 |
| ***R* indices (all data)** | R1=0.0975, wR2=0.2744 | *R*1=0.1837, *wR2*=0.3416 | *R*1=0.2839, *wR2*=0.4618 | *R*1=0.1092, *wR2*=0.1389 |
| **GOF on $F^2$** | 1.087 | 1.317 | 1.371 | 1.017 |
| **parameters/restraints** | 2154/47 | 728/0 | 1449/361 | 1369/0 |

| | **5**[18] | **6**[18] | **7**[16] | **8**[18] |
|---|---|---|---|---|
| **structural formula** | $[Cu_{24}(m\text{-BDC})_{24}(Py)_{12}(MeOH)_{12}]\cdot xS$ | $[Cu_{24}(m\text{-BDC})_{24}(MeOH)_{24}]\cdot xS$ | $[Cu_{24}(m\text{-BDC})_{24}(H_2O)_{24}]\cdot 42(H_2O)$ | $[Cu_{24}(m\text{-BDC})_{24}(MeOH)_{24}]\cdot xS$ |
| **empirical formula** | $C_{249.33}Cu_{16}N_{16}O_{64}$ | $C_{245.84}H_{96}Cu_{24}O_{120}$ | $C_{191.5}H_{180}Cu_{24}O_{162}$ | $C_{208}Cu_{24}O_{112}$ |
| $F_w$, g mol$^{-1}$ | 5259.29 | 6494.21 | 6598.31 | 6259.65 |
| **cryst system** | Triclinic | Cubic | Cubic | Monoclinic |
| **space group** | $P\bar{1}$ | *Im*-3*m* | *Im*-3*m* | *C2/c* |
| ***a*, Å** | 26.202(9) | 27.6895(17) | 27.722(3) | 33.933(7) |
| ***b*, Å** | 27.756(10) | | | 36.925(8) |
| ***c*, Å** | 28.407(10) | | | 29.577(6) |
| **$\alpha$, deg** | 92.583(5) | | | 90 |
| **$\beta$, deg** | 96.393(5) | | | 93.460(3) |
| **$\gamma$, deg** | 92.643(5) | | | 90 |
| ***V*, Å$^3$** | 20483(12) | 21230(2) | 21306(4) | 36991(13) |
| ***Z*** | 2 | 2 | 2 | 4 |
| $\rho_{obs}$, $\rho_{cal}$, g·cm$^{-3}$ | none, 1.279 | none, 1.016 | none, 1.029 | none, 1.353 |
| $\mu$, mm$^{-1}$ | 1.291 | 1.235 | 1.238 | 0.762 |
| **absorption correction** | SADABS | ---- | ---- | ---- |
| **radiation, $\lambda$, Å** | 0.71073 | 0.71073 | 0.71073 | 0.71073 |
| **temperature, K** | 173(2) | 173(2) | 163(2) | 293(2) |
| **reflns collected, unique** | 31316, 10314 | 1501, 996 | 30726, 1116 | 11089, 3512 |
| **final *R* indices [I > 2σ(I)]** | *R*1=0.1379, *wR*2=0.3499 | *R*1=0.0784, *wR*2=0.2725 | *R*1=0.1004, *wR*2=0.3212 | *R*1=0.1353, *wR*2=0.3382 |
| ***R* indices (all data)** | *R*1=0.2849, *wR*2=0.4223 | *R*1=0.1069, *wR*2=0.2953 | *R*1=0.1908, *wR*2=0.3427 | *R*1=0.3056, *wR*2=0.4226 |
| **GOF on $F^2$** | 1.089 | 1.138 | 1.053 | 1.031 |
| **parameters/restraints** | 2529/0 | 100/0 | 90/0 | 823/0 |

**Table S2.** Fractional atomic coordinates and equivalent thermal factors for compound **1** (Å$^2$).

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4574 (2) | 0.0455 (2) | -0.1777 (2) | 0.0374 (9) |
| C2 | 0.3895 (2) | 0.0135 (2) | -0.2231 (3) | 0.044 (2) |
| C3 | 0.3637 (3) | -0.0528 (3) | -0.2510 (4) | 0.071 (2) |
| H3 | 0.3888 | -0.0768 | -0.2392 | 0.085* |
| C4 | 0.3002 (3) | -0.0828 (4) | -0.2967 (6) | 0.098 (3) |
| H4 | 0.2826 | -0.1281 | -0.3178 | 0.117* |
| C5 | 0.2629 (3) | -0.0468 (3) | -0.3114 (5) | 0.075 (2) |
| H5 | 0.2198 | -0.0674 | -0.3416 | 0.09* |
| C6 | 0.2885 (2) | 0.0190 (2) | -0.2821 (3) | 0.0471 (2) |
| C7 | 0.3516 (2) | 0.0494 (2) | -0.2377 (3) | 0.0398 (1) |
| H7 | 0.3689 | 0.0946 | -0.2173 | 0.048* |
| C8 | 0.2486 (2) | 0.0571 (2) | -0.3011 (3) | 0.0447 (1) |
| C9 | 0.6855 (3) | 0.1573 (2) | -0.0144 (2) | 0.0458 (1) |
| C10 | 0.7505 (3) | 0.1908 (3) | 0.0424 (3) | 0.0564 (1) |
| C11 | 0.7873 (4) | 0.1548 (4) | 0.0589 (5) | 0.098 (3) |
| H11 | 0.7724 | 0.1087 | 0.0324 | 0.118* |

| | | | | |
|---|---|---|---|---|
| C12 | 0.8461 (4) | 0.1878 (4) | 0.1150 (6) | 0.130 (5) |
| H12 | 0.8718 | 0.164 | 0.1263 | 0.156* |
| C13 | 0.8672 (4) | 0.2552 (4) | 0.1543 (5) | 0.101 (3) |
| H13 | 0.9074 | 0.2771 | 0.1924 | 0.121* |
| C14 | 0.8308 (3) | 0.2906 (3) | 0.1389 (3) | 0.064 (2) |
| C15 | 0.7725 (3) | 0.2587 (3) | 0.0833 (3) | 0.0497 (1) |
| H15 | 0.7471 | 0.2831 | 0.0727 | 0.06* |
| C16 | 0.8528 (3) | 0.3635 (3) | 0.1826 (3) | 0.056 (2) |
| C17 | 0.4154 (2) | 0.9155 (2) | 0.1993 (2) | 0.0323 (9) |
| C18 | 0.4176 (2) | 0.9302 (2) | 0.2653 (2) | 0.0328 (9) |
| C19 | 0.4095 (2) | 0.9882 (2) | 0.3070 (2) | 0.0361 (9) |
| H19 | 0.3998 | 1.0169 | 0.2924 | 0.043* |
| C20 | 0.4158 (3) | 1.0037 (2) | 0.3700 (3) | 0.0450 (1) |
| H20 | 0.4105 | 1.0432 | 0.3985 | 0.054* |
| C21 | 0.4298 (2) | 0.9619 (2) | 0.3912 (2) | 0.040 (1) |
| H21 | 0.4342 | 0.9728 | 0.4344 | 0.047* |
| C22 | 0.4376 (2) | 0.9035 (2) | 0.3493 (2) | 0.0347 (9) |
| C23 | 0.4305 (2) | 0.8879 (2) | 0.2860 (2) | 0.0326 (9) |
| H23 | 0.4346 | 0.8479 | 0.2568 | 0.039* |
| C24 | 0.4539 (2) | 0.8578 (2) | 0.3712 (2) | 0.0354 (9) |
| C25 | 0.5557 (3) | 0.1208 (2) | 0.0007 (2) | 0.044 (2) |
| C26 | 0.5464 (3) | 0.1304 (2) | 0.0597 (2) | 0.041 (2) |
| C27 | 0.5450 (3) | 0.0818 (2) | 0.0722 (3) | 0.054 (2) |
| H27 | 0.5489 | 0.0418 | 0.0426 | 0.065* |
| C28 | 0.5382 (3) | 0.0903 (3) | 0.1268 (3) | 0.058 (2) |
| H28 | 0.5362 | 0.056 | 0.1343 | 0.07* |
| C29 | 0.5342 (3) | 0.1493 (2) | 0.1711 (3) | 0.049 (2) |
| H29 | 0.5303 | 0.1556 | 0.2096 | 0.059* |
| C30 | 0.5357 (2) | 0.1992 (2) | 0.1598 (2) | 0.039 (2) |
| C31 | 0.5406 (2) | 0.1892 (2) | 0.1028 (2) | 0.0367 (9) |
| H31 | 0.5399 | 0.2223 | 0.0934 | 0.044* |
| C32 | 0.5332 (2) | 0.2632 (2) | 0.2089 (2) | 0.036 (2) |
| C33 | 0.8820 (2) | 0.8199 (2) | 0.3755 (2) | 0.042 (2) |
| C34 | 0.9209 (2) | 0.7826 (2) | 0.3977 (3) | 0.046 (2) |
| C35 | 0.9779 (3) | 0.8145 (3) | 0.4558 (3) | 0.059 (2) |
| H35 | 0.9923 | 0.8607 | 0.4831 | 0.072* |
| C36 | 1.0134 (3) | 0.7803 (3) | 0.4740 (4) | 0.071 (12) |
| H36 | 1.0519 | 0.8026 | 0.5145 | 0.084* |
| C37 | 0.9934 (3) | 0.7126 (3) | 0.4333 (4) | 0.065 (2) |
| H37 | 1.0188 | 0.6887 | 0.4451 | 0.078* |
| C38 | 0.9362 (2) | 0.6802 (2) | 0.3754 (3) | 0.0472 (1) |

| | | | | |
|---|---|---|---|---|
| C39 | 0.8998 (2) | 0.7144 (2) | 0.3572 (3) | 0.045 (2) |
| H39 | 0.8607 | 0.6921 | 0.3175 | 0.055* |
| C40 | 0.9150 (2) | 0.6067 (2) | 0.3303 (3) | 0.047 (2) |
| C41 | 0.7729 (2) | 0.8999 (2) | 0.4178 (3) | 0.045 (2) |
| C42 | 0.7451 (2) | 0.9121 (2) | 0.4655 (3) | 0.049 (2) |
| C43 | 0.7766 (3) | 0.9651 (3) | 0.5329 (3) | 0.073 (2) |
| H43 | 0.8159 | 0.9929 | 0.5492 | 0.088* |
| C44 | 0.7506 (4) | 0.9771 (4) | 0.5760 (4) | 0.085 (2) |
| H44 | 0.7723 | 1.0127 | 0.6221 | 0.102* |
| C45 | 0.6925 (3) | 0.9369 (3) | 0.5512 (3) | 0.071 (2) |
| H45 | 0.6747 | 0.9451 | 0.5808 | 0.086* |
| C46 | 0.6602 (3) | 0.8847 (3) | 0.4839 (3) | 0.048 (2) |
| C47 | 0.6874 (2) | 0.8714 (2) | 0.4413 (3) | 0.044 (2) |
| H47 | 0.6665 | 0.8346 | 0.3958 | 0.053* |
| C48 | 0.5965 (2) | 0.8432 (2) | 0.4563 (2) | 0.042 (2) |
| C49 | 0.1356 (2) | 0.1317 (2) | -0.2608 (3) | 0.042 (2) |
| C50 | 0.1083 (2) | 0.1426 (2) | -0.2135 (3) | 0.047 (2) |
| C51 | 0.0602 (3) | 0.0938 (3) | -0.2305 (3) | 0.068 (2) |
| H51 | 0.0454 | 0.0525 | -0.2718 | 0.082* |
| C52 | 0.0338 (4) | 0.1043 (4) | -0.1887 (4) | 0.090 (3) |
| H52 | 0.0016 | 0.0702 | -0.2003 | 0.108* |
| C53 | 0.0548 (3) | 0.1667 (3) | -0.1276 (3) | 0.069 (2) |
| H53 | 0.0361 | 0.175 | -0.0987 | 0.083* |
| C54 | 0.1029 (2) | 0.2150 (3) | -0.1110 (3) | 0.049 (2) |
| C55 | 0.1308 (2) | 0.2028 (2) | -0.1532 (3) | 0.044 (2) |
| H55 | 0.1648 | 0.2356 | -0.1406 | 0.053* |
| C56 | 0.1245 (2) | 0.2818 (3) | -0.0482 (2) | 0.045 (2) |
| C57 | 0.8394 (2) | 0.4704 (3) | 0.3257 (3) | 0.059 (2) |
| C58 | 0.8125 (3) | 0.4585 (3) | 0.3647 (3) | 0.060 (2) |
| C59 | 0.8492 (3) | 0.4608 (5) | 0.4232 (4) | 0.084 (2) |
| H59 | 0.8928 | 0.4722 | 0.4399 | 0.101* |
| C60 | 0.8241 (4) | 0.4471 (6) | 0.4581 (5) | 0.098 (3) |
| H60 | 0.8501 | 0.4487 | 0.4981 | 0.117* |
| C61 | 0.7602 (3) | 0.4310 (5) | 0.4336 (4) | 0.080 (2) |
| H61 | 0.7422 | 0.4214 | 0.4568 | 0.096* |
| C62 | 0.7227 (3) | 0.4289 (3) | 0.3750 (3) | 0.054 (2) |
| C63 | 0.7487 (3) | 0.4436 (3) | 0.3412 (3) | 0.051 (2) |
| H63 | 0.723 | 0.4434 | 0.302 | 0.062* |
| C64 | 0.6534 (2) | 0.4084 (3) | 0.3466 (3) | 0.045 (2) |
| C65 | 0.9209 (2) | 0.4998 (3) | 0.1816 (3) | 0.047 (2) |
| C66 | 0.9458 (2) | 0.5135 (2) | 0.1412 (2) | 0.047 (2) |

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|---|---|---|---|---|
| C67 | 1.0050 (3) | 0.5119 (3) | 0.1505 (3) | 0.058 (2) |
| H67 | 1.0289 | 0.4999 | 0.1802 | 0.07* |
| C68 | 1.0296 (3) | 0.5279 (4) | 0.1163 (3) | 0.072 (2) |
| H68 | 1.07 | 0.5262 | 0.122 | 0.087* |
| C69 | 0.9944 (3) | 0.5464 (4) | 0.0734 (3) | 0.060 (2) |
| H69 | 1.0114 | 0.5592 | 0.0513 | 0.073* |
| C70 | 0.9341 (2) | 0.5463 (3) | 0.0628 (2) | 0.047 (2) |
| C71 | 0.9101 (2) | 0.5294 (2) | 0.0968 (3) | 0.044 (2) |
| H71 | 0.869 | 0.5287 | 0.0894 | 0.053* |
| C72 | 0.8977 (2) | 0.5674 (3) | 0.0176 (2) | 0.043 (1) |
| C73 | 0.5414 (2) | 0.4822 (2) | 0.3868 (2) | 0.038 (2) |
| C74 | 0.5401 (2) | 0.5485 (2) | 0.4357 (2) | 0.0352 (9) |
| C75 | 0.5448 (2) | 0.5636 (2) | 0.4981 (2) | 0.0379 (9) |
| H75 | 0.5505 | 0.5332 | 0.5112 | 0.045* |
| C76 | 0.5409 (2) | 0.6235 (2) | 0.5413 (2) | 0.039 (2) |
| H76 | 0.544 | 0.6339 | 0.584 | 0.048* |
| C77 | 0.5325 (2) | 0.6676 (2) | 0.5226 (2) | 0.0353 (9) |
| H77 | 0.5309 | 0.7088 | 0.5527 | 0.042* |
| C78 | 0.5264 (2) | 0.6519 (2) | 0.4594 (2) | 0.0311 (8) |
| C79 | 0.5321 (2) | 0.5928 (2) | 0.4166 (2) | 0.0325 (9) |
| H79 | 0.5305 | 0.5829 | 0.3747 | 0.039* |
| C80 | 0.5138 (2) | 0.6989 (2) | 0.4375 (2) | 0.0294 (8) |
| C81 | 0.4229 (2) | 0.3392 (2) | 0.2600 (2) | 0.041 (2) |
| C82 | 0.3551 (2) | 0.3270 (3) | 0.2390 (3) | 0.048 (2) |
| C83 | 0.3279 (3) | 0.3007 (4) | 0.2654 (4) | 0.067 (2) |
| H83 | 0.3517 | 0.2877 | 0.2942 | 0.081* |
| C84 | 0.2654 (4) | 0.2941 (5) | 0.2486 (5) | 0.091 (3) |
| H84 | 0.2469 | 0.2779 | 0.2674 | 0.109* |
| C85 | 0.2307 (3) | 0.3108 (4) | 0.2051 (4) | 0.078 (2) |
| H85 | 0.188 | 0.305 | 0.1932 | 0.094* |
| C86 | 0.2563 (3) | 0.3358 (3) | 0.1785 (3) | 0.056 (2) |
| C87 | 0.3190 (2) | 0.3447 (3) | 0.1964 (2) | 0.046 (2) |
| H87 | 0.3372 | 0.3631 | 0.179 | 0.056* |
| C88 | 0.2193 (3) | 0.3566 (3) | 0.1327 (3) | 0.052 (2) |
| C89 | 0.1987 (2) | 0.5068 (3) | 0.1627 (2) | 0.041 (2) |
| C90 | 0.2231 (2) | 0.5737 (3) | 0.2260 (2) | 0.041 (2) |
| C91 | 0.1874 (2) | 0.5956 (3) | 0.2589 (3) | 0.054 (2) |
| H91 | 0.1473 | 0.5685 | 0.2414 | 0.065* |
| C92 | 0.2108 (2) | 0.6576 (3) | 0.3177 (3) | 0.059 (2) |
| H92 | 0.1856 | 0.6735 | 0.3389 | 0.071* |
| C93 | 0.2701 (2) | 0.6962 (3) | 0.3455 (2) | 0.048 (2) |

| | | | | |
|---|---|---|---|---|
| H93 | 0.286 | 0.7381 | 0.3863 | 0.058* |
| C94 | 0.3070 (2) | 0.6735 (2) | 0.3133 (2) | 0.0364 (9) |
| C95 | 0.2822 (2) | 0.6124 (2) | 0.2530 (2) | 0.038 (2) |
| H95 | 0.3063 | 0.5971 | 0.2301 | 0.046* |
| C96 | 0.3723 (2) | 0.7129 (2) | 0.3444 (2) | 0.0345 (9) |
| Cu1 | 0.86286 (3) | 0.93644 (3) | 0.38630 (3) | 0.0393 (2) |
| Cu2 | 0.77208 (3) | 0.82753 (3) | 0.29008 (3) | 0.0361 (2) |
| Cu3 | 0.48325 (3) | 0.81649 (3) | 0.46025 (3) | 0.0332 (2) |
| Cu4 | 0.48660 (3) | 0.73892 (3) | 0.34583 (3) | 0.0321 (2) |
| Cu5 | 0.11265 (3) | 0.37996 (4) | 0.06460 (3) | 0.0423 (2) |
| Cu6 | 0.20963 (3) | 0.40909 (3) | 0.04999 (3) | 0.0374 (2) |
| Cu7 | 0.54399 (3) | 0.35410 (3) | 0.34253 (3) | 0.0358 (2) |
| Cu8 | 0.53151 (3) | 0.39094 (3) | 0.25717 (3) | 0.0351 (2) |
| Cu9 | 0.93738 (3) | 0.48505 (4) | 0.29243 (4) | 0.0474 (2) |
| Cu10 | 0.82768 (3) | 0.48521 (3) | 0.21703 (4) | 0.0440 (2) |
| Cu11 | 0.58022 (3) | 0.04578 (3) | -0.11101 (3) | 0.0335 (2) |
| Cu12 | 0.56519 (3) | 0.15946 (3) | -0.08519 (3) | 0.0324 (2) |
| O1 | 0.4907 (2) | 0.0100 (2) | -0.1714 (2) | 0.0372 (7) |
| O2 | 0.4774 (2) | 0.1073 (2) | -0.1472 (2) | 0.0442 (8) |
| O3 | 0.6663 (2) | 0.0959 (2) | -0.0463 (2) | 0.0532 (9) |
| O4 | 0.6550 (2) | 0.1924 (2) | -0.0255 (2) | 0.0447 (8) |
| O5 | 0.4078 (2) | 0.9578 (2) | 0.1855 (2) | 0.0387 (7) |
| O6 | 0.4232 (2) | 0.8623 (2) | 0.1645 (2) | 0.0383 (7) |
| O7 | 0.5635 (2) | 0.0675 (2) | -0.0339 (2) | 0.0519 (9) |
| O8 | 0.5541 (2) | 0.1660 (2) | -0.0096 (2) | 0.0468 (8) |
| O9 | 0.1940 (2) | 0.0253 (2) | -0.3469 (2) | 0.0547 (9) |
| O10 | 0.2731 (2) | 0.1170 (2) | -0.2685 (2) | 0.0471 (8) |
| O11 | 0.9052 (2) | 0.8803 (2) | 0.4097 (2) | 0.0516 (9) |
| O12 | 0.8290 (2) | 0.7873 (2) | 0.3255 (2) | 0.0514 (9) |
| O13 | 0.8213 (2) | 0.9416 (2) | 0.4407 (2) | 0.0554 (9) |
| O14 | 0.7457 (2) | 0.8477 (2) | 0.3608 (2) | 0.0502 (9) |
| O15 | 0.1068 (2) | 0.0822 (2) | -0.3197 (2) | 0.0538 (9) |
| O16 | 0.1859 (12) | 0.1726 (2) | -0.2365 (2) | 0.0486 (8) |
| O17 | 0.9531 (2) | 0.5785 (2) | 0.3450 (2) | 0.0550 (9) |
| O18 | 0.8598 (2) | 0.5799 (2) | 0.2827 (2) | 0.063 (2) |
| O19 | 0.9064 (2) | 0.3901 (2) | 0.2316 (2) | 0.071 (2) |
| O20 | 0.8157 (2) | 0.3910 (2) | 0.1650 (2) | 0.0542 (9) |
| O21 | 0.8955 (2) | 0.4765 (3) | 0.3432 (3) | 0.070 (2) |
| O22 | 0.8033 (2) | 0.4744 (2) | 0.2776 (2) | 0.059 (2) |
| O23 | 0.9573 (2) | 0.4932 (2) | 0.2268 (2) | 0.057 (2) |
| O24 | 0.8652 (2) | 0.4966 (2) | 0.1659 (2) | 0.060 (2) |

| | | | | |
|---|---|---|---|---|
| O25 | 0.5420 (2) | 0.2735 (2) | 0.2657 (2) | 0.0423 (7) |
| O26 | 0.5232 (2) | 0.3024 (2) | 0.1901 (2) | 0.0471 (8) |
| O27 | 0.5428 (2) | 0.4418 (2) | 0.4039 (1) | 0.0470 (8) |
| O28 | 0.5417 (2) | 0.4744 (2) | 0.3342 (2) | 0.0445 (8) |
| O29 | 0.6321 (2) | 0.3914 (2) | 0.3761 (2) | 0.0511 (8) |
| O30 | 0.6221 (2) | 0.4111 (2) | 0.2957 (2) | 0.0481 (8) |
| O31 | 0.4542 (2) | 0.3253 (2) | 0.3020 (2) | 0.0418 (7) |
| O32 | 0.4436 (2) | 0.3630 (2) | 0.2345 (2) | 0.0481 (8) |
| O33 | 0.1642 (2) | 0.3525 (2) | 0.1223 (2) | 0.0613 (1) |
| O34 | 0.2456 (2) | 0.3755 (2) | 0.1074 (2) | 0.0555 (9) |
| O35 | 0.9243 (2) | 0.5885 (2) | -0.0054 (2) | 0.0537 (9) |
| O36 | 0.8419 (2) | 0.5619 (2) | 0.0059 (2) | 0.0516 (9) |
| O37 | 0.1487 (2) | 0.4695 (2) | 0.1442 (2) | 0.0496 (9) |
| O38 | 0.2314 (2) | 0.4935 (2) | 0.1324 (2) | 0.0483 (8) |
| O39 | 0.0930 (2) | 0.2934 (2) | -0.0164 (2) | 0.0568 (1) |
| O40 | 0.1733 (2) | 0.3206 (2) | -0.0309 (2) | 0.0496 (8) |
| O41 | 0.5035 (2) | 0.7481 (2) | 0.47573 (2) | 0.0395 (7) |
| O42 | 0.5133 (2) | 0.6847 (2) | 0.3822 (2) | 0.0385 (7) |
| O43 | 0.4633 (2) | 0.8761 (1) | 0.4314 (2) | 0.0436 (8) |
| O44 | 0.4582 (2) | 0.8060 (2) | 0.3305 (2) | 0.0433 (8) |
| O45 | 0.5720 (2) | 0.8583 (2) | 0.49580 (18) | 0.0495 (8) |
| O46 | 0.5721 (2) | 0.7957 (2) | 0.39606 (17) | 0.0440 (8) |
| O47 | 0.3951 (2) | 0.7638 (2) | 0.40348 (15) | 0.0382 (7) |
| O48 | 0.4014 (2) | 0.6917 (2) | 0.31058 (16) | 0.0407 (7) |
| O1W | 0.5 | 0.5 | 0 | 0.39 (2)* |
| O2WA | 0.5619 (4) | 0.2590 (4) | -0.0444 (4) | 0.0522 (2)* |
| O2WB | 0.5340 (2) | 0.2398 (4) | -0.0863 (5) | 0.063 (2)* |
| O3WA | 0.316 (2) | 0.261 (2) | 0.0324 (2) | 0.249 (2)* |
| O3WB | 0.374 (2) | 0.321 (2) | 0.0563 (2) | 0.175 (2)* |
| O4WA | 0.1570 (7) | 0.7394 (8) | 0.5138 (8) | 0.091 (4)* |
| O4WB | 0.1243 (5) | 0.6777 (6) | 0.4019 (6) | 0.050 (3)* |
| O4WC | 0.156 (2) | 0.744 (2) | 0.458 (2) | 0.094 (5)* |
| O5WA | 0.9930 (6) | 0.6227 (6) | 0.5525 (7) | 0.098 (3)* |
| O5WB | 1.0387 (8) | 0.5737 (9) | 0.4927 (9) | 0.063 (4)* |
| O5WC | 0.9995 (6) | 0.5899 (6) | 0.4960 (7) | 0.042 (3)* |
| O6WA | 0.0674 (8) | 0.3506 (9) | 0.2274 (9) | 0.128 (5)* |
| O6WB | 0.092 (2) | 0.418 (2) | 0.244 (2) | 0.199 (2)* |
| O7WA | 0.322 (4) | 0.729 (4) | 0.120 (5) | 0.26 (4)* |
| O7WB | 0.306 (4) | 0.644 (4) | 0.020 (4) | 0.23 (3)* |
| O7WC | 0.349 (2) | 0.702 (2) | 0.138 (2) | 0.174 (2)* |
| O7WD | 0.310 (2) | 0.650 (2) | 0.088 (2) | 0.070 (5)* |

| | | | | |
|---|---|---|---|---|
| O8WA | 0.370 (2) | 0.245 (2) | -0.101 (2) | 0.123 (6)* |
| O8WB | 0.414 (2) | 0.175 (2) | -0.047 (2) | 0.123 (8)* |
| O8WC | 0.349 (2) | 0.165 (2) | -0.094 (2) | 0.092 (5)* |
| O9WA | 1.1214 (7) | 0.5515 (8) | 0.3578 (8) | 0.093 (4)* |
| O9WB | 1.123 (2) | 0.647 (2) | 0.422 (2) | 0.139 (2)* |
| O9WC | 1.132 (2) | 0.585 (2) | 0.418 (2) | 0.140 (2)* |
| O10W | 1.0265 (2) | 0.4908 (2) | 0.3576 (2) | 0.0639 (1)* |
| O12W | 0.7400 (8) | 0.5936 (8) | 0.0393 (9) | 0.126 (5)* |
| O13W | 0.5957 (7) | 0.2957 (8) | 0.0207 (8) | 0.115 (4)* |
| N1 | 0.2292 (5) | 0.8065 (5) | 0.2978 (6) | 0.076 (3)* |
| O100 | 0.2258 (9) | 0.7464 (9) | 0.1966 (1) | 0.166 (6)* |
| C100 | 0.2014 (8) | 0.7570 (8) | 0.2328 (9) | 0.098 (4)* |
| C101 | 0.2935 (7) | 0.8423 (7) | 0.3297 (8) | 0.089 (4)* |
| C102 | 0.1983 (6) | 0.8210 (7) | 0.3389 (7) | 0.078 (3)* |
| N2 | 0.9298 (2) | 1.0880 (2) | 0.5646 (3) | 0.062 (2) |
| O101 | 0.93589 (2) | 1.0245 (2) | 0.46724 (2) | 0.0519 (9) |
| C103 | 0.9547 (2) | 1.0480 (3) | 0.528 (3) | 0.056 (2) |
| C104 | 0.8784 (4) | 1.1055 (4) | 0.5334 (5) | 0.087 (2) |
| C105 | 0.9570 (4) | 1.1166 (4) | 0.6375 (4) | 0.097 (3) |
| N3 | 0.6626 (3) | -0.1053 (3) | -0.1418 (4) | 0.087 (2) |
| O102 | 0.5985 (2) | -0.0436 (2) | -0.1296 (2) | 0.0429 (8) |
| C106 | 0.6488 (3) | -0.0501 (3) | -0.1232 (4) | 0.069 (2) |
| C107 | 0.6183 (5) | -0.1635 (4) | -0.1694 (7) | 0.119 (4) |
| C108 | 0.7216 (6) | -0.1102 (6) | -0.1365 (9) | 0.152 (6) |
| N4 | 0.6454 (3) | 0.0565 (3) | 0.4578 (3) | 0.067 (2) |
| O103 | 0.7097 (4) | 0.1589 (3) | 0.5127 (4) | 0.108 (2) |
| C109 | 0.6647 (5) | 0.1216 (4) | 0.5027 (5) | 0.090 (2) |
| C110 | 0.6777 (5) | 0.0284 (4) | 0.4198 (5) | 0.099 (3) |
| C111 | 0.5894 (5) | 0.0157 (4) | 0.4443 (5) | 0.092 (3) |
| N5 | 0.4941 (3) | 0.8655 (2) | 0.6484 (2) | 0.068 (2) |
| O104 | 0.4748 (2) | 0.8628 (2) | 0.5516 (2) | 0.0457 (8) |
| C112 | 0.5045 (3) | 0.8532 (2) | 0.5969 (2) | 0.0564 (2) |
| C113 | 0.5314 (5) | 0.8515 (4) | 0.6988 (3) | 0.097 (3) |
| C114 | 0.4457 (5) | 0.8907 (4) | 0.6562 (4) | 0.095 (3) |
| N6A | 0.720 (2) | 0.643 (2) | 0.113 (2) | 0.030 (2)* |
| N6B | 0.720 (2) | 0.6342 (8) | 0.131 (2) | 0.079 (6)* |
| N6C | 0.7152 (2) | 0.702 (2) | 0.129 (2) | 0.082* |
| O105 | 0.713 (2) | 0.730 (2) | 0.203 (2) | 0.07* |
| O195 | 0.7049 (5) | 0.7345 (5) | 0.2082 (5) | 0.011 (2)* |
| C115 | 0.7409 (5) | 0.6924 (5) | 0.1800 (5) | 0.053 (2)* |
| C116 | 0.671 (2) | 0.641 (2) | 0.0624 (2) | 0.088 (2)* |

| | | | | |
|---|---|---|---|---|
| C186 | 0.664 (2) | 0.706 (3) | 0.079 (2) | 0.080 (2)* |
| C196 | 0.758 (2) | 0.596 (2) | 0.140 (2) | 0.042 (5)* |
| C117 | 0.7431 (8) | 0.5869 (7) | 0.0886 (8) | 0.083 (4)* |
| N7 | 0.6416 (2) | 0.2849 (2) | 0.4582 (2) | 0.0491 (1) |
| O106 | 0.5665 (2) | 0.3159 (2) | 0.4056 (2) | 0.0382 (7) |
| C118 | 0.6119 (2) | 0.2962 (3) | 0.4109 (3) | 0.0450 (1) |
| C119 | 0.6996 (3) | 0.2689 (5) | 0.4660 (5) | 0.081 (2) |
| C120 | 0.6227 (3) | 0.2926 (4) | 0.5080 (3) | 0.060 (2) |
| N8 | 0.2531 (6) | 0.9140 (7) | 0.1791 (7) | 0.081 (3)* |
| O107 | 0.2576 (9) | 0.9724 (2) | 0.280 (2) | 0.148 (6)* |
| C121 | 0.254 (2) | 0.9583 (2) | 0.162 (2) | 0.112 (6)* |
| C122 | 0.2482 (2) | 0.8478 (2) | 0.130 (2) | 0.130 (8)* |
| C123 | 0.2517 (7) | 0.9213 (8) | 0.2339 (8) | 0.077 (4)* |
| N9 | -0.0981 (6) | 0.1336 (6) | -0.1733 (6) | 0.061 (3)* |
| O108 | -0.120 (2) | 0.0843 (9) | -0.2843 (8) | 0.128 (6)* |
| C124 | -0.1000 (2) | 0.0828 (2) | -0.1602 (2) | 0.083 (5)* |
| C125 | -0.1083 (2) | 0.1333 (9) | -0.2322 (2) | 0.084 (5)* |
| C126 | -0.0847 (9) | 0.2003 (2) | -0.1226 (2) | 0.079 (5)* |
| N10 | 0.6848 (6) | -0.0020 (7) | 0.0466 (8) | 0.094 (4)* |
| O109 | 0.725 (2) | -0.0813 (2) | 0.011 (3) | 0.152 (1)* |
| O199 | 0.7827 (9) | 0.0171 (2) | 0.0664 (2) | 0.101 (6)* |
| C127 | 0.7314 (8) | -0.0229 (2) | 0.0384 (2) | 0.120 (7)* |
| C128 | 0.6953 (2) | 0.0663 (8) | 0.0937 (2) | 0.119 (7)* |
| C129 | 0.6235 (7) | -0.0475 (9) | 0.0106 (2) | 0.106 (6)* |
| N11 | 0.7215 (6) | 0.2558 (6) | 0.2452 (6) | 0.128 (3) |
| O110 | 0.7052 (5) | 0.2308 (4) | 0.3146 (5) | 0.143 (3) |
| C130 | 0.6931 (5) | 0.2537 (5) | 0.2802 (5) | 0.095 (3) |
| C131 | 0.7000 (6) | 0.2829 (6) | 0.2032 (6) | 0.122 (4) |
| C132 | 0.792 (2) | 0.2541 (2) | 0.260 (2) | 0.20 (2) |
| C192 | 0.736 (3) | 0.195 (2) | 0.215 (3) | 0.29 (5) |
| N12 | 0.6357 (7) | 0.3959 (7) | 0.1046 (9) | 0.102 (4)* |
| O111 | 0.7319 (3) | 0.4714 (3) | 0.1534 (3) | 0.036 (2)* |
| C133 | 0.6926 (5) | 0.4183 (6) | 0.1405 (7) | 0.062 (3)* |
| C134 | 0.5908 (6) | 0.3358 (6) | 0.0756 (7) | 0.068 (3)* |
| C135 | 0.603 (2) | 0.440 (2) | 0.086 (2) | 0.089 (2)* |
| C195 | 0.609 (2) | 0.372 (2) | 0.134 (2) | 0.075 (6)* |
| N13A | 0.572 (3) | 0.762 (4) | 0.245 (5) | 0.10 (2)* |
| N13B | 0.5317 (6) | 0.7353 (6) | 0.2003 (7) | 0.142 (4)* |
| O112 | 0.4939 (2) | 0.6922 (3) | 0.2529 (2) | 0.077 (2) |
| C136 | 0.5234 (5) | 0.7418 (5) | 0.2510 (5) | 0.098 (3) |
| C137 | 0.516 (2) | 0.6711 (8) | 0.140 (2) | 0.16 (2) |

| | | | | |
|---|---|---|---|---|
| C197 | 0.526 (2) | 0.7658 (9) | 0.161 (2) | 0.25 (3) |
| C138 | 0.571 (2) | 0.7850 (8) | 0.207 (2) | 0.23 (2) |
| N14 | 0.3443 (8) | 0.4704 (8) | 0.1308 (8) | 0.127 (6)* |
| O113 | 0.2796 (4) | 0.4270 (4) | 0.0221 (4) | 0.011 (2)* |
| O123 | 0.2988 (4) | 0.4392 (4) | 0.0608 (5) | 0.026 (2)* |
| C139 | 0.3260 (6) | 0.4684 (7) | 0.0734 (7) | 0.09* |
| C140 | 0.3960 (8) | 0.5256 (8) | 0.1939 (8) | 0.091 (4)* |
| C141 | 0.334 (6) | 0.408 (2) | 0.125 (2) | 0.19 (7)* |
| C151 | 0.3982 (7) | 0.5057 (8) | 0.1562 (8) | 0.066 (3)* |
| N15 | -0.0775 (5) | 0.3446 (6) | 0.0209 (6) | 0.107 (3)* |
| O114 | 0.0285 (2) | 0.3548 (2) | 0.0672 (2) | 0.053 (2)* |
| C142 | -0.0199 (6) | 0.3551 (6) | 0.0275 (6) | 0.091 (3)* |
| C143 | -0.0807 (2) | 0.327 (2) | 0.065 (2) | 0.160 (7)* |
| C144 | -0.129 (2) | 0.356 (2) | -0.0256 (2) | 0.166 (7)* |
| N16 | 0.0152 (4) | 0.3035 (3) | -0.2284 (4) | 0.099 (2) |
| O115 | -0.0560 (7) | 0.283 (12) | -0.1971 (2) | 0.097 (8) |
| O185 | -0.0716 (7) | 0.302 (2) | -0.290 (2) | 0.080 (6) |
| C145 | -0.0191 (6) | 0.3125 (6) | -0.2763 (6) | 0.126 (4) |
| C146 | -0.0015 (7) | 0.2794 (8) | -0.1946 (7) | 0.150 (5) |
| C147 | 0.0856 (5) | 0.3178 (5) | -0.2068 (5) | 0.107 (3) |
| N17 | 0.6807 (3) | 0.4706 (3) | 0.6080 (3) | 0.078 (2) |
| O116 | 0.7538 (3) | 0.4429 (5) | 0.5755 (5) | 0.126 (3) |
| C148 | 0.7049 (7) | 0.4499 (8) | 0.564 (2) | 0.41 (3) |
| C149 | 0.6213 (6) | 0.4758 (8) | 0.5822 (2) | 0.30 (2) |
| C150 | 0.718 (2) | 0.488 (2) | 0.6753 (9) | 0.114 (2) |
| N18 | 0.4447 (6) | 0.4964 (6) | 0.1821 (7) | 0.066 (3)* |
| O117 | 0.5020 (4) | 0.4306 (3) | 0.1939 (4) | 0.0440 (2)* |
| O197 | 0.5292 (6) | 0.4310 (5) | 0.1976 (6) | 0.075 (3)* |
| C160 | 0.4676 (5) | 0.4630 (6) | 0.2058 (6) | 0.049 (2)* |
| C161 | 0.443 (2) | 0.495 (2) | 0.1202 (2) | 0.108 (7)* |
| C162 | 0.436 (2) | 0.537 (2) | 0.225 (2) | 0.124 (8)* |

**Table S3.** Anisotropic displacement parameters ($A^2$) for compound **1**.

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.059 (3) | 0.034 (2) | 0.041 (2) | 0.025 (2) | 0.030 (2) | 0.028 (2) |
| C2 | 0.056 (3) | 0.039 (2) | 0.060 (3) | 0.024 (2) | 0.037 (2) | 0.035 (2) |
| C3 | 0.065 (4) | 0.049 (3) | 0.117 (6) | 0.028 (3) | 0.042 (4) | 0.058 (4) |
| C4 | 0.059 (4) | 0.058 (4) | 0.188 (1) | 0.021 (3) | 0.047 (5) | 0.082 (6) |
| C5 | 0.049 (3) | 0.051 (3) | 0.111 (6) | 0.011 (3) | 0.026 (3) | 0.044 (4) |
| C6 | 0.051 (3) | 0.041 (2) | 0.065 (3) | 0.023 (2) | 0.032 (2) | 0.035 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.047 (2) | 0.036 (2) | 0.051 (3) | 0.019 (2) | 0.030 (2) | 0.028 (2) |
| C8 | 0.038 (2) | 0.042 (2) | 0.059 (3) | 0.019 (2) | 0.024 (2) | 0.028 (2) |
| C9 | 0.066 (3) | 0.034 (2) | 0.034 (2) | 0.017 (2) | 0.018 (2) | 0.020 (2) |
| C10 | 0.057 (3) | 0.037 (3) | 0.055 (3) | 0.011 (2) | 0.012 (3) | 0.022 (2) |
| C11 | 0.084 (5) | 0.055 (4) | 0.104 (6) | 0.028 (4) | 0.004 (4) | 0.037 (4) |
| C12 | 0.087 (6) | 0.059 (4) | 0.142 (9) | 0.016 (4) | -0.026 (6) | 0.045 (5) |
| C13 | 0.080 (5) | 0.055 (4) | 0.103 (6) | 0.024 (3) | -0.010 (4) | 0.039 (4) |
| C14 | 0.055 (3) | 0.039 (3) | 0.066 (4) | 0.010 (2) | 0.004 (3) | 0.025 (3) |
| C15 | 0.057 (3) | 0.043 (3) | 0.050 (3) | 0.019 (2) | 0.019 (2) | 0.030 (2) |
| C16 | 0.049 (3) | 0.047 (3) | 0.054 (3) | 0.007 (2) | 0.005 (2) | 0.032 (3) |
| C17 | 0.047 (2) | 0.027 (2) | 0.024 (2) | 0.008 (2) | 0.016 (2) | 0.016 (2) |
| C18 | 0.044 (2) | 0.030 (2) | 0.032 (2) | 0.011 (2) | 0.023 (2) | 0.018 (2) |
| C19 | 0.053 (2) | 0.025 (2) | 0.038 (2) | 0.0109 (2) | 0.030 (2) | 0.016 (2) |
| C20 | 0.077 (3) | 0.027 (2) | 0.046 (3) | 0.020 (2) | 0.044 (3) | 0.018 (2) |
| C21 | 0.065 (3) | 0.029 (2) | 0.031 (2) | 0.012 (2) | 0.033 (2) | 0.0143 (2) |
| C22 | 0.053 (2) | 0.027 (2) | 0.029 (2) | 0.008 (2) | 0.025 (2) | 0.016 (2) |
| C23 | 0.052 (2) | 0.023 (2) | 0.0267 (2) | 0.009 (1) | 0.024 (2) | 0.011 (2) |
| C24 | 0.058 (3) | 0.025 (2) | 0.026 (2) | 0.008 (2) | 0.0231 (2) | 0.014 (2) |
| C25 | 0.082 (3) | 0.021 (2) | 0.025 (2) | 0.013 (2) | 0.029 (2) | 0.009 (2) |
| C26 | 0.072 (3) | 0.027 (2) | 0.031 (2) | 0.015 (2) | 0.033 (2) | 0.014 (2) |
| C27 | 0.099 (4) | 0.031 (2) | 0.041 (2) | 0.022 (2) | 0.039 (3) | 0.019 (2) |
| C28 | 0.110 (5) | 0.035 (2) | 0.048 (3) | 0.025 (3) | 0.046 (3) | 0.028 (2) |
| C29 | 0.090 (4) | 0.038 (2) | 0.039 (2) | 0.022 (2) | 0.042 (3) | 0.024 (2) |
| C30 | 0.060 (3) | 0.033 (2) | 0.029 (2) | 0.016 (2) | 0.027 (2) | 0.015 (2) |
| C31 | 0.058 (3) | 0.027 (2) | 0.028 (2) | 0.012 (2) | 0.024 (2) | 0.014 (2) |
| C32 | 0.058 (3) | 0.036 (2) | 0.039 (2) | 0.024 (2) | 0.033 (2) | 0.027 (2) |
| C33 | 0.038 (2) | 0.032 (2) | 0.039 (2) | 0.007 (2) | 0.012 (2) | 0.011 (2) |
| C34 | 0.044 (2) | 0.041 (2) | 0.046 (3) | 0.011 (2) | 0.014 (2) | 0.023 (2) |
| C35 | 0.057 (3) | 0.043 (3) | 0.054 (3) | 0.010 (2) | 0.010 (3) | 0.022 (2) |
| C36 | 0.053 (3) | 0.058 (3) | 0.066 (4) | 0.011 (3) | 0.001 (3) | 0.031 (3) |
| C37 | 0.056 (3) | 0.055 (3) | 0.073 (4) | 0.018 (3) | 0.011 (3) | 0.040 (3) |
| C38 | 0.046 (3) | 0.041 (3) | 0.053 (3) | 0.015 (2) | 0.018 (2) | 0.028 (2) |
| C39 | 0.041 (2) | 0.039 (2) | 0.047 (3) | 0.011 (2) | 0.015 (2) | 0.022 (2) |
| C40 | 0.043 (3) | 0.041 (3) | 0.054 (3) | 0.014 (2) | 0.011 (2) | 0.031 (2) |
| C41 | 0.033 (2) | 0.040 (2) | 0.053 (3) | 0.005 (2) | 0.020 (2) | 0.020 (2) |
| C42 | 0.045 (3) | 0.040 (2) | 0.045 (3) | 0.005 (2) | 0.023 (2) | 0.011 (2) |
| C43 | 0.056 (3) | 0.068 (4) | 0.052 (3) | -0.005 (3) | 0.027 (3) | 0.006 (3) |
| C44 | 0.075 (4) | 0.075 (4) | 0.051 (3) | -0.005 (3) | 0.033 (3) | 0.000 (3) |
| C45 | 0.069 (4) | 0.066 (4) | 0.051 (3) | 0.005 (3) | 0.035 (3) | 0.009 (3) |
| C46 | 0.057 (3) | 0.043 (3) | 0.042 (2) | 0.012 (2) | 0.028 (2) | 0.017 (2) |
| C47 | 0.048 (3) | 0.040 (2) | 0.044 (2) | 0.014 (2) | 0.024 (2) | 0.019 (2) |

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|---|---|---|---|---|---|---|
| C48 | 0.059 (3) | 0.034 (2) | 0.037 (2) | 0.010 (2) | 0.031 (2) | 0.016 (2) |
| C49 | 0.037 (2) | 0.032 (2) | 0.043 (2) | 0.007 (2) | 0.015 (2) | 0.012 (2) |
| C50 | 0.048 (3) | 0.042 (2) | 0.039 (2) | 0.008 (2) | 0.016 (2) | 0.016 (2) |
| C51 | 0.076 (4) | 0.056 (3) | 0.047 (3) | -0.002 (3) | 0.029 (3) | 0.014 (3) |
| C52 | 0.091 (5) | 0.073 (4) | 0.069 (4) | -0.018 (4) | 0.044 (4) | 0.014 (4) |
| C53 | 0.065 (4) | 0.067 (4) | 0.058 (3) | 0.001 (3) | 0.035 (3) | 0.020 (3) |
| C54 | 0.046 (3) | 0.051 (3) | 0.043 (3) | 0.012 (2) | 0.023 (2) | 0.020 (2) |
| C55 | 0.040 (2) | 0.045 (3) | 0.043 (2) | 0.009 (2) | 0.019 (2) | 0.021 (2) |
| C56 | 0.035 (2) | 0.054 (3) | 0.038 (2) | 0.007 (2) | 0.014 (2) | 0.022 (2) |
| C57 | 0.037 (3) | 0.064 (3) | 0.073 (4) | 0.010 (2) | 0.013 (2) | 0.045 (3) |
| C58 | 0.052 (3) | 0.074 (4) | 0.068 (4) | 0.019 (3) | 0.020 (3) | 0.054 (3) |
| C59 | 0.056 (4) | 0.130 (7) | 0.082 (5) | 0.028 (4) | 0.018 (3) | 0.079 (5) |
| C60 | 0.072 (5) | 0.157 (9) | 0.099 (6) | 0.038 (5) | 0.029 (4) | 0.101 (7) |
| C61 | 0.065 (4) | 0.122 (6) | 0.080 (5) | 0.029 (4) | 0.027 (3) | 0.079 (5) |
| C62 | 0.054 (3) | 0.062 (3) | 0.051 (3) | 0.016 (2) | 0.018 (2) | 0.039 (3) |
| C63 | 0.049 (3) | 0.058 (3) | 0.052 (3) | 0.016 (2) | 0.017 (2) | 0.038 (3) |
| C64 | 0.056 (3) | 0.053 (3) | 0.051 (3) | 0.027 (2) | 0.031 (2) | 0.039 (2) |
| C65 | 0.041 (2) | 0.047 (3) | 0.048 (3) | 0.017 (2) | 0.012 (2) | 0.028 (2) |
| C66 | 0.048 (3) | 0.044 (3) | 0.034 (2) | 0.016 (2) | 0.011 (2) | 0.015 (2) |
| C67 | 0.052 (3) | 0.074 (4) | 0.048 (3) | 0.038 (3) | 0.022 (2) | 0.031 (3) |
| C68 | 0.057 (3) | 0.116 (6) | 0.057 (3) | 0.053 (4) | 0.033 (3) | 0.046 (4) |
| C69 | 0.049 (3) | 0.099 (5) | 0.042 (3) | 0.040 (3) | 0.026 (2) | 0.039 (3) |
| C70 | 0.046 (3) | 0.058 (3) | 0.032 (2) | 0.023 (2) | 0.015 (2) | 0.022 (2) |
| C71 | 0.041 (2) | 0.046 (3) | 0.042 (2) | 0.016 (2) | 0.016 (2) | 0.023 (2) |
| C72 | 0.032 (2) | 0.059 (3) | 0.028 (2) | 0.016 (2) | 0.010 (2) | 0.018 (2) |
| C73 | 0.055 (3) | 0.042 (2) | 0.038 (2) | 0.029 (2) | 0.031 (2) | 0.027 (2) |
| C74 | 0.048 (2) | 0.032 (2) | 0.033 (2) | 0.016 (2) | 0.023 (2) | 0.018 (2) |
| C75 | 0.054 (3) | 0.039 (2) | 0.031 (2) | 0.018 (2) | 0.023 (2) | 0.022 (2) |
| C76 | 0.055 (3) | 0.044 (2) | 0.031 (2) | 0.021 (2) | 0.025 (2) | 0.024 (2) |
| C77 | 0.048 (2) | 0.035 (2) | 0.027 (2) | 0.0165 (2) | 0.022 (2) | 0.016 (2) |
| C78 | 0.039 (2) | 0.0295 (2) | 0.0271 (1) | 0.013 (2) | 0.019 (2) | 0.013 (2) |
| C79 | 0.045 (2) | 0.031 (2) | 0.026 (2) | 0.0129 (2) | 0.020 (2) | 0.014 (2) |
| C80 | 0.043 (2) | 0.0229 (1) | 0.025 (2) | 0.011 (2) | 0.019 (2) | 0.011 (2) |
| C81 | 0.058 (3) | 0.044 (2) | 0.027 (2) | 0.028 (2) | 0.022 (2) | 0.019 (2) |
| C82 | 0.052 (3) | 0.053 (3) | 0.038 (2) | 0.021 (2) | 0.019 (2) | 0.025 (2) |
| C83 | 0.071 (4) | 0.080 (4) | 0.070 (4) | 0.025 (3) | 0.031 (3) | 0.054 (4) |
| C84 | 0.067 (4) | 0.144 (8) | 0.108 (6) | 0.030 (5) | 0.038 (4) | 0.103 (7) |
| C85 | 0.058 (4) | 0.115 (6) | 0.089 (5) | 0.026 (4) | 0.031 (3) | 0.077 (5) |
| C86 | 0.055 (3) | 0.065 (3) | 0.050 (3) | 0.019 (3) | 0.022 (2) | 0.034 (3) |
| C87 | 0.055 (3) | 0.054 (3) | 0.036 (2) | 0.024 (2) | 0.021 (2) | 0.027 (2) |
| C88 | 0.051 (3) | 0.064 (3) | 0.041 (2) | 0.019 (2) | 0.017 (2) | 0.030 (2) |

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|---|---|---|---|---|---|---|
| C89 | 0.029 (2) | 0.055 (3) | 0.031 (2) | 0.014 (2) | 0.009 (2) | 0.020 (2) |
| C90 | 0.030 (2) | 0.058 (3) | 0.033 (2) | 0.018 (2) | 0.012 (2) | 0.024 (2) |
| C91 | 0.032 (2) | 0.072 (3) | 0.040 (2) | 0.017 (2) | 0.012 (2) | 0.020 (2) |
| C92 | 0.043 (3) | 0.084 (4) | 0.040 (3) | 0.029 (3) | 0.021 (2) | 0.023 (3) |
| C93 | 0.050 (3) | 0.060 (3) | 0.034 (2) | 0.031 (2) | 0.019 (2) | 0.023 (2) |
| C94 | 0.041 (2) | 0.048 (2) | 0.029 (2) | 0.023 (2) | 0.018 (2) | 0.023 (2) |
| C95 | 0.042 (2) | 0.044 (2) | 0.032 (2) | 0.017 (2) | 0.016 (2) | 0.022 (2) |
| C96 | 0.056 (3) | 0.028 (2) | 0.0270 (2) | 0.018 (2) | 0.022 (2) | 0.017 (2) |
| Cu1 | 0.0354 (3) | 0.0277 (3) | 0.0382 (3) | 0.0044 (2) | 0.0131 (3) | 0.0103 (3) |
| Cu2 | 0.0325 (3) | 0.0266 (3) | 0.0365 (3) | 0.0069 (2) | 0.0123 (3) | 0.0116 (3) |
| Cu3 | 0.0555 (4) | 0.0263 (3) | 0.0239 (3) | 0.0143 (3) | 0.0252 (3) | 0.0125 (2) |
| Cu4 | 0.0518 (4) | 0.0238 (3) | 0.0253 (3) | 0.0114 (2) | 0.0245 (3) | 0.0116 (2) |
| Cu5 | 0.0297 (3) | 0.0596 (4) | 0.0375 (3) | 0.0121 (3) | 0.0171 (3) | 0.0254 (3) |
| Cu6 | 0.0275 (3) | 0.0506 (4) | 0.0300 (3) | 0.0111 (3) | 0.0128 (2) | 0.0197 (3) |
| Cu7 | 0.0598 (4) | 0.0351 (3) | 0.0274 (3) | 0.0238 (3) | 0.0254 (3) | 0.0222 (3) |
| Cu8 | 0.0585 (4) | 0.0374 (3) | 0.0282 (3) | 0.0268 (3) | 0.0275 (3) | 0.0234 (3) |
| Cu9 | 0.0377 (3) | 0.0460 (4) | 0.0486 (4) | 0.0125 (3) | 0.0047 (3) | 0.0304 (3) |
| Cu10 | 0.0354 (3) | 0.0422 (4) | 0.0495 (4) | 0.0099 (3) | 0.0068 (3) | 0.0313 (3) |
| Cu11 | 0.0588 (4) | 0.0241 (3) | 0.0276 (3) | 0.0203 (3) | 0.0245 (3) | 0.0166 (2) |
| Cu12 | 0.0578 (4) | 0.0232 (3) | 0.0263 (3) | 0.0195 (3) | 0.0246 (3) | 0.0160 (2) |
| O1 | 0.055 (2) | 0.033 (2) | 0.043 (2) | 0.023 (2) | 0.029 (2) | 0.028 (2) |
| O2 | 0.056 (2) | 0.036 (2) | 0.051 (2) | 0.024 (2) | 0.025 (2) | 0.029 (2) |
| O3 | 0.065 (2) | 0.030 (2) | 0.047 (2) | 0.014 (2) | 0.014 (2) | 0.0184 (2) |
| O4 | 0.062 (2) | 0.028 (2) | 0.038 (2) | 0.013 (2) | 0.019 (2) | 0.017 (2) |
| O5 | 0.062 (2) | 0.036 (2) | 0.041 (2) | 0.0249 (2) | 0.035 (2) | 0.028 (2) |
| O6 | 0.065 (2) | 0.029 (2) | 0.027 (2) | 0.018 (2) | 0.024 (2) | 0.017 (2) |
| O7 | 0.107 (3) | 0.027 (2) | 0.035 (2) | 0.027 (2) | 0.042 (2) | 0.018 (2) |
| O8 | 0.092 (3) | 0.028 (2) | 0.043 (2) | 0.025 (2) | 0.046 (2) | 0.023 (2) |
| O9 | 0.044 (2) | 0.036 (2) | 0.065 (2) | 0.008 (2) | 0.014 (2) | 0.024 (2) |
| O10 | 0.039 (2) | 0.036 (2) | 0.059 (2) | 0.013 (2) | 0.018 (2) | 0.025 (2) |
| O11 | 0.046 (2) | 0.034 (2) | 0.050 (2) | 0.010 (2) | 0.010 (2) | 0.016 (2) |
| O12 | 0.051 (2) | 0.031 (2) | 0.051 (2) | 0.011 (2) | 0.012 (2) | 0.016 (2) |
| O13 | 0.051 (2) | 0.0441 (2) | 0.053 (2) | 0.001 (2) | 0.025 (2) | 0.010 (2) |
| O14 | 0.042 (2) | 0.045 (2) | 0.044 (2) | -0.001 (2) | 0.020 (2) | 0.016 (2) |
| O15 | 0.049 (2) | 0.043 (2) | 0.041 (2) | 0.005 (2) | 0.017 (2) | 0.009 (2) |
| O16 | 0.047 (2) | 0.0371 (2) | 0.042 (2) | 0.010 (2) | 0.019 (2) | 0.009 (2) |
| O17 | 0.052 (2) | 0.049 (2) | 0.059 (2) | 0.023 (2) | 0.016 (2) | 0.031 (2) |
| O18 | 0.053 (2) | 0.041 (2) | 0.068 (3) | 0.0164 (2) | 0.003 (2) | 0.029 (2) |
| O19 | 0.061 (2) | 0.044 (2) | 0.071 (3) | 0.011 (2) | -0.004 (2) | 0.031 (2) |
| O20 | 0.040 (2) | 0.044 (2) | 0.055 (2) | 0.010 (2) | 0.000 (2) | 0.028 (2) |
| O21 | 0.042 (2) | 0.095 (3) | 0.085 (3) | 0.015 (2) | 0.016 (2) | 0.067 (3) |

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|---|---|---|---|---|---|---|
| O22 | 0.043 (2) | 0.077 (3) | 0.061 (2) | 0.016 (2) | 0.014 (2) | 0.048 (2) |
| O23 | 0.058 (2) | 0.068 (2) | 0.049 (2) | 0.029 (2) | 0.016 (2) | 0.037 (2) |
| O24 | 0.044 (2) | 0.082 (3) | 0.069 (2) | 0.019 (2) | 0.016 (2) | 0.057 (2) |
| O25 | 0.073 (2) | 0.044 (2) | 0.032 (2) | 0.030 (2) | 0.036 (2) | 0.026 (2) |
| O26 | 0.080 (2) | 0.044 (1) | 0.033 (2) | 0.028 (2) | 0.038 (2) | 0.022 (2) |
| O27 | 0.085 (3) | 0.035 (2) | 0.036 (2) | 0.025 (2) | 0.034 (2) | 0.024 (2) |
| O28 | 0.078 (2) | 0.039 (2) | 0.037 (2) | 0.032 (2) | 0.037 (2) | 0.026 (2) |
| O29 | 0.066 (2) | 0.053 (2) | 0.049 (2) | 0.020 (1) | 0.027 (2) | 0.037 (2) |
| O30 | 0.058 (2) | 0.057 (2) | 0.047 (2) | 0.022 (1) | 0.030 (2) | 0.035 (2) |
| O31 | 0.058 (2) | 0.041 (2) | 0.030 (2) | 0.023 (1) | 0.020 (2) | 0.022 (2) |
| O32 | 0.058 (2) | 0.060 (2) | 0.039 (2) | 0.028 (1) | 0.021 (2) | 0.035 (2) |
| O33 | 0.048 (2) | 0.081 (3) | 0.06 (2) | 0.0231 (2) | 0.023 (2) | 0.045 (2) |
| O34 | 0.047 (2) | 0.079 (3) | 0.051 (2) | 0.029 (1) | 0.021 (2) | 0.043 (2) |
| O35 | 0.040 (2) | 0.084 (3) | 0.046 (2) | 0.024 (1) | 0.024 (2) | 0.038 (2) |
| O36 | 0.039 (2) | 0.072 (2) | 0.048 (2) | 0.016 (1) | 0.020 (2) | 0.037 (2) |
| O37 | 0.029 (2) | 0.065 (2) | 0.037 (2) | 0.011 (1) | 0.011 (2) | 0.019 (1) |
| O38 | 0.039 (2) | 0.054 (2) | 0.037 (2) | 0.007 (1) | 0.018 (2) | 0.015 (1) |
| O39 | 0.051 (2) | 0.063 (2) | 0.049 (2) | 0.009 (1) | 0.028 (2) | 0.021 (1) |
| O40 | 0.048 (2) | 0.057 (2) | 0.041 (2) | 0.012 (1) | 0.027 (2) | 0.020 (1) |
| O41 | 0.064 (2) | 0.033 (2) | 0.030 (2) | 0.025 (1) | 0.0297 (2) | 0.017 (1) |
| O42 | 0.063 (2) | 0.032 (2) | 0.034 (2) | 0.021 (1) | 0.033 (2) | 0.019 (1) |
| O43 | 0.080 (2) | 0.032 (2) | 0.030 (2) | 0.019 (1) | 0.034 (2) | 0.019 (1) |
| O44 | 0.077 (2) | 0.033 (2) | 0.031 (2) | 0.026 (1) | 0.034 (2) | 0.018 (1) |
| O45 | 0.059 (2) | 0.042 (2) | 0.0385 (2) | 0.009 (1) | 0.030 (2) | 0.012 (1) |
| O46 | 0.054 (2) | 0.041 (2) | 0.039 (2) | 0.012 (1) | 0.028 (2) | 0.019 (1) |
| O47 | 0.057 (2) | 0.036 (2) | 0.030 (2) | 0.020 (1) | 0.024 (2) | 0.021 (1) |
| O48 | 0.052 (2) | 0.029 (2) | 0.035 (2) | 0.015 (1) | 0.025 (2) | 0.011 (1) |
| N2 | 0.054 (3) | 0.043 (2) | 0.050 (3) | 0.018 (1) | 0.017 (2) | 0.001 (2) |
| O101 | 0.044 (2) | 0.031 (2) | 0.048 (2) | -0.003 (1) | 0.016 (2) | 0.006 (1) |
| C103 | 0.036 (2) | 0.046 (3) | 0.056 (3) | 0.005 (2) | 0.017 (2) | 0.012 (2) |
| C104 | 0.075 (4) | 0.070 (4) | 0.095 (6) | 0.035 (4) | 0.041 (4) | 0.028 (4) |
| C105 | 0.090 (5) | 0.088 (5) | 0.055 (4) | 0.022 (4) | 0.024 (4) | 0.008 (4) |
| N3 | 0.086 (4) | 0.048 (3) | 0.107 (5) | 0.031 (3) | 0.031 (4) | 0.037 (3) |
| O102 | 0.064 (2) | 0.027 (2) | 0.040 (2) | 0.024 (1) | 0.023 (2) | 0.020 (1) |
| C106 | 0.076 (4) | 0.051 (3) | 0.076 (4) | 0.030 (3) | 0.029 (3) | 0.034 (3) |
| C107 | 0.119 (7) | 0.052 (4) | 0.19 (2) | 0.048 (5) | 0.081 (8) | 0.065 (6) |
| C108 | 0.106 (8) | 0.097 (7) | 0.23 (2) | 0.063 (6) | 0.08 (2) | 0.072 (9) |
| N4 | 0.098 (4) | 0.053 (3) | 0.068 (3) | 0.039 (3) | 0.054 (3) | 0.032 (3) |
| O103 | 0.128 (5) | 0.063 (3) | 0.105 (5) | 0.017 (3) | 0.048 (4) | 0.032 (3) |
| C109 | 0.112 (7) | 0.061 (4) | 0.080 (5) | 0.035 (4) | 0.038 (5) | 0.031 (4) |
| C110 | 0.124 (7) | 0.074 (5) | 0.112 (7) | 0.048 (5) | 0.085 (6) | 0.034 (5) |

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|---|---|---|---|---|---|---|
| C111 | 0.135 (7) | 0.071 (4) | 0.110 (6) | 0.039 (5) | 0.088 (6) | 0.054 (5) |
| N5 | 0.105 (4) | 0.055 (3) | 0.027 (2) | -0.005 (3) | 0.036 (2) | 0.009 (2) |
| O104 | 0.071 (2) | 0.038 (2) | 0.029 (2) | 0.017 (1) | 0.034 (2) | 0.012 (1) |
| C112 | 0.100 (4) | 0.035 (2) | 0.025 (2) | 0.003 (2) | 0.034 (3) | 0.008 (2) |
| C113 | 0.145 (8) | 0.086 (5) | 0.035 (3) | -0.005 (5) | 0.027 (4) | 0.032 (3) |
| C114 | 0.125 (7) | 0.092 (5) | 0.054 (4) | 0.022 (5) | 0.061 (5) | 0.018 (4) |
| N7 | 0.046 (2) | 0.067 (3) | 0.056 (2) | 0.025 (2) | 0.024 (2) | 0.046 (2) |
| O106 | 0.054 (2) | 0.045 (2) | 0.035 (2) | 0.029 (1) | 0.027 (2) | 0.029 (2) |
| C118 | 0.057 (3) | 0.051 (3) | 0.046 (3) | 0.025 (2) | 0.031 (2) | 0.034 (2) |
| C119 | 0.060 (4) | 0.126 (7) | 0.111 (6) | 0.055 (4) | 0.049 (4) | 0.091 (6) |
| C120 | 0.054 (3) | 0.092 (4) | 0.056 (3) | 0.023 (3) | 0.023 (3) | 0.057 (3) |
| N11 | 0.162 (9) | 0.148 (9) | 0.127 (8) | 0.082 (8) | 0.094 (7) | 0.085 (7) |
| O110 | 0.22 (2) | 0.135 (7) | 0.141 (7) | 0.107 (7) | 0.106 (7) | 0.105 (6) |
| C130 | 0.122 (7) | 0.079 (5) | 0.091 (6) | 0.028 (5) | 0.053 (6) | 0.050 (5) |
| C131 | 0.142 (9) | 0.111 (7) | 0.091 (6) | -0.009 (7) | 0.059 (7) | 0.044 (6) |
| C132 | 0.17 (2) | 0.15 (2) | 0.36 (5) | 0.11 (2) | 0.17 (3) | 0.14 (3) |
| C192 | 0.27 (7) | 0.5 (2) | 0.26 (7) | 0.33 (9) | 0.22 (6) | 0.30 (9) |
| O112 | 0.091 (3) | 0.101 (4) | 0.032 (2) | 0.036 (3) | 0.041 (2) | 0.020 (2) |
| C136 | 0.125 (7) | 0.11 (7) | 0.078 (5) | 0.027 (6) | 0.066 (5) | 0.058 (5) |
| C137 | 0.37 (4) | 0.070 (2) | 0.12 (1) | 0.07 (2) | 0.19 (3) | 0.05 (2) |
| C197 | 0.43 (6) | 0.09 (2) | 0.12 (2) | -0.13 (3) | 0.20 (3) | -0.03 (2) |
| C138 | 0.24 (2) | 0.11 (2) | 0.34 (3) | -0.01 (2) | 0.22 (2) | 0.05 (2) |
| N16 | 0.125 (6) | 0.064 (4) | 0.062 (4) | 0.004 (4) | 0.021 (4) | 0.023 (3) |
| O115 | 0.015 (6) | 0.11 (2) | 0.13 (2) | -0.022 (8) | -0.010 (8) | 0.08 (2) |
| O185 | 0.034 (8) | 0.11 (2) | 0.09 (1) | 0.033 (9) | 0.023 (8) | 0.05 (2) |
| C145 | 0.123 (9) | 0.101 (7) | 0.094 (7) | 0.033 (6) | 0.018 (6) | 0.037 (6) |
| C146 | 0.14 (2) | 0.18 (2) | 0.100 (8) | 0.019 (1) | 0.034 (8) | 0.078 (9) |
| C147 | 0.101 (7) | 0.094 (6) | 0.090 (6) | 0.031 (5) | 0.039 (5) | 0.030 (5) |
| N17 | 0.072 (4) | 0.077 (4) | 0.076 (4) | 0.025 (3) | 0.025 (3) | 0.041 (3) |
| O116 | 0.098 (5) | 0.184 (8) | 0.146 (7) | 0.058 (5) | 0.069 (5) | 0.113 (7) |
| C148 | 0.33 (3) | 0.13 (2) | 0.94 (9) | 0.13 (2) | 0.51 (5) | 0.24 (3) |
| C149 | 0.16 (2) | 0.18 (2) | 0.36 (3) | -0.02 (2) | -0.12 (2) | 0.21 (2) |
| C150 | 0.12 (2) | 0.21 (3) | 0.06 (2) | 0.07 (2) | 0.04 (2) | 0.11 (2) |

**Table S4.** Bond distances (Å) and angles (º) for compound **1**.

**Distances**

| | | | |
|---|---|---|---|
| C1—C2 | 1.490 (7) | C95—H95 | 0.95 |
| C1—O1 | 1.259 (6) | C96—O47 | 1.265 (5) |
| C1—O2 | 1.279 (6) | C96—O48 | 1.262 (6) |
| C2—C3 | 1.404 (8) | Cu1—Cu2 | 2.6266 (8) |

| | | | |
|---|---|---|---|
| C2—C7 | 1.397 (7) | Cu1—O9$^{i}$ | 1.963 (4) |
| C3—H3 | 0.95 | Cu1—O11 | 1.963 (4) |
| C3—C4 | 1.404 (1) | Cu1—O13 | 1.957 (4) |
| C4—H4 | 0.95 | Cu1—O15 | 1.957 (4) |
| C4—C5 | 1.390 (1) | Cu1—O101 | 2.132 (3) |
| C5—H5 | 0.95 | Cu2—O10$^{i}$ | 1.964 (4) |
| C5—C6 | 1.387 (8) | Cu2—O12 | 1.958 (4) |
| C6—C7 | 1.393 (7) | Cu2—O14 | 1.969 (4) |
| C6—C8 | 1.508 (7) | Cu2—O16 | 1.978 (4) |
| C7—H7 | 0.95 | Cu2—O105 | 2.17 (3) |
| C8—O9 | 1.249 (6) | Cu2—O195 | 2.14 (1) |
| C8—O10 | 1.248 (6) | Cu3—Cu4 | 2.6340 (7) |
| C9—C10 | 1.497 (8) | Cu3—O41 | 1.958 (3) |
| C9—O3 | 1.264 (6) | Cu3—O43 | 1.944 (3) |
| C9—O4 | 1.244 (6) | Cu3—O45 | 1.981 (4) |
| C10—C11 | 1.398 (1) | Cu3—O47 | 1.972 (3) |
| C10—C15 | 1.397 (8) | Cu3—O104 | 2.133 (3) |
| C11—H11 | 0.95 | Cu4—O42 | 1.973 (3) |
| C11—C12 | 1.39 (1) | Cu4—O44 | 1.984 (3) |
| C12—H12 | 0.95 | Cu4—O46 | 1.960 (3) |
| C12—C13 | 1.386 (1) | Cu4—O48 | 1.938 (3) |
| C13—H13 | 0.95 | Cu4—O112 | 2.152 (4) |
| C13—C14 | 1.372 (9) | Cu5—Cu6 | 2.6346 (9) |
| C14—C15 | 1.383 (8) | Cu5—O33 | 1.963 (4) |
| C14—C16 | 1.500 (8) | Cu5—O35 | 1.962 (4) |
| C15—H15 | 0.95 | Cu5—O37 | 1.960 (4) |
| C16—O19 | 1.253 (7) | Cu5—O39 | 1.977 (4) |
| C16—O20 | 1.246 (7) | Cu5—O114 | 2.141 (5) |
| C17—C18 | 1.503 (6) | Cu6—O34 | 1.962 (4) |
| C17—O5 | 1.251 (6) | Cu6—O36 | 1.964 (4) |
| C17—O6 | 1.260 (5) | Cu6—O38 | 1.954 (3) |
| C18—C19 | 1.395 (6) | Cu6—O40 | 1.954 (4) |
| C18—C23 | 1.376 (7) | Cu6—O113 | 2.169 (8) |
| C19—H19 | 0.95 | Cu6—O123 | 2.124 (9) |
| C19—C20 | 1.387 (7) | Cu7—Cu8 | 2.6387 (9) |
| C20—H20 | 0.95 | Cu7—O25 | 1.986 (3) |
| C20—C21 | 1.377 (8) | Cu7—O27 | 1.978 (3) |
| C21—H21 | 0.95 | Cu7—O29 | 1.953 (4) |
| C21—C22 | 1.401 (6) | Cu7—O31 | 1.943 (4) |
| C22—C23 | 1.389 (6) | Cu7—O106 | 2.136 (3) |
| C22—C24 | 1.490 (7) | Cu8—O26 | 1.953 (3) |

| | | | |
|---|---|---|---|
| C23—H23 | 0.95 | Cu8—O28 | 1.956 (3) |
| C24—O43 | 1.278 (5) | Cu8—O30 | 1.970 (4) |
| C24—O44 | 1.242 (5) | Cu8—O32 | 1.977 (4) |
| C25—C26 | 1.499 (6) | Cu8—O117 | 2.178 (8) |
| C25—O7 | 1.262 (6) | Cu8—O197 | 2.14 (1) |
| C25—O8 | 1.259 (6) | Cu9—Cu10 | 2.6493 (9) |
| C26—C27 | 1.376 (7) | Cu9—O17 | 1.944 (4) |
| C26—C31 | 1.393 (6) | Cu9—O19 | 1.959 (4) |
| C27—H27 | 0.95 | Cu9—O21 | 1.985 (5) |
| C27—C28 | 1.368 (8) | Cu9—O23 | 1.981 (4) |
| C28—H28 | 0.95 | Cu9—O10W | 2.128 (5) |
| C28—C29 | 1.388 (7) | Cu10—O18 | 1.967 (4) |
| C29—H29 | 0.95 | Cu10—O20 | 1.972 (4) |
| C29—C30 | 1.386 (7) | Cu10—O22 | 1.952 (4) |
| C30—C31 | 1.392 (6) | Cu10—O24 | 1.945 (4) |
| C30—C32 | 1.494 (6) | Cu10—O111 | 2.175 (6) |
| C31—H31 | 0.95 | Cu11—Cu12 | 2.6406 (8) |
| C32—O25 | 1.256 (5) | Cu11—O1 | 1.960 (3) |
| C32—O26 | 1.266 (6) | Cu11—O3 | 1.939 (4) |
| C33—C34 | 1.510 (8) | Cu11—O5$^{i}$ | 1.972 (3) |
| C33—O11 | 1.251 (6) | Cu11—O7 | 1.967 (3) |
| C33—O12 | 1.254 (6) | Cu11—O102 | 2.140 (3) |
| C34—C35 | 1.387 (8) | Cu12—O2 | 1.969 (4) |
| C34—C39 | 1.404 (7) | Cu12—O4 | 1.964 (4) |
| C35—H35 | 0.95 | Cu12—O6$^{i}$ | 1.950 (3) |
| C35—C36 | 1.361 (9) | Cu12—O8 | 1.958 (3) |
| C36—H36 | 0.95 | Cu12—O2WA | 2.180 (8) |
| C36—C37 | 1.393 (9) | Cu12—O2WB | 2.179 (9) |
| C37—H37 | 0.95 | O5—Cu11$^{i}$ | 1.972 (3) |
| C37—C38 | 1.387 (8) | O6—Cu12$^{i}$ | 1.950 (3) |
| C38—C39 | 1.375 (8) | O9—Cu1$^{i}$ | 1.963 (4) |
| C38—C40 | 1.513 (7) | O10—Cu2$^{i}$ | 1.964 (4) |
| C39—H39 | 0.95 | O15—C49$^{i}$ | 1.247 (6) |
| C40—O17 | 1.252 (6) | O16—C49$^{i}$ | 1.256 (6) |
| C40—O18 | 1.265 (6) | O2WB—C197$^{i}$ | 1.84 (3) |
| C41—C42 | 1.516 (7) | O4WB—O9WB$^{ii}$ | 1.08 (3) |
| C41—O13 | 1.239 (6) | O8WA—C186$^{i}$ | 1.52 (5) |
| C41—O14 | 1.253 (6) | O9WB—O4WB$^{iii}$ | 1.08 (3) |
| C42—C43 | 1.395 (8) | O12W—C117 | 1.31 (2) |
| C42—C47 | 1.392 (7) | O12W—O113$^{i}$ | 1.24 (2) |
| C43—H43 | 0.95 | O13W—C134 | 1.32 (2) |

| | | | |
|---|---|---|---|
| C43—C44 | 1.38 (1) | N1—C100 | 1.33 (2) |
| C44—H44 | 0.95 | N1—C101 | 1.44 (2) |
| C44—C45 | 1.38 (1) | N1—C102 | 1.43 (2) |
| C45—H45 | 0.95 | O100—C100 | 1.21 (2) |
| C45—C46 | 1.389 (8) | N2—C103 | 1.345 (7) |
| C46—C47 | 1.390 (7) | N2—C104 | 1.43 (1) |
| C46—C48 | 1.495 (7) | N2—C105 | 1.44 (2) |
| C47—H47 | 0.95 | O101—C103 | 1.238 (7) |
| C48—O45 | 1.271 (6) | N3—C106 | 1.326 (8) |
| C48—O46 | 1.248 (6) | N3—C107 | 1.40 (1) |
| C49—C50 | 1.505 (7) | N3—C108 | 1.42 (1) |
| C49—O15$^{i}$ | 1.247 (6) | O102—C106 | 1.211 (8) |
| C49—O16$^{i}$ | 1.256 (6) | N4—C109 | 1.35 (1) |
| C50—C51 | 1.391 (8) | N4—C110 | 1.428 (9) |
| C50—C55 | 1.386 (7) | N4—C111 | 1.45 (2) |
| C51—H51 | 0.95 | O103—C109 | 1.24 (2) |
| C51—C52 | 1.37 (1) | N5—C112 | 1.318 (7) |
| C52—H52 | 0.95 | N5—C113 | 1.47 (2) |
| C52—C53 | 1.42 (1) | N5—C114 | 1.41 (2) |
| C53—H53 | 0.95 | O104—C112 | 1.246 (7) |
| C53—C54 | 1.388 (8) | N6A—C115 | 1.36 (2) |
| C54—C55 | 1.399 (7) | N6A—C116 | 1.36 (2) |
| C54—C56 | 1.502 (7) | N6A—C196 | 1.79 (3) |
| C55—H55 | 0.95 | N6A—C117 | 1.49 (2) |
| C56—O39 | 1.263 (6) | N6B—C115 | 1.25 (2) |
| C56—O40 | 1.257 (6) | N6B—C116 | 1.81 (3) |
| C57—C58 | 1.489 (9) | N6B—C196 | 1.39 (2) |
| C57—O21 | 1.249 (7) | N6B—C117 | 1.47 (2) |
| C57—O22 | 1.259 (7) | N6C—C115 | 1.33 (2) |
| C58—C59 | 1.381 (9) | N6C—C116 | 1.51 (5) |
| C58—C63 | 1.392 (8) | N6C—C186 | 1.46 (2) |
| C59—H59 | 0.95 | O105—C115 | 1.24 (1) |
| C59—C60 | 1.38 (2) | O195—C115 | 1.50 (1) |
| C60—H60 | 0.95 | C116—C186 | 1.49 (6) |
| C60—C61 | 1.39 (1) | C186—O8WA$^{i}$ | 1.52 (5) |
| C61—H61 | 0.95 | C196—C117 | 1.13 (3) |
| C61—C62 | 1.393 (9) | N7—C118 | 1.312 (7) |
| C62—C63 | 1.388 (8) | N7—C119 | 1.470 (7) |
| C62—C64 | 1.506 (8) | N7—C120 | 1.432 (7) |
| C63—H63 | 0.95 | O106—C118 | 1.232 (6) |
| C64—O29 | 1.249 (6) | N8—C121 | 1.35 (3) |

| | | | |
|---|---|---|---|
| C64—O30 | 1.262 (6) | N8—C122 | 1.46 (3) |
| C65—C66 | 1.512 (8) | N8—C123 | 1.32 (2) |
| C65—O23 | 1.250 (6) | O107—C123 | 1.19 (2) |
| C65—O24 | 1.253 (6) | N9—C124 | 1.44 (3) |
| C66—C67 | 1.384 (8) | N9—C125 | 1.41 (2) |
| C66—C71 | 1.382 (8) | N9—C126 | 1.43 (2) |
| C67—H67 | 0.95 | O108—C125 | 1.19 (1) |
| C67—C68 | 1.39 (1) | N10—C127 | 1.32 (1) |
| C68—H68 | 0.95 | N10—C128 | 1.45 (1) |
| C68—C69 | 1.398 (9) | N10—C129 | 1.44 (1) |
| C69—H69 | 0.95 | O109—C127 | 1.22 (2) |
| C69—C70$^{i}$ | 1.396 (7) | O199—C127 | 1.24 (2) |
| C70—C69$^{i}$ | 1.396 (7) | N11—C130 | 1.32 (2) |
| C70—C71$^{i}$ | 1.391 (8) | N11—C131 | 1.46 (12) |
| C70—C72 | 1.495 (7) | N11—C132 | 1.64 (3) |
| C71—C70$^{i}$ | 1.391 (8) | N11—C192 | 1.46 (2) |
| C71—H71 | 0.95 | O110—C130 | 1.20 (2) |
| C72—O35 | 1.247 (7) | N12—C133 | 1.23 (2) |
| C72—O36 | 1.266 (6) | N12—C134 | 1.43 (2) |
| C73—C74 | 1.518 (6) | N12—C135 | 1.53 (2) |
| C73—O27 | 1.256 (6) | N12—C195 | 1.42 (3) |
| C73—O28 | 1.249 (6) | O111—C133 | 1.38 (2) |
| C74—C75 | 1.391 (6) | C134—C195 | 1.17 (3) |
| C74—C79 | 1.383 (7) | N13A—C136 | 1.36 (2) |
| C75—H75 | 0.95 | N13A—C138 | 1.29 (8) |
| C75—C76 | 1.391 (7) | N13B—C136 | 1.30 (2) |
| C76—H76 | 0.95 | N13B—C137 | 1.45 (2) |
| C76—C77 | 1.376 (7) | N13B—C197 | 1.47 (2) |
| C77—H77 | 0.95 | N13B—C138 | 1.40 (2) |
| C77—C78 | 1.392 (6) | O112—C136 | 1.40 (2) |
| C78—C79 | 1.396 (6) | C197—O2WB$^{i}$ | 1.84 (3) |
| C78—C80 | 1.508 (6) | C197—C138 | 1.12 (4) |
| C79—H79 | 0.95 | N14—O123 | 1.43 (2) |
| C80—O41 | 1.254 (5) | N14—C139 | 1.32 (2) |
| C80—O42 | 1.261 (5) | N14—C140 | 1.47 (2) |
| C81—C82 | 1.496 (7) | N14—C141 | 1.47 (1) |
| C81—O31 | 1.264 (6) | N14—C151 | 1.25 (2) |
| C81—O32 | 1.255 (6) | O113—O12W$^{i}$ | 1.24 (1) |
| C82—C83 | 1.408 (9) | O113—O123 | 0.78 (1) |
| C82—C87 | 1.384 (8) | O113—C139 | 1.21 (1) |
| C83—H83 | 0.95 | O123—C139 | 0.78 (1) |

| | | | |
|---|---|---|---|
| C83—C84 | 1.401(1) | C139—C151 | 1.87 (2) |
| C84—H84 | 0.95 | C140—C151 | 0.86 (2) |
| C84—C85 | 1.37 (1) | C140—N18 | 1.49 (2) |
| C85—H85 | 0.95 | C140—C162 | 0.93 (3) |
| C85—C86 | 1.36 (1) | C151—N18 | 1.18 (2) |
| C86—C87 | 1.394 (8) | C151—C161 | 1.64 (3) |
| C86—C88 | 1.506 (8) | C151—C162 | 1.39 (4) |
| C87—H87 | 0.95 | N15—C142 | 1.34 (2) |
| C88—O33 | 1.260 (7) | N15—C143 | 1.39 (2) |
| C88—O34 | 1.258 (7) | N15—C144 | 1.53 (2) |
| C89—C90 | 1.501 (7) | O114—C142 | 1.23 (1) |
| C89—O37 | 1.246 (6) | N16—C145 | 1.31 (1) |
| C89—O38 | 1.262 (6) | N16—C146 | 1.39 (2) |
| C90—C91 | 1.391 (7) | N16—C147 | 1.55 (2) |
| C90—C95 | 1.379 (7) | O115—C146 | 1.32 (3) |
| C91—H91 | 0.95 | O185—C145 | 1.17 (2) |
| C91—C92 | 1.390 (8) | N17—C148 | 1.35 (2) |
| C92—H92 | 0.95 | N17—C149 | 1.39 (2) |
| C92—C93 | 1.381 (8) | N17—C150 | 1.41 (2) |
| C93—H93 | 0.95 | O116—C148 | 1.16 (4) |
| C93—C94 | 1.405 (6) | O197—C160 | 1.78 (2) |
| C94—C95 | 1.394 (6) | C160—C162 | 1.94 (3) |
| C94—C96 | 1.492 (7) | | |

**Angles**

| | | | |
|---|---|---|---|
| O1—C1—C2 | 117.8 (4) | O35—Cu5—O39 | 89.9 (1) |
| O1—C1—O2 | 125.0 (5) | O35—Cu5—O114 | 93.1 (1) |
| O2—C1—C2 | 117.2 (4) | O37—Cu5—Cu6 | 84.0 (1) |
| C3—C2—C1 | 119.9 (5) | O37—Cu5—O33 | 88.7 (2) |
| C7—C2—C1 | 120.0 (4) | O37—Cu5—O35 | 89.9 (2) |
| C7—C2—C3 | 120.1 (5) | O37—Cu5—O39 | 167.7 (2) |
| C2—C3—H3 | 120.5 | O37—Cu5—O114 | 98.5 (2) |
| C2—C3—C4 | 118.9 (6) | O39—Cu5—Cu6 | 83.8 (2) |
| C4—C3—H3 | 120.5 | O39—Cu5—O114 | 93.7 (2) |
| C3—C4—H4 | 119.7 | O114—Cu5—Cu6 | 174.5 (2) |
| C5—C4—C3 | 120.5 (6) | O34—Cu6—Cu5 | 81.7 (2) |
| C5—C4—H4 | 119.7 | O34—Cu6—O36 | 168.0 (2) |
| C4—C5—H5 | 120 | O34—Cu6—O113 | 104.6 (3) |
| C6—C5—C4 | 120.1 (6) | O34—Cu6—O123 | 88.4 (3) |
| C6—C5—H5 | 120 | O36—Cu6—Cu5 | 86.3 (2) |
| C5—C6—C7 | 120.2 (5) | O36—Cu6—O113 | 87.2 (3) |

| | | | |
|---|---|---|---|
| C5—C6—C8 | 120.0 (5) | O36—Cu6—O123 | 103.4 (3) |
| C7—C6—C8 | 119.8 (4) | O38—Cu6—Cu5 | 84.1 (2) |
| C2—C7—H7 | 120 | O38—Cu6—O34 | 88.9 (2) |
| C6—C7—C2 | 120.0 (4) | O38—Cu6—O36 | 90.1 (2) |
| C6—C7—H7 | 120 | O38—Cu6—O40 | 168.8 (2) |
| O9—C8—C6 | 116.5 (4) | O38—Cu6—O113 | 101.5 (2) |
| O10—C8—C6 | 116.6 (4) | O38—Cu6—O123 | 87.9 (3) |
| O10—C8—O9 | 126.9 (5) | O40—Cu6—Cu5 | 84.6 (1) |
| O3—C9—C10 | 117.0 (5) | O40—Cu6—O34 | 90.1 (2) |
| O4—C9—C10 | 117.0 (4) | O40—Cu6—O36 | 88.5 (2) |
| O4—C9—O3 | 126.0 (5) | O40—Cu6—O113 | 89.5 (2) |
| C11—C10—C9 | 120.4 (5) | O40—Cu6—O123 | 103.2 (3) |
| C15—C10—C9 | 119.7 (5) | O113—Cu6—Cu5 | 171.4 (2) |
| C15—C10—C11 | 119.6 (6) | O123—Cu6—Cu5 | 167.5 (3) |
| C10—C11—H11 | 120.5 | O123—Cu6—O113 | 21.1 (3) |
| C12—C11—C10 | 118.9 (7) | O25—Cu7—Cu8 | 80.12 (9) |
| C12—C11—H11 | 120.5 | O25—Cu7—O106 | 91.5 (2) |
| C11—C12—H12 | 119.8 | O27—Cu7—Cu8 | 85.8 (2) |
| C13—C12—C11 | 120.4 (7) | O27—Cu7—O25 | 165.9 (2) |
| C13—C12—H12 | 119.8 | O27—Cu7—O106 | 102.4 (2) |
| C12—C13—H13 | 119.6 | O29—Cu7—Cu8 | 82.9 (2) |
| C14—C13—C12 | 120.8 (7) | O29—Cu7—O25 | 90.3 (2) |
| C14—C13—H13 | 119.6 | O29—Cu7—O27 | 88.4 (2) |
| C13—C14—C15 | 119.5 (6) | O29—Cu7—O106 | 89.7 (2) |
| C13—C14—C16 | 120.9 (6) | O31—Cu7—Cu8 | 87.7 (2) |
| C15—C14—C16 | 119.5 (5) | O31—Cu7—O25 | 91.0 (2) |
| C10—C15—H15 | 119.6 | O31—Cu7—O27 | 87.9 (2) |
| C14—C15—C10 | 120.7 (5) | O31—Cu7—O29 | 170.2 (2) |
| C14—C15—H15 | 119.6 | O31—Cu7—O106 | 99.8 (2) |
| O19—C16—C14 | 117.0 (5) | O106—Cu7—Cu8 | 168.85 (9) |
| O20—C16—C14 | 115.9 (5) | O26—Cu8—Cu7 | 88.23 (1) |
| O20—C16—O19 | 127.1 (5) | O26—Cu8—O28 | 170.58 (1) |
| O5—C17—C18 | 117.0 (4) | O26—Cu8—O30 | 88.91 (1) |
| O5—C17—O6 | 126.6 (4) | O26—Cu8—O32 | 90.13 (1) |
| O6—C17—C18 | 116.3 (4) | O26—Cu8—O117 | 101.2 (2) |
| C19—C18—C17 | 120.0 (4) | O26—Cu8—O197 | 96.8 (3) |
| C23—C18—C17 | 120.0 (4) | O28—Cu8—Cu7 | 82.35 (1) |
| C23—C18—C19 | 120.0 (4) | O28—Cu8—O30 | 89.94 (1) |
| C18—C19—H19 | 120.1 | O28—Cu8—O32 | 88.62 (1) |
| C20—C19—C18 | 119.8 (4) | O28—Cu8—O117 | 88.1 (2) |
| C20—C19—H19 | 120.1 | O28—Cu8—O197 | 92.5 (3) |

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| C19—C20—H20 | 119.9 | O30—Cu8—Cu7 | 84.80 (1) |
| C21—C20—C19 | 120.2 (4) | O30—Cu8—O32 | 165.30 (1) |
| C21—C20—H20 | 119.9 | O30—Cu8—O117 | 107.5 (2) |
| C20—C21—H21 | 119.9 | O30—Cu8—O197 | 91.2 (3) |
| C20—C21—C22 | 120.2 (4) | O32—Cu8—Cu7 | 80.51 (1) |
| C22—C21—H21 | 119.9 | O32—Cu8—O117 | 87.1 (2) |
| C21—C22—C24 | 121.7 (4) | O32—Cu8—O197 | 103.5 (3) |
| C23—C22—C21 | 119.2 (4) | O117—Cu8—Cu7 | 164.5 (2) |
| C23—C22—C24 | 119.1 (4) | O197—Cu8—Cu7 | 173.5 (3) |
| C18—C23—C22 | 120.5 (4) | O197—Cu8—O117 | 16.9 (3) |
| C18—C23—H23 | 119.7 | O17—Cu9—Cu10 | 83.3 (2) |
| C22—C23—H23 | 119.7 | O17—Cu9—O19 | 169.9 (2) |
| O43—C24—C22 | 116.5 (4) | O17—Cu9—O21 | 89.2 (2) |
| O44—C24—C22 | 117.9 (4) | O17—Cu9—O23 | 89.2 (2) |
| O44—C24—O43 | 125.6 (4) | O17—Cu9—O10W | 93.7 (1) |
| O7—C25—C26 | 116.2 (4) | O19—Cu9—Cu10 | 86.7 (2) |
| O8—C25—C26 | 117.1 (4) | O19—Cu9—O21 | 87.7 (2) |
| O8—C25—O7 | 126.7 (4) | O19—Cu9—O23 | 91.2 (1) |
| C27—C26—C25 | 120.1 (4) | O19—Cu9—O10W | 96.5 (1) |
| C27—C26—C31 | 119.8 (4) | O21—Cu9—Cu10 | 83.0 (1) |
| C31—C26—C25 | 120.1 (4) | O21—Cu9—O10W | 96.1 (1) |
| C26—C27—H27 | 119.5 | O23—Cu9—Cu10 | 81.8 (1) |
| C28—C27—C26 | 121.0 (5) | O23—Cu9—O21 | 164.8 (1) |
| C28—C27—H27 | 119.5 | O23—Cu9—O10W | 98.9 (2) |
| C27—C28—H28 | 120.2 | O10W—Cu9—Cu10 | 176.5 (2) |
| C27—C28—C29 | 119.6 (5) | O18—Cu10—Cu9 | 84.8 (2) |
| C29—C28—H28 | 120.2 | O18—Cu10—O20 | 165.9 (2) |
| C28—C29—H29 | 119.7 | O18—Cu10—O111 | 102.1 (2) |
| C30—C29—C28 | 120.6 (4) | O20—Cu10—Cu9 | 81.0 (2) |
| C30—C29—H29 | 119.7 | O20—Cu10—O111 | 91.8 (2) |
| C29—C30—C31 | 119.3 (4) | O22—Cu10—Cu9 | 84.5 (2) |
| C29—C30—C32 | 120.2 (4) | O22—Cu10—O18 | 90.1 (2) |
| C31—C30—C32 | 120.5 (4) | O22—Cu10—O20 | 88.9 (2) |
| C26—C31—C30 | 119.7 (4) | O22—Cu10—O111 | 90.0 (2) |
| C26—C31—H31 | 120.1 | O24—Cu10—Cu9 | 86.1 (2) |
| C30—C31—H31 | 120.1 | O24—Cu10—O18 | 88.7 (2) |
| O25—C32—C30 | 116.9 (4) | O24—Cu10—O20 | 89.9 (19) |
| O25—C32—O26 | 125.8 (4) | O24—Cu10—O22 | 170.6 (2) |
| O26—C32—C30 | 117.3 (4) | O24—Cu10—O111 | 99.3 (2) |
| O11—C33—C34 | 116.7 (4) | O111—Cu10—Cu9 | 171.1 (2) |
| O11—C33—O12 | 126.5 (5) | O1—Cu11—Cu12 | 85.41 (9) |

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| O12—C33—C34 | 116.8 (4) | O1—Cu11—O5$^{i}$ | 88.7 (2) |
| C35—C34—C33 | 121.3 (5) | O1—Cu11—O7 | 88.8 (2) |
| C35—C34—C39 | 119.6 (5) | O1—Cu11—O102 | 98.0 (3) |
| C39—C34—C33 | 119.1 (4) | O3—Cu11—Cu12 | 84.4 (1) |
| C34—C35—H35 | 119.7 | O3—Cu11—O1 | 169.8 (2) |
| C36—C35—C34 | 120.7 (5) | O3—Cu11—O5$^{i}$ | 91.41 (5) |
| C36—C35—H35 | 119.7 | O3—Cu11—O7 | 88.7 (2) |
| C35—C36—H36 | 119.9 | O3—Cu11—O102 | 92.2 (2) |
| C35—C36—C37 | 120.1 (6) | O5$^{i}$—Cu11—Cu12 | 83.85 (9) |
| C37—C36—H36 | 119.9 | O5$^{i}$—Cu11—O102 | 94.90 (2) |
| C36—C37—H37 | 120.1 | O7—Cu11—Cu12 | 83.1 (2) |
| C38—C37—C36 | 119.7 (6) | O7—Cu11—O5$^{i}$ | 166.8 (2) |
| C38—C37—H37 | 120.1 | O7—Cu11—O102 | 98.22 (2) |
| C37—C38—C40 | 119.9 (5) | O102—Cu11—Cu12 | 176.3 (1) |
| C39—C38—C37 | 120.5 (5) | O2—Cu12—Cu11 | 83.20 (9) |
| C39—C38—C40 | 119.6 (5) | O2—Cu12—O2WA | 103.0 (2) |
| C34—C39—H39 | 120.3 | O2—Cu12—O2WB | 84.9 (3) |
| C38—C39—C34 | 119.4 (5) | O4—Cu12—Cu11 | 83.6 (1) |
| C38—C39—H39 | 120.3 | O4—Cu12—O2 | 166.7 (1) |
| O17—C40—C38 | 116.8 (5) | O4—Cu12—O2WA | 89.9 (2) |
| O17—C40—O18 | 126.6 (5) | O4—Cu12—O2WB | 108.4 (3) |
| O18—C40—C38 | 116.6 (4) | O6$^{i}$—Cu12—Cu11 | 84.50 (9) |
| O13—C41—C42 | 116.4 (4) | O6$^{i}$—Cu12—O2 | 88.6 (1) |
| O13—C41—O14 | 126.9 (5) | O6$^{i}$—Cu12—O4 | 91.6 (1) |
| O14—C41—C42 | 116.6 (4) | O6$^{i}$—Cu12—O8 | 170.0 (1) |
| C43—C42—C41 | 120.0 (5) | O6$^{i}$—Cu12—O2WA | 103.9 (2) |
| C47—C42—C41 | 119.9 (4) | O6$^{i}$—Cu12—O2WB | 89.8 (3) |
| C47—C42—C43 | 120.1 (5) | O8—Cu12—Cu11 | 85.53 (9) |
| C42—C43—H43 | 120 | O8—Cu12—O2 | 89.3 (1) |
| C44—C43—C42 | 120.0 (6) | O8—Cu12—O4 | 88.1 (1) |
| C44—C43—H43 | 120 | O8—Cu12—O2WA | 86.1 (2) |
| C43—C44—H44 | 120.2 | O8—Cu12—O2WB | 99.8 (3) |
| C43—C44—C45 | 119.6 (6) | O2WA—Cu12—Cu11 | 169.5 (2) |
| C45—C44—H44 | 120.2 | O2WB—Cu12—Cu11 | 166.9 (3) |
| C44—C45—H45 | 119.5 | O2WB—Cu12—O2WA | 22.8 (3) |
| C46—C45—C44 | 120.9 (6) | C1—O1—Cu11 | 122.4 (3) |
| C46—C45—H45 | 119.5 | C1—O2—Cu12 | 124.0 (3) |
| C45—C46—C48 | 121.0 (5) | C9—O3—Cu11 | 122.5 (4) |
| C47—C46—C45 | 119.3 (5) | C9—O4—Cu12 | 122.6 (3) |
| C47—C46—C48 | 119.6 (4) | C17—O5—Cu11$^{i}$ | 122.1 (3) |
| C42—C47—H47 | 120 | C17—O6—Cu12$^{i}$ | 122.4 (3) |

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| C46—C47—C42 | 120.0 (5) | C25—O7—Cu11 | 123.4 (3) |
| C46—C47—H47 | 120 | C25—O8—Cu12 | 121.2 (3) |
| O45—C48—C46 | 117.9 (4) | C8—O9—Cu1$^{i}$ | 123.0 (3) |
| O46—C48—C46 | 116.4 (4) | C8—O10—Cu2$^{i}$ | 121.2 (3) |
| O46—C48—O45 | 125.6 (5) | C33—O11—Cu1 | 122.4 (3) |
| O15$^{i}$—C49—C50 | 117.1 (4) | C33—O12—Cu2 | 122.4 (3) |
| O15$^{i}$—C49—O16$^{i}$ | 126.3 (5) | C41—O13—Cu1 | 122.7 (4) |
| O16$^{i}$—C49—C50 | 116.6 (4) | C41—O14—Cu2 | 121.7 (3) |
| C51—C50—C49 | 120.8 (5) | C49$^{i}$—O15—Cu1 | 120.8 (3) |
| C55—C50—C49 | 118.9 (5) | C49$^{i}$—O16—Cu2 | 124.2 (3) |
| C55—C50—C51 | 120.3 (5) | C40—O17—Cu9 | 124.1 (3) |
| C50—C51—H51 | 119.5 | C40—O18—Cu10 | 120.9 (3) |
| C52—C51—C50 | 121.0 (6) | C16—O19—Cu9 | 119.3 (4) |
| C52—C51—H51 | 119.5 | C16—O20—Cu10 | 125.3 (3) |
| C51—C52—H52 | 120.2 | C57—O21—Cu9 | 123.8 (4) |
| C51—C52—C53 | 119.6 (6) | C57—O22—Cu10 | 123.6 (4) |
| C53—C52—H52 | 120.2 | C65—O23—Cu9 | 124.0 (4) |
| C52—C53—H53 | 120.5 | C65—O24—Cu10 | 120.8 (4) |
| C54—C53—C52 | 119.0 (6) | C32—O25—Cu7 | 126.8 (3) |
| C54—C53—H53 | 120.5 | C32—O26—Cu8 | 118.4 (3) |
| C53—C54—C55 | 120.7 (5) | C73—O27—Cu7 | 119.1 (3) |
| C53—C54—C56 | 120.0 (5) | C73—O28—Cu8 | 124.3 (3) |
| C55—C54—C56 | 119.2 (5) | C64—O29—Cu7 | 124.1 (4) |
| C50—C55—C54 | 119.4 (5) | C64—O30—Cu8 | 121.0 (3) |
| C50—C55—H55 | 120.3 | C81—O31—Cu7 | 119.1 (3) |
| C54—C55—H55 | 120.3 | C81—O32—Cu8 | 126.3 (3) |
| O39—C56—C54 | 117.4 (4) | C88—O33—Cu5 | 119.9 (4) |
| O40—C56—C54 | 116.8 (4) | C88—O34—Cu6 | 125.8 (4) |
| O40—C56—O39 | 125.8 (5) | C72—O35—Cu5 | 125.8 (3) |
| O21—C57—C58 | 118.4 (6) | C72—O36—Cu6 | 120.2 (4) |
| O21—C57—O22 | 124.8 (6) | C89—O37—Cu5 | 123.2 (3) |
| O22—C57—C58 | 116.8 (5) | C89—O38—Cu6 | 122.9 (3) |
| C59—C58—C57 | 121.6 (6) | C56—O39—Cu5 | 122.5 (3) |
| C59—C58—C63 | 119.0 (6) | C56—O40—Cu6 | 123.0 (3) |
| C63—C58—C57 | 119.4 (5) | C80—O41—Cu3 | 126.3 (3) |
| C58—C59—H59 | 119.1 | C80—O42—Cu4 | 118.7 (3) |
| C58—C59—C60 | 121.8 (7) | C24—O43—Cu3 | 117.0 (3) |
| C60—C59—H59 | 119.1 | C24—O44—Cu4 | 128.5 (3) |
| C59—C60—H60 | 120.6 | C48—O45—Cu3 | 120.9 (3) |
| C59—C60—C61 | 118.9 (7) | C48—O46—Cu4 | 124.2 (3) |
| C61—C60—H60 | 120.6 | C96—O47—Cu3 | 125.1 (3) |

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| C60—C61—H61 | 120.1 | C96—O48—Cu4 | 121.1 (3) |
| C60—C61—C62 | 119.9 (7) | C197$^{i}$—O2WB—Cu12 | 125.5 (8) |
| C62—C61—H61 | 120.1 | O113$^{i}$—O12W—C117 | 152.1 (1) |
| C61—C62—C64 | 119.9 (6) | C100—N1—C101 | 119.8 (1) |
| C63—C62—C61 | 120.4 (6) | C100—N1—C102 | 121.3 (1) |
| C63—C62—C64 | 119.7 (5) | C102—N1—C101 | 118.6 (1) |
| C58—C63—H63 | 120 | O100—C100—N1 | 121.8 (1) |
| C62—C63—C58 | 119.9 (5) | C103—N2—C104 | 121.9 (6) |
| C62—C63—H63 | 120 | C103—N2—C105 | 119.5 (6) |
| O29—C64—C62 | 117.2 (5) | C104—N2—C105 | 118.5 (6) |
| O29—C64—O30 | 125.9 (5) | C103—O101—Cu1 | 125.8 (4) |
| O30—C64—C62 | 116.9 (5) | O101—C103—N2 | 123.0 (6) |
| O23—C65—C66 | 117.4 (5) | C106—N3—C107 | 121.1 (7) |
| O23—C65—O24 | 126.9 (6) | C106—N3—C108 | 123.2 (8) |
| O24—C65—C66 | 115.7 (5) | C107—N3—C108 | 115.7 (7) |
| C67—C66—C65 | 119.8 (5) | C106—O102—Cu11 | 121.4 (4) |
| C71—C66—C65 | 119.8 (5) | O102—C106—N3 | 126.1 (7) |
| C71—C66—C67 | 120.4 (6) | C109—N4—C110 | 119.5 (8) |
| C66—C67—H67 | 119.8 | C109—N4—C111 | 120.4 (7) |
| C66—C67—C68 | 120.3 (6) | C110—N4—C111 | 120.0 (6) |
| C68—C67—H67 | 119.8 | O103—C109—N4 | 122.9 (9) |
| C67—C68—H68 | 120.4 | C112—N5—C113 | 120.9 (7) |
| C67—C68—C69 | 119.3 (5) | C112—N5—C114 | 121.4 (7) |
| C69—C68—H68 | 120.4 | C114—N5—C113 | 117.7 (6) |
| C68—C69—H69 | 119.9 | C112—O104—Cu3 | 118.0 (3) |
| C70$^{i}$—C69—C68 | 120.2 (6) | O104—C112—N5 | 125.1 (7) |
| C70$^{i}$—C69—H69 | 119.9 | C115—N6A—C196 | 89.2 (1) |
| C69$^{i}$—C70—C72 | 119.2 (5) | C115—N6A—C117 | 125.6 (1) |
| C71$^{i}$—C70—C69$^{i}$ | 119.6 (5) | C116—N6A—C115 | 121.3 (1) |
| C71$^{i}$—C70—C72 | 121.1 (4) | C116—N6A—C196 | 144 (3) |
| C66—C71—C70$^{i}$ | 120.2 (5) | C116—N6A—C117 | 112.9 (1) |
| C66—C71—H71 | 119.9 | C115—N6B—C116 | 100.2 (1) |
| C70$^{i}$—C71—H71 | 119.9 | C115—N6B—C196 | 115 (2) |
| O35—C72—C70 | 117.8 (4) | C115—N6B—C117 | 139 (2) |
| O35—C72—O36 | 125.7 (5) | C196—N6B—C116 | 138 (2) |
| O36—C72—C70 | 116.5 (5) | C196—N6B—C117 | 46.3 (1) |
| O27—C73—C74 | 116.7 (4) | C117—N6B—C116 | 92.5 (1) |
| O28—C73—C74 | 115.8 (4) | C115—N6C—C116 | 114 (3) |
| O28—C73—O27 | 127.4 (4) | C115—N6C—C186 | 155 (4) |
| C75—C74—C73 | 120.1 (4) | C186—N6C—C116 | 60 (3) |
| C79—C74—C73 | 119.4 (4) | C115—O105—Cu2 | 116.0 (1) |

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| C79—C74—C75 | 120.5 (4) | C115—O195—Cu2 | 105.5 (6) |
| C74—C75—H75 | 120.2 | N6A—C115—O195 | 125.6 (1) |
| C76—C75—C74 | 119.6 (4) | N6B—C115—N6C | 82 (2) |
| C76—C75—H75 | 120.2 | N6B—C115—O195 | 128.2 (1) |
| C75—C76—H76 | 119.8 | N6C—C115—N6A | 58 (2) |
| C77—C76—C75 | 120.3 (4) | N6C—C115—O195 | 82.7 (1) |
| C77—C76—H76 | 119.8 | O105—C115—N6A | 126.5 (1) |
| C76—C77—H77 | 120 | O105—C115—N6B | 131.4 (1) |
| C76—C77—C78 | 120.1 (4) | O105—C115—N6C | 80 (2) |
| C78—C77—H77 | 120 | N6A—C116—N6C | 54 (2) |
| C77—C78—C79 | 120.0 (4) | N6A—C116—C186 | 113 (3) |
| C77—C78—C80 | 119.9 (4) | N6C—C116—N6B | 60.9 (12) |
| C79—C78—C80 | 120.1 (4) | C186—C116—N6B | 118 (2) |
| C74—C79—C78 | 119.4 (4) | C186—C116—N6C | 59 (2) |
| C74—C79—H79 | 120.3 | N6C—C186—O8WA$^{i}$ | 121 (4) |
| C78—C79—H79 | 120.3 | N6C—C186—C116 | 61 (2) |
| O41—C80—C78 | 116.3 (4) | C116—C186—O8WA$^{i}$ | 146 (5) |
| O41—C80—O42 | 126.2 (4) | C117—C196—N6A | 56.4 (1) |
| O42—C80—C78 | 117.5 (3) | C117—C196—N6B | 70.3 (1) |
| O31—C81—C82 | 117.8 (5) | O12W—C117—N6A | 89 (2) |
| O32—C81—C82 | 116.6 (4) | O12W—C117—N6B | 111.9 (1) |
| O32—C81—O31 | 125.6 (5) | C196—C117—O12W | 162 (2) |
| C83—C82—C81 | 120.4 (5) | C196—C117—N6A | 84.7 (1) |
| C87—C82—C81 | 120.5 (5) | C196—C117—N6B | 63.4 (1) |
| C87—C82—C83 | 119.0 (5) | C118—N7—C119 | 120.8 (5) |
| C82—C83—H83 | 120.4 | C118—N7—C120 | 122.7 (5) |
| C84—C83—C82 | 119.1 (6) | C120—N7—C119 | 116.3 (5) |
| C84—C83—H83 | 120.4 | C118—O106—Cu7 | 115.2 (3) |
| C83—C84—H84 | 119.9 | O106—C118—N7 | 124.3 (5) |
| C85—C84—C83 | 120.2 (7) | C121—N8—C122 | 118.2 (1) |
| C85—C84—H84 | 119.9 | C123—N8—C121 | 128.2 (1) |
| C84—C85—H85 | 119.4 | C123—N8—C122 | 113.5 (1) |
| C86—C85—C84 | 121.2 (7) | O107—C123—N8 | 122.9 (1) |
| C86—C85—H85 | 119.4 | C125—N9—C124 | 132.5 (1) |
| C85—C86—C87 | 119.3 (6) | C125—N9—C126 | 104.4 (1) |
| C85—C86—C88 | 121.8 (6) | C126—N9—C124 | 123.1 (1) |
| C87—C86—C88 | 118.9 (5) | O108—C125—N9 | 121 (2) |
| C82—C87—C86 | 121.1 (5) | C127—N10—C128 | 120.5 (1) |
| C82—C87—H87 | 119.5 | C127—N10—C129 | 120.3 (1) |
| C86—C87—H87 | 119.5 | C129—N10—C128 | 119.2 (1) |
| O33—C88—C86 | 116.7 (5) | O109—C127—N10 | 118 (3) |

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| O34—C88—C86 | 117.5 (5) | O109—C127—O199 | 121 (3) |
| O34—C88—O33 | 125.8 (5) | O199—C127—N10 | 119.5 (1) |
| O37—C89—C90 | 118.7 (4) | C130—N11—C131 | 120.3 (1) |
| O37—C89—O38 | 125.7 (5) | C130—N11—C132 | 127.2 (1) |
| O38—C89—C90 | 115.7 (4) | C130—N11—C192 | 109 (2) |
| C91—C90—C89 | 120.2 (4) | C131—N11—C132 | 109.5 (1) |
| C95—C90—C89 | 119.8 (4) | C192—N11—C131 | 117 (2) |
| C95—C90—C91 | 120.0 (5) | C192—N11—C132 | 57 (2) |
| C90—C91—H91 | 120.2 | O110—C130—N11 | 126.3 (1) |
| C92—C91—C90 | 119.6 (5) | C133—N12—C134 | 133.8 (1) |
| C92—C91—H91 | 120.2 | C133—N12—C135 | 116.2 (1) |
| C91—C92—H92 | 119.6 | C133—N12—C195 | 108.9 (1) |
| C93—C92—C91 | 120.7 (5) | C134—N12—C135 | 109.9 (1) |
| C93—C92—H92 | 119.6 | C195—N12—C134 | 48.2 (1) |
| C92—C93—H93 | 120.1 | C195—N12—C135 | 114 (2) |
| C92—C93—C94 | 119.8 (5) | C133—O111—Cu10 | 110.6 (6) |
| C94—C93—H93 | 120.1 | N12—C133—O111 | 127.3 (1) |
| C93—C94—C96 | 120.8 (4) | O13W—C134—N12 | 102.7 (1) |
| C95—C94—C93 | 119.0 (5) | C195—C134—O13W | 154 (2) |
| C95—C94—C96 | 120.2 (4) | C195—C134—N12 | 65.5 (1) |
| C90—C95—C94 | 120.9 (4) | C134—C195—N12 | 66.3 (1) |
| C90—C95—H95 | 119.6 | C138—N13A—C136 | 127 (7) |
| C94—C95—H95 | 119.6 | C136—N13B—C137 | 120.9 (1) |
| O47—C96—C94 | 117.7 (4) | C136—N13B—C197 | 140.7 (1) |
| O48—C96—C94 | 117.5 (4) | C136—N13B—C138 | 122.1 (1) |
| O48—C96—O47 | 124.8 (4) | C137—N13B—C197 | 91.7 (1) |
| O9$^{i}$—Cu1—Cu2 | 83.3 (1) | C138—N13B—C137 | 114.3 (1) |
| O9$^{i}$—Cu1—O101 | 97.4 (1) | C138—N13B—C197 | 45.9 (1) |
| O11—Cu1—Cu2 | 84.1 (1) | C136—O112—Cu4 | 106.5 (4) |
| O11—Cu1—O9$^{i}$ | 167.5 (1) | N13A—C136—O112 | 143 (4) |
| O11—Cu1—O101 | 95.0 (1) | N13B—C136—N13A | 45 (4) |
| O13—Cu1—Cu2 | 84.1 (1) | N13B—C136—O112 | 126.6 (1) |
| O13—Cu1—O9$^{i}$ | 89.4 (1) | N13B—C197—O2WB$^{i}$ | 137.9 (1) |
| O13—Cu1—O11 | 89.6 (1) | C138—C197—O2WB$^{i}$ | 158.3 (1) |
| O13—Cu1—O101 | 93.7 (1) | C138—C197—N13B | 63.6 (1) |
| O15—Cu1—Cu2 | 86.2 (1) | C197—C138—N13A | 114 (3) |
| O15—Cu1—O9$^{i}$ | 89.3 (1) | C197—C138—N13B | 70.5 (1) |
| O15—Cu1—O11 | 89.4 (1) | O123—N14—C140 | 151.7 (1) |
| O15—Cu1—O13 | 170.43 (15) | O123—N14—C141 | 90.2 (18) |
| O15—Cu1—O101 | 95.81 (15) | C139—N14—C140 | 119.8 (14) |
| O101—Cu1—Cu2 | 177.79 (12) | C139—N14—C141 | 117 (2) |

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| O10$^{i}$—Cu2—Cu1 | 85.09 (10) | C140—N14—C141 | 117.1 (19) |
| O10$^{i}$—Cu2—O14 | 88.32 (17) | C151—N14—O123 | 124.5 (16) |
| O10$^{i}$—Cu2—O16 | 89.80 (16) | C151—N14—C139 | 93.2 (15) |
| O10$^{i}$—Cu2—O105 | 102.4 (7) | C151—N14—C141 | 120 (5) |
| O10$^{i}$—Cu2—O195 | 98.7 (3) | O12W$^{i}$—O113—Cu6 | 115.1 (9) |
| O12—Cu2—Cu1 | 84.40 (10) | O123—O113—Cu6 | 76.2 (9) |
| O12—Cu2—O10$^{i}$ | 169.45 (1) | O123—O113—O12W$^{i}$ | 167.5 (2) |
| O12—Cu2—O14 | 89.82 (1) | C139—O113—Cu6 | 109.1 (9) |
| O12—Cu2—O16 | 89.57 (1) | C139—O113—O12W$^{i}$ | 133.0 (1) |
| O12—Cu2—O105 | 88.0 (6) | N14—O123—Cu6 | 109.6 (9) |
| O12—Cu2—O195 | 91.8 (3) | O113—O123—Cu6 | 82.7 (9) |
| O14—Cu2—Cu1 | 84.16 (1) | O113—O123—N14 | 166.6 (1) |
| O14—Cu2—O16 | 166.36 (1) | C139—O123—Cu6 | 146.5 (1) |
| O14—Cu2—O105 | 107.1 (7) | C139—O123—N14 | 65.6 (1) |
| O14—Cu2—O195 | 100.6 (3) | C139—O123—O113 | 101.2 (1) |
| O16—Cu2—Cu1 | 82.21 (1) | O113—C139—N14 | 121.1 (1) |
| O16—Cu2—O105 | 86.5 (7) | O113—C139—C151 | 158.3 (1) |
| O16—Cu2—O195 | 93.0 (3) | O123—C139—N14 | 81.6 (1) |
| O105—Cu2—Cu1 | 166.4 (5) | N14—C140—N18 | 94.6 (1) |
| O195—Cu2—Cu1 | 173.9 (2) | C151—C140—N14 | 58.2 (1) |
| O195—Cu2—O105 | 7.6 (6) | C151—C140—N18 | 52.7 (1) |
| O41—Cu3—Cu4 | 81.43 (9) | C151—C140—C162 | 102 (3) |
| O41—Cu3—O45 | 90.40 (1) | C162—C140—N14 | 143 (3) |
| O41—Cu3—O47 | 89.97 (1) | C162—C140—N18 | 53 (2) |
| O41—Cu3—O104 | 89.33 (1) | N14—C151—C161 | 127.2 (1) |
| O43—Cu3—Cu4 | 89.57 (9) | N14—C151—C162 | 119.4 (1) |
| O43—Cu3—O41 | 171.0 (1) | C140—C151—N14 | 85.9 (1) |
| O43—Cu3—O45 | 88.6 (3) | C140—C151—C139 | 119.5 (1) |
| O43—Cu3—O47 | 88.79 (2) | C140—C151—N18 | 92 (2) |
| O43—Cu3—O104 | 99.63 (2) | C140—C151—C161 | 146 (2) |
| O45—Cu3—Cu4 | 84.78 (2) | N18—C151—N14 | 126.2 (1) |
| O45—Cu3—O104 | 100.86 (2) | N18—C151—C139 | 141.8 (1) |
| O47—Cu3—Cu4 | 81.50 (2) | N18—C151—C161 | 63.3 (1) |
| O47—Cu3—O45 | 166.0 (2) | N18—C151—C162 | 54.0 (1) |
| O47—Cu3—O104 | 93.0 (2) | C161—C151—C139 | 93.2 (2) |
| O104—Cu3—Cu4 | 169.2 (2) | C162—C151—C139 | 160.3 (2) |
| O42—Cu4—Cu3 | 86.97 (8) | C162—C151—C161 | 106.4 (2) |
| O42—Cu4—O44 | 165.7 (2) | C142—N15—C143 | 111.1 (2) |
| O42—Cu4—O112 | 102.2 (2) | C142—N15—C144 | 121.8 (2) |
| O44—Cu4—Cu3 | 78.79 (9) | C143—N15—C144 | 126.8 (2) |
| O44—Cu4—O112 | 91.9 (2) | C142—O114—Cu5 | 118.9 (7) |

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| O46—Cu4—Cu3 | 83.6 (2) | O114—C142—N15 | 130.9 (2) |
| O46—Cu4—O42 | 90.4 (2) | C145—N16—C146 | 130.5 (2) |
| O46—Cu4—O44 | 88.8 (2) | C145—N16—C147 | 117.2 (2) |
| O46—Cu4—O112 | 90.5 (2) | C146—N16—C147 | 112.2 (2) |
| O48—Cu4—Cu3 | 86.60 (9) | O185—C145—N16 | 115.3 (2) |
| O48—Cu4—O42 | 88.6 (2) | O115—C146—N16 | 113.5 (2) |
| O48—Cu4—O44 | 89.6 (2) | C148—N17—C149 | 115.4 (2) |
| O48—Cu4—O46 | 170.2 (2) | C148—N17—C150 | 117.7 (2) |
| O48—Cu4—O112 | 99.1 (2) | C149—N17—C150 | 126.8 (2) |
| O112—Cu4—Cu3 | 169.1 (2) | O116—C148—N17 | 127 (2) |
| O33—Cu5—Cu6 | 86.7 (2) | C160—O197—Cu8 | 94.3 (7) |
| O33—Cu5—O39 | 88.9 (2) | O197—C160—C162 | 146.8 (2) |
| O33—Cu5—O114 | 98.1 (2) | C140—C162—C160 | 112 (3) |
| O35—Cu5—Cu6 | 82.0 (2) | C151—C162—C160 | 87.7 (2) |
| O35—Cu5—O33 | 168.7 (2) | | |

Symmetry codes: (i) -*x*+1, -*y*+1, -*z*; (ii) *x*-1, *y*, *z*; (iii) *x*+1, *y*, *z*.