supporting information

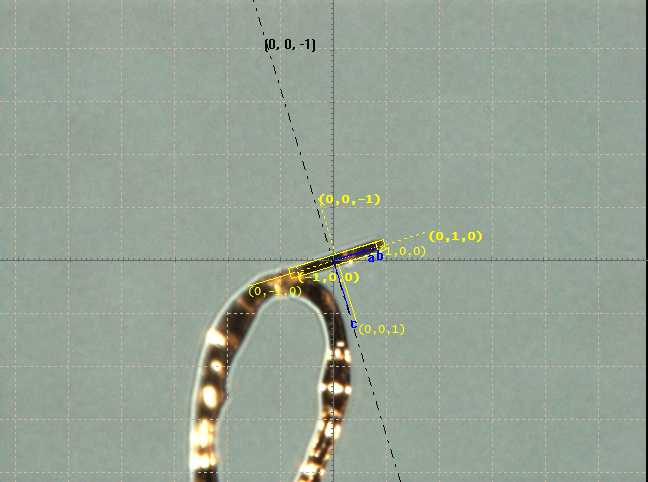
Characterization and Structural Analysis of Genkwanin, a Natural Product from *Callicarpa americana*

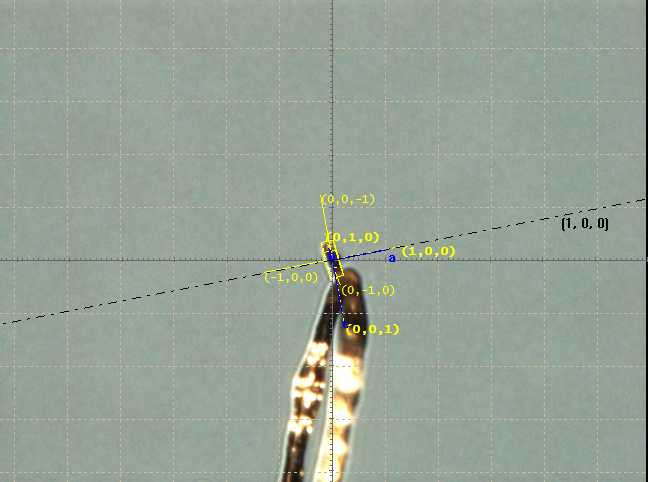
Gina Porras 1,†, John Bacsa 2,†, Huaqiao Tang 1 and Cassandra L. Quave 1,3,4,\*

**Figure S1.** 1H NMR (600 MHz, DMSO-*d6*) spectrum of Genkwanin (**1**).

**Crystal Morphology**

Photographs of the crystal on the diffractometer showing the needle-like growth morphology. The (010) and (0-10) faces correspond to the needle axis. The (001), (00-1), (100) and (-100) faces have distances that are much shorter than the distance to the (010) face (even after the crystal was cut).

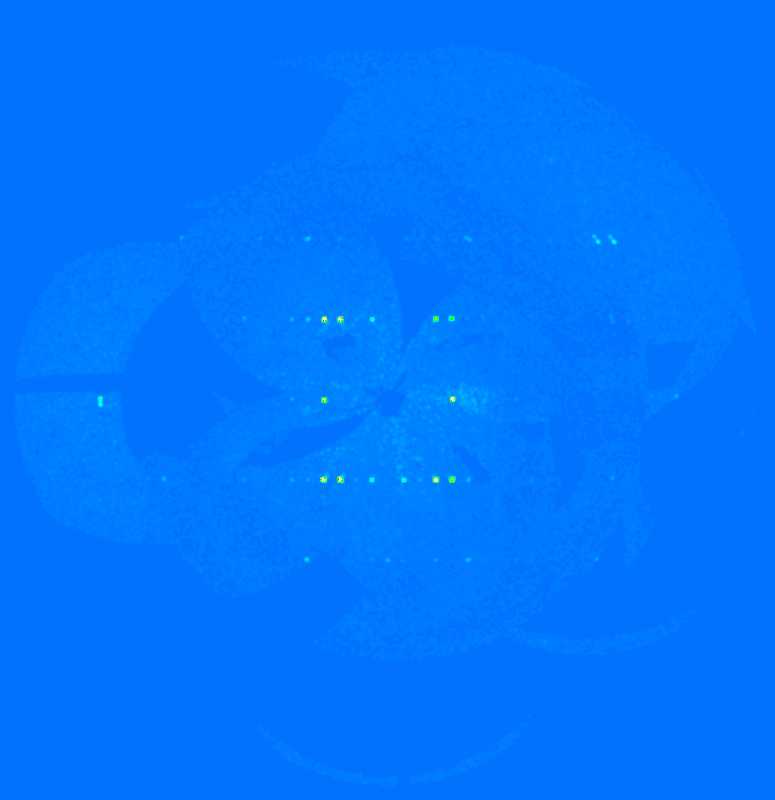




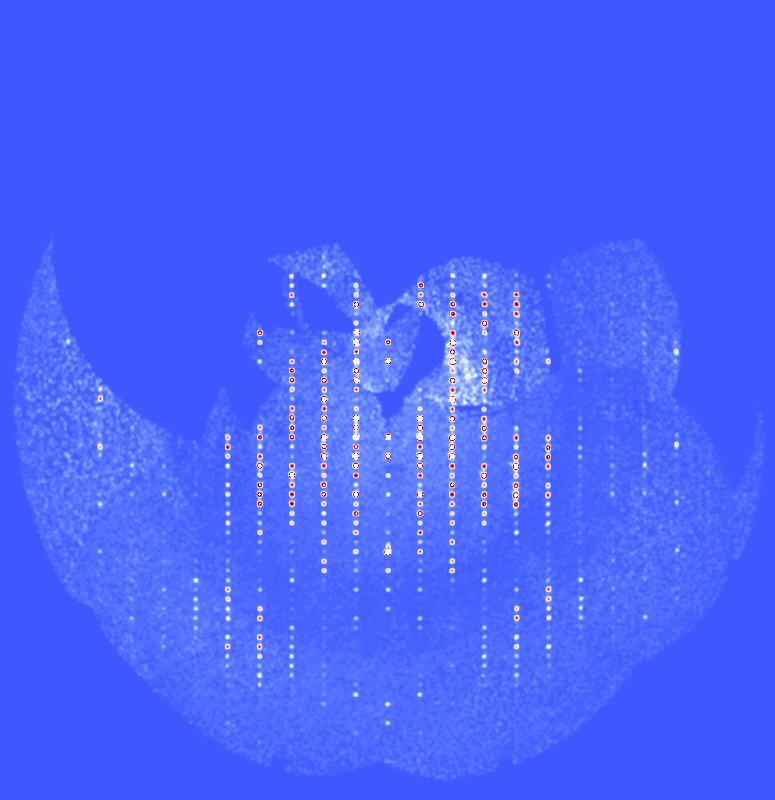
**Precession Images**

Reconstructed precession photographs for the Genkwanin crystal 2 in the (a) hk0 and (b) h0l layers and (c) 0kl layers showing the weak diffraction except along the needle (the b\*direction).

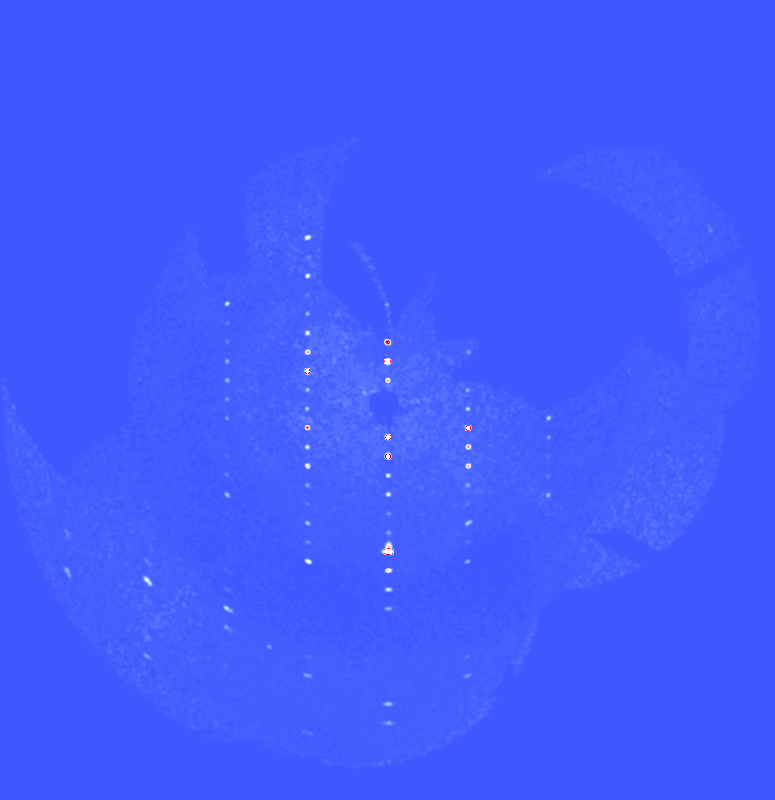
**(a) hk0 plane**

****

**(b) h0l plane**

****

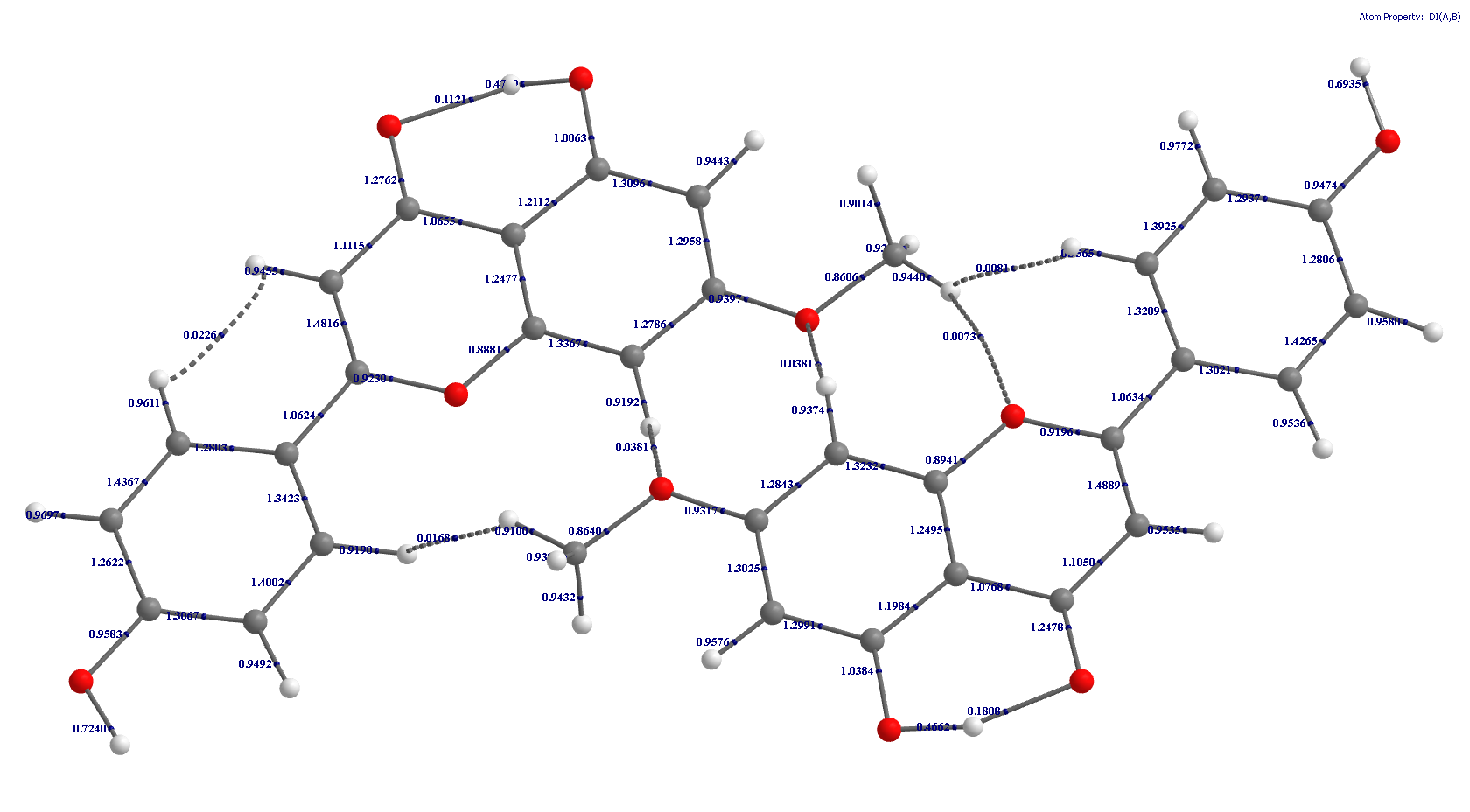
**(c) 0kl plane**

****

**Quantum Mechanical Calculations**

A Hirshfeld atom refinement was performed using Olex2 [35] to determine the accurate geometry with optimised hydrogen atom positions. The molecular orbitals of the asymmetric unit of the crystal were obtained with Gaussian 16 software [37], and the local and integrated properties of electron density were calculated with the AIMAll suite of programs [38] to investigate the conjugation in the X-ray structure. The Kohn-Sham molecular orbitals were calculated using a b3lyp/SCCF calculation and a TZVP basis set.

The molecular graph of the asymmetric unit is shown in the Figure 1s. The small spheres are bond critical points and the values of the bond delocalization indices (DI’s) between the bonded pairs of atoms are shown. The most important DI’s for the discussion are for the C-C bond that links the two planar moieties (highlighted in the table below).

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**Figure S4.** The molecular graph of the asymmetric unit with the bond critical points and the values of the bond delocalization indices (DI’s).

**Table S1.** The properties of the bond critical points between atoms. The bond localization indices (DI) are shown in the last column.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atoms** | **Rho** | **DelSqRho** | **Ellipticity** | **DI(A|B)** |
| C21 - C24 | 0.283722 | -0.797947 | 0.133561 | 1.062404 |
| C54 - C57 | 0.287365 | -0.818474 | 0.129315 | 1.063396 |
| O1 - H3 | 0.051956 | +0.139246 | 0.035351 | 0.112146 |
| O2 - H3 | 0.363746 | -2.603211 | 0.016272 | 0.471887 |
| O1 - C8 | 0.384818 | -0.386162 | 0.043297 | 1.276169 |
| O6 - H7 | 0.242314 | -0.921748 | 0.027301 | 0.724041 |
| C9 - C10 | 0.303496 | -0.855840 | 0.207807 | 1.211197 |
| C8 - C9 | 0.285594 | -0.789705 | 0.140928 | 1.065486 |
| C10 - C11 | 0.317576 | -0.922030 | 0.244347 | 1.309626 |
| O2 - C10 | 0.310619 | -0.601335 | 0.018877 | 1.006312 |
| C11 - C13 | 0.311115 | -0.883007 | 0.239726 | 1.295835 |
| C9 - C20 | 0.311604 | -0.889425 | 0.229755 | 1.247714 |
| C18 - H19 | 0.289022 | -1.019442 | 0.031992 | 0.919243 |
| C11 - H12 | 0.301577 | -1.087571 | 0.033430 | 0.944268 |
| O4 - C13 | 0.295763 | -0.476129 | 0.006345 | 0.939699 |
| C18 - C20 | 0.320003 | -0.929559 | 0.273797 | 1.336683 |
| O4 - C14 | 0.242729 | -0.394551 | 0.016804 | 0.860642 |
| H17 - O38 | 0.002119 | +0.008086 | 1.063406 | 0.007302 |
| C14 - H17 | 0.365685 | -1.588082 | 0.048082 | 0.943988 |
| H17 - H59 | 0.003317 | +0.012196 | 0.109597 | 0.008099 |
| C14 - H15 | 0.258539 | -0.835609 | 0.041494 | 0.901413 |
| C14 - H16 | 0.329964 | -1.294284 | 0.048726 | 0.939288 |
| C13 - C18 | 0.316236 | -0.921228 | 0.239847 | 1.278585 |
| O4 - H52 | 0.010017 | +0.039408 | 0.159345 | 0.038091 |
| O5 - C20 | 0.280657 | -0.291931 | 0.010553 | 0.888092 |
| C8 - C22 | 0.302520 | -0.882546 | 0.144982 | 1.111532 |
| O5 - C21 | 0.290068 | -0.325968 | 0.016468 | 0.923040 |
| C21 - C22 | 0.328964 | -0.952168 | 0.314949 | 1.481648 |
| C22 - H23 | 0.309724 | -1.146961 | 0.027003 | 0.945467 |
| C25 - H26 | 0.268351 | -0.897348 | 0.013372 | 0.919027 |
| C24 - C25 | 0.316515 | -0.913429 | 0.193480 | 1.342257 |
| C24 - C32 | 0.297183 | -0.817746 | 0.172309 | 1.280294 |
| C27 - C29 | 0.315986 | -0.914861 | 0.232068 | 1.306723 |
| C25 - C27 | 0.315296 | -0.904496 | 0.208268 | 1.400230 |
| C27 - H28 | 0.264675 | -0.870332 | 0.027517 | 0.949176 |
| C30 - C32 | 0.318892 | -0.916116 | 0.218059 | 1.436695 |
| O6 - C29 | 0.300141 | -0.459071 | 0.006116 | 0.958266 |
| C32 - H33 | 0.343673 | -1.396887 | 0.004526 | 0.961110 |
| H23 - H33 | 0.011829 | +0.047497 | 1.077493 | 0.022648 |
| C29 - C30 | 0.314885 | -0.922858 | 0.207738 | 1.262189 |
| C30 - H31 | 0.335005 | -1.331167 | 0.019032 | 0.969713 |
| O34 - H36 | 0.076145 | +0.103142 | 0.018200 | 0.180762 |
| O35 - H36 | 0.248079 | -1.174941 | 0.019566 | 0.466190 |
| H19 - O37 | 0.010051 | +0.038533 | 0.164242 | 0.038063 |
| O39 - H40 | 0.277540 | -1.383590 | 0.023412 | 0.693471 |
| C51 - C53 | 0.316224 | -0.908592 | 0.266906 | 1.323195 |
| O34 - C41 | 0.388558 | -0.309944 | 0.040161 | 1.247793 |
| C46 - C51 | 0.320368 | -0.944035 | 0.240557 | 1.284319 |
| C41 - C42 | 0.283362 | -0.774100 | 0.150270 | 1.076817 |
| O35 - C43 | 0.317446 | -0.634481 | 0.023391 | 1.038377 |
| C44 - C46 | 0.314542 | -0.900722 | 0.239847 | 1.302469 |
| C42 - C53 | 0.313998 | -0.902544 | 0.229076 | 1.249547 |
| C51 - H52 | 0.325581 | -1.258841 | 0.032342 | 0.937385 |
| C42 - C43 | 0.306907 | -0.877985 | 0.201070 | 1.198412 |
| O37 - C46 | 0.288420 | -0.485145 | 0.009146 | 0.931677 |
| C43 - C44 | 0.318833 | -0.931544 | 0.242250 | 1.299074 |
| C44 - H45 | 0.326906 | -1.259176 | 0.034181 | 0.957595 |
| H26 - H48 | 0.006098 | +0.018684 | 0.086392 | 0.016778 |
| O37 - C47 | 0.251016 | -0.425903 | 0.042690 | 0.863969 |
| C47 - H48 | 0.282260 | -0.980253 | 0.054252 | 0.910040 |
| C47 - H49 | 0.329242 | -1.286060 | 0.055673 | 0.937205 |
| C47 - H50 | 0.350446 | -1.442188 | 0.058693 | 0.943197 |
| O38 - C53 | 0.282473 | -0.296650 | 0.014037 | 0.894070 |
| C41 - C55 | 0.297477 | -0.856882 | 0.143921 | 1.105040 |
| O38 - C54 | 0.283778 | -0.358147 | 0.025520 | 0.919585 |
| C54 - C55 | 0.337589 | -1.001537 | 0.309634 | 1.488941 |
| C55 - H56 | 0.330787 | -1.289810 | 0.027232 | 0.953549 |
| C60 - C62 | 0.315481 | -0.914268 | 0.221908 | 1.293668 |
| C57 - C58 | 0.308698 | -0.872856 | 0.191862 | 1.320932 |
| C58 - H59 | 0.343267 | -1.395560 | 0.008261 | 0.956534 |
| C58 - C60 | 0.313578 | -0.892944 | 0.203817 | 1.392452 |
| C60 - H61 | 0.335759 | -1.331444 | 0.021448 | 0.977171 |
| O39 - C62 | 0.294917 | -0.418723 | 0.011872 | 0.947395 |
| C57 - C65 | 0.304971 | -0.858137 | 0.182846 | 1.302095 |
| C62 - C63 | 0.319594 | -0.948767 | 0.212022 | 1.280594 |
| C63 - C65 | 0.323585 | -0.944041 | 0.212238 | 1.426451 |
| C63 - H64 | 0.301548 | -1.097461 | 0.019166 | 0.958024 |
| C65 - H66 | 0.315328 | -1.193110 | 0.010349 | 0.953591 |

**Computing details**

Data collection: *CrysAlis PRO* 1.171.40.53 (Rigaku OD, 2019); cell refinement: *CrysAlis PRO* 1.171.40.53 (Rigaku OD, 2019); data reduction: *CrysAlis PRO* 1.171.40.53 (Rigaku OD, 2019); program(s) used to solve structure: ShelXT [34]; program(s) used to refine structure: SHELXL [36]; molecular graphics: Olex2 [35]; software used to prepare material for publication: Olex2 [35]. The molecular orbitals of the asymmetric unit of the crystal were obtained with Gaussian 16 software [37], and the local and integrated properties of electron density were calculated with the AIMAll suite of programs [38] to investigate the conjugation in the X-ray structure. The Kohn-Sham molecular orbitals were calculated using a b3lyp/SCCF calculation and a TZVP basis set.

**Table S2.** Crystal data Genkwanin **1**.

|  |  |
| --- | --- |
| C16H12O5 | *D*x = 1.546 Mg m-3 |
| *Mr* = 284.26 | Cu *K* radiation,  = 1.54184 Å |
| Orthorhombic, *Pna*21 | Cell parameters from 4515 reflections |
| *a* = 19.3911 (7) Å |  = 2.7–72.0° |
| *b* = 3.86568 (19) Å |  = 0.97 mm-1 |
| *c* = 32.5877 (11) Å | *T* = 102 K |
| *V* = 2442.77 (17) Å3 | Needle, yellowish colourless |
| *Z* = 8 | 0.28 × 0.03 × 0.02 mm |
| *F*(000) = 1184 |  |

**Table S2.** Data collection Genkwanin **1**.

|  |  |
| --- | --- |
| XtaLAB Synergy, Dualflex, HyPix  diffractometer | 3900 independent reflections |
| Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source | 2676 reflections with *I* > 2(*I*) |
| Mirror monochromator | *R*int = 0.098 |
| Detector resolution: 10.0000 pixels mm-1 | max = 73.5°, min = 2.7° |
|  scans | *h* = -2222 |
| Absorption correction: multi-scan  *CrysAlis PRO* 1.171.40.53 (Rigaku Oxford Diffraction, 2019) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. | *k* = -44 |
| *T*min = 0.386, *T*max = 1.000 | *l* = -3926 |
| 16725 measured reflections |  |

**Table S3.** Refinement**.**

|  |  |
| --- | --- |
| Refinement on *F*2 | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| *R*[*F*2 > 2(*F*2)] = 0.058 | *w* = 1/[2(*F*o2) + (0.0754*P*)2 + 0.5445*P*]  where *P* = (*F*o2 + 2*F*c2)/3 |
| *wR*(*F*2) = 0.159 | (/)max < 0.001 |
| *S* = 1.06 | max = 0.27 e Å-3 |
| 3900 reflections | min = -0.27 e Å-3 |
| 384 parameters | Absolute structure: Flack x determined using 734 quotients [(I+)-(I-)]/[(I+)+(I-)] [37]. |
| 431 restraints | Absolute structure parameter: 0.3 (4) |
| Primary atom site location: dual |  |

**Special details**

*Geometry*. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Table S4.** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å2) for Genkwanin **1**.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | *x* | *y* | *z* | *U*iso\*/*U*eq |
| O1\_1 | 0.17958 (17) | 0.6569 (12) | 0.08599 (10) | 0.0319 (10) |
| O2\_1 | 0.13768 (17) | 0.3982 (11) | 0.15456 (10) | 0.0324 (11) |
| H2\_1 | 0.135150 | 0.472679 | 0.125237 | 0.049\* |
| O3\_1 | 0.29374 (18) | 0.4700 (12) | 0.26797 (8) | 0.0318 (10) |
| O4\_1 | 0.35947 (17) | 0.9391 (10) | 0.14243 (8) | 0.0288 (9) |
| O5\_1 | 0.57824 (18) | 1.6711 (11) | 0.03081 (11) | 0.0348 (11) |
| H5\_1 | 0.616080 | 1.704920 | 0.051220 | 0.052\* |
| C1\_1 | 0.2357 (2) | 0.7430 (15) | 0.10265 (11) | 0.0275 (12) |
| C2\_1 | 0.2474 (2) | 0.6725 (15) | 0.14616 (11) | 0.0267 (12) |
| C3\_1 | 0.1982 (2) | 0.5027 (15) | 0.17087 (12) | 0.0264 (11) |
| C4\_1 | 0.2113 (2) | 0.4377 (16) | 0.21200 (12) | 0.0306 (13) |
| H4\_1 | 0.178361 | 0.331085 | 0.228414 | 0.037\* |
| C5\_1 | 0.2747 (2) | 0.5346 (16) | 0.22823 (11) | 0.0281 (12) |
| C6\_1 | 0.2460 (3) | 0.2874 (17) | 0.29367 (15) | 0.0344 (15) |
| H6A\_1 | 0.233370 | 0.073220 | 0.280784 | 0.052\* |
| H6B\_1 | 0.205453 | 0.426148 | 0.297681 | 0.052\* |
| H6C\_1 | 0.267078 | 0.240791 | 0.319729 | 0.052\* |
| C7\_1 | 0.3245 (2) | 0.7025 (16) | 0.20517 (11) | 0.0285 (12) |
| H7\_1 | 0.366520 | 0.766987 | 0.216602 | 0.034\* |
| C8\_1 | 0.3093 (2) | 0.7707 (16) | 0.16446 (11) | 0.0272 (12) |
| C9\_1 | 0.3496 (2) | 1.0062 (15) | 0.10156 (11) | 0.0276 (12) |
| C10\_1 | 0.2909 (2) | 0.9110 (16) | 0.08208 (12) | 0.0306 (13) |
| H10\_1 | 0.286642 | 0.957341 | 0.054188 | 0.037\* |
| C11\_1 | 0.4089 (2) | 1.1820 (16) | 0.08406 (12) | 0.0289 (13) |
| C12\_1 | 0.4658 (2) | 1.2742 (15) | 0.10770 (13) | 0.0284 (12) |
| H12\_1 | 0.465459 | 1.225625 | 0.135646 | 0.034\* |
| C13\_1 | 0.5229 (3) | 1.4361 (16) | 0.09084 (12) | 0.0310 (14) |
| H13\_1 | 0.560260 | 1.494269 | 0.107334 | 0.037\* |
| C14\_1 | 0.5239 (2) | 1.5110 (16) | 0.04927 (13) | 0.0293 (13) |
| C15\_1 | 0.4676 (2) | 1.4268 (16) | 0.02508 (13) | 0.0312 (14) |
| H15\_1 | 0.468123 | 1.479063 | -0.002774 | 0.037\* |
| C16\_1 | 0.4109 (3) | 1.2669 (16) | 0.04185 (12) | 0.0306 (13) |
| H16\_1 | 0.373364 | 1.213817 | 0.025238 | 0.037\* |
| O1\_2 | 0.59789 (17) | 0.3332 (11) | 0.41353 (10) | 0.0326 (10) |
| O2\_2 | 0.63982 (17) | 0.5990 (10) | 0.34514 (10) | 0.0310 (10) |
| H2\_2 | 0.640913 | 0.537005 | 0.374901 | 0.046\* |
| O3\_2 | 0.48472 (18) | 0.5269 (11) | 0.23121 (9) | 0.0313 (10) |
| O4\_2 | 0.41631 (16) | 0.0761 (10) | 0.35705 (8) | 0.0282 (9) |
| O5\_2 | 0.18930 (18) | -0.5689 (12) | 0.46987 (11) | 0.0353 (11) |
| H5\_2 | 0.163592 | -0.719663 | 0.450227 | 0.053\* |
| C1\_2 | 0.5417 (2) | 0.2509 (15) | 0.39663 (12) | 0.0268 (11) |
| C2\_2 | 0.5297 (2) | 0.3289 (15) | 0.35334 (12) | 0.0267 (12) |
| C3\_2 | 0.5793 (2) | 0.4973 (15) | 0.32874 (12) | 0.0263 (12) |
| C4\_2 | 0.5663 (2) | 0.5624 (15) | 0.28759 (12) | 0.0286 (12) |
| H4\_2 | 0.599591 | 0.666959 | 0.271209 | 0.034\* |
| C5\_2 | 0.5028 (2) | 0.4688 (14) | 0.27123 (11) | 0.0246 (10) |
| C6\_2 | 0.5328 (3) | 0.7075 (17) | 0.20553 (15) | 0.0326 (14) |
| H6A\_2 | 0.511198 | 0.762886 | 0.179852 | 0.049\* |
| H6B\_2 | 0.572318 | 0.563579 | 0.200649 | 0.049\* |
| H6C\_2 | 0.547102 | 0.916862 | 0.218892 | 0.049\* |
| C7\_2 | 0.4530 (2) | 0.2997 (15) | 0.29408 (11) | 0.0276 (12) |
| H7\_2 | 0.411285 | 0.232445 | 0.282440 | 0.033\* |
| C8\_2 | 0.4676 (2) | 0.2345 (16) | 0.33493 (11) | 0.0270 (12) |
| C9\_2 | 0.4261 (2) | 0.0077 (15) | 0.39788 (11) | 0.0257 (11) |
| C10\_2 | 0.4861 (2) | 0.0847 (15) | 0.41702 (12) | 0.0291 (12) |
| H10\_2 | 0.491034 | 0.026817 | 0.444560 | 0.035\* |
| C11\_2 | 0.3652 (2) | -0.1520 (15) | 0.41568 (11) | 0.0267 (11) |
| C12\_2 | 0.3120 (2) | -0.2824 (16) | 0.39154 (12) | 0.0298 (12) |
| H12\_2 | 0.316124 | -0.273786 | 0.363128 | 0.036\* |
| C13\_2 | 0.2532 (2) | -0.4248 (15) | 0.40871 (12) | 0.0289 (11) |
| H13\_2 | 0.218474 | -0.511778 | 0.391920 | 0.035\* |
| C14\_2 | 0.2462 (2) | -0.4369 (16) | 0.45100 (13) | 0.0290 (11) |
| C15\_2 | 0.2980 (3) | -0.3043 (17) | 0.47569 (13) | 0.0351 (15) |
| H15\_2 | 0.292931 | -0.308663 | 0.504069 | 0.042\* |
| C16\_2 | 0.3567 (3) | -0.1663 (17) | 0.45874 (12) | 0.0347 (14) |
| H16\_2 | 0.391255 | -0.081286 | 0.475772 | 0.042\* |

**Table S5.** Atomic displacement parameters (Å2) for Genkwanin **1**.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | *U*11 | *U*22 | *U*33 | *U*12 | *U*13 | *U*23 |
| O1\_1 | 0.0234 (18) | 0.049 (3) | 0.023 (2) | 0.0017 (17) | -0.0038 (14) | 0.0009 (19) |
| O2\_1 | 0.0253 (17) | 0.049 (3) | 0.023 (2) | -0.0039 (16) | -0.0019 (14) | -0.0016 (18) |
| O3\_1 | 0.026 (2) | 0.051 (3) | 0.0190 (14) | -0.0035 (19) | -0.0012 (12) | 0.0054 (16) |
| O4\_1 | 0.0253 (19) | 0.043 (2) | 0.0181 (14) | -0.0031 (16) | -0.0007 (12) | 0.0000 (14) |
| O5\_1 | 0.029 (2) | 0.054 (3) | 0.021 (2) | -0.0072 (19) | -0.0004 (16) | 0.0033 (18) |
| C1\_1 | 0.0210 (18) | 0.040 (3) | 0.0214 (16) | 0.0060 (18) | -0.0019 (12) | -0.0012 (17) |
| C2\_1 | 0.0228 (18) | 0.035 (3) | 0.0221 (16) | 0.0022 (18) | -0.0025 (12) | 0.0001 (17) |
| C3\_1 | 0.0232 (16) | 0.033 (2) | 0.0235 (15) | 0.0017 (15) | -0.0018 (11) | -0.0013 (15) |
| C4\_1 | 0.023 (2) | 0.046 (3) | 0.0238 (15) | 0.001 (2) | -0.0013 (13) | 0.0015 (18) |
| C5\_1 | 0.022 (2) | 0.044 (3) | 0.0182 (15) | 0.002 (2) | 0.0003 (12) | 0.0017 (17) |
| C6\_1 | 0.028 (3) | 0.052 (4) | 0.023 (3) | -0.002 (3) | 0.002 (2) | 0.007 (3) |
| C7\_1 | 0.021 (2) | 0.045 (3) | 0.0200 (16) | 0.002 (2) | 0.0001 (13) | 0.0019 (17) |
| C8\_1 | 0.0224 (18) | 0.039 (3) | 0.0201 (15) | 0.0004 (19) | -0.0008 (12) | 0.0012 (17) |
| C9\_1 | 0.0266 (18) | 0.038 (3) | 0.0175 (15) | 0.0028 (19) | 0.0002 (13) | -0.0020 (15) |
| C10\_1 | 0.0258 (18) | 0.047 (4) | 0.019 (2) | 0.0019 (19) | 0.0004 (14) | -0.003 (2) |
| C11\_1 | 0.0269 (19) | 0.040 (3) | 0.0198 (17) | 0.0027 (19) | 0.0004 (13) | 0.0003 (17) |
| C12\_1 | 0.028 (2) | 0.037 (3) | 0.020 (2) | 0.002 (2) | -0.0007 (15) | 0.002 (2) |
| C13\_1 | 0.029 (2) | 0.043 (4) | 0.0202 (18) | -0.002 (2) | -0.0013 (15) | 0.0015 (18) |
| C14\_1 | 0.025 (2) | 0.042 (3) | 0.0207 (17) | 0.0001 (19) | 0.0004 (14) | 0.0022 (17) |
| C15\_1 | 0.027 (2) | 0.046 (4) | 0.020 (2) | -0.002 (2) | -0.0002 (15) | 0.002 (2) |
| C16\_1 | 0.027 (2) | 0.045 (4) | 0.0200 (17) | -0.002 (2) | -0.0013 (15) | 0.0011 (19) |
| O1\_2 | 0.0265 (17) | 0.048 (3) | 0.0234 (19) | -0.0021 (16) | -0.0030 (13) | 0.0010 (19) |
| O2\_2 | 0.0231 (18) | 0.046 (3) | 0.024 (2) | -0.0029 (16) | -0.0018 (14) | 0.0027 (19) |
| O3\_2 | 0.024 (2) | 0.049 (3) | 0.0214 (13) | -0.0014 (18) | -0.0005 (12) | 0.0043 (15) |
| O4\_2 | 0.0211 (18) | 0.046 (2) | 0.0174 (14) | -0.0003 (16) | -0.0009 (12) | 0.0019 (14) |
| O5\_2 | 0.0298 (18) | 0.055 (3) | 0.0216 (19) | -0.0081 (18) | 0.0011 (15) | -0.0034 (18) |
| C1\_2 | 0.0246 (15) | 0.034 (2) | 0.0222 (14) | 0.0030 (15) | -0.0015 (11) | -0.0014 (14) |
| C2\_2 | 0.0203 (18) | 0.038 (3) | 0.0220 (15) | 0.0030 (17) | 0.0001 (12) | -0.0001 (16) |
| C3\_2 | 0.0207 (18) | 0.036 (3) | 0.0219 (16) | 0.0022 (18) | 0.0004 (12) | -0.0018 (16) |
| C4\_2 | 0.0232 (19) | 0.040 (3) | 0.0220 (17) | 0.0027 (18) | 0.0005 (13) | -0.0006 (18) |
| C5\_2 | 0.0228 (17) | 0.031 (2) | 0.0206 (13) | 0.0051 (15) | 0.0006 (11) | -0.0005 (14) |
| C6\_2 | 0.030 (3) | 0.048 (3) | 0.021 (2) | -0.003 (3) | 0.004 (2) | 0.001 (2) |
| C7\_2 | 0.025 (2) | 0.038 (3) | 0.0200 (15) | 0.000 (2) | -0.0003 (13) | -0.0009 (17) |
| C8\_2 | 0.0207 (18) | 0.040 (3) | 0.0200 (15) | 0.0015 (18) | 0.0011 (12) | -0.0003 (16) |
| C9\_2 | 0.0247 (15) | 0.035 (3) | 0.0171 (14) | 0.0032 (17) | -0.0008 (12) | -0.0002 (15) |
| C10\_2 | 0.0256 (16) | 0.042 (3) | 0.020 (2) | 0.0012 (18) | -0.0025 (13) | 0.002 (2) |
| C11\_2 | 0.0254 (16) | 0.033 (2) | 0.0218 (15) | 0.0032 (15) | 0.0007 (12) | -0.0001 (14) |
| C12\_2 | 0.0274 (17) | 0.039 (3) | 0.0231 (19) | 0.0005 (19) | -0.0001 (14) | -0.001 (2) |
| C13\_2 | 0.0269 (18) | 0.035 (2) | 0.0250 (14) | 0.0016 (16) | 0.0004 (12) | -0.0015 (14) |
| C14\_2 | 0.0263 (18) | 0.036 (2) | 0.0253 (14) | 0.0009 (16) | 0.0013 (11) | -0.0009 (13) |
| C15\_2 | 0.029 (2) | 0.052 (4) | 0.023 (2) | -0.007 (2) | 0.0025 (14) | -0.002 (2) |
| C16\_2 | 0.028 (2) | 0.054 (4) | 0.0217 (16) | -0.007 (2) | 0.0002 (14) | -0.0003 (17) |

**Table S6.** Geometric parameters (Å, º) for Genkwanin **1**.

|  |  |  |  |
| --- | --- | --- | --- |
| O1\_1—C1\_1 | 1.261 (4) | O1\_2—C1\_2 | 1.261 (4) |
| O2\_1—H2\_1 | 0.9991 | O2\_2—H2\_2 | 0.9991 |
| O2\_1—C3\_1 | 1.349 (4) | O2\_2—C3\_2 | 1.349 (4) |
| O3\_1—C5\_1 | 1.369 (4) | O3\_2—C5\_2 | 1.369 (4) |
| O3\_1—C6\_1 | 1.434 (4) | O3\_2—C6\_2 | 1.434 (4) |
| O4\_1—C8\_1 | 1.373 (4) | O4\_2—C8\_2 | 1.373 (4) |
| O4\_1—C9\_1 | 1.370 (4) | O4\_2—C9\_2 | 1.370 (4) |
| O5\_1—H5\_1 | 0.9990 | O5\_2—H5\_2 | 0.9990 |
| O5\_1—C14\_1 | 1.362 (5) | O5\_2—C14\_2 | 1.362 (5) |
| C1\_1—C2\_1 | 1.461 (5) | C1\_2—C2\_2 | 1.461 (5) |
| C1\_1—C10\_1 | 1.421 (5) | C1\_2—C10\_2 | 1.421 (5) |
| C2\_1—C3\_1 | 1.411 (5) | C2\_2—C3\_2 | 1.411 (5) |
| C2\_1—C8\_1 | 1.394 (5) | C2\_2—C8\_2 | 1.393 (5) |
| C3\_1—C4\_1 | 1.388 (5) | C3\_2—C4\_2 | 1.387 (5) |
| C4\_1—H4\_1 | 0.9300 | C4\_2—H4\_2 | 0.9300 |
| C4\_1—C5\_1 | 1.390 (5) | C4\_2—C5\_2 | 1.389 (5) |
| C5\_1—C7\_1 | 1.385 (5) | C5\_2—C7\_2 | 1.384 (5) |
| C6\_1—H6A\_1 | 0.9600 | C6\_2—H6A\_2 | 0.9600 |
| C6\_1—H6B\_1 | 0.9600 | C6\_2—H6B\_2 | 0.9600 |
| C6\_1—H6C\_1 | 0.9600 | C6\_2—H6C\_2 | 0.9600 |
| C7\_1—H7\_1 | 0.9300 | C7\_2—H7\_2 | 0.9300 |
| C7\_1—C8\_1 | 1.384 (5) | C7\_2—C8\_2 | 1.384 (5) |
| C9\_1—C10\_1 | 1.353 (5) | C9\_2—C10\_2 | 1.352 (5) |
| C9\_1—C11\_1 | 1.453 (5) | C9\_2—C11\_2 | 1.453 (5) |
| C10\_1—H10\_1 | 0.9300 | C10\_2—H10\_2 | 0.9300 |
| C11\_1—C12\_1 | 1.392 (5) | C11\_2—C12\_2 | 1.392 (5) |
| C11\_1—C16\_1 | 1.415 (5) | C11\_2—C16\_2 | 1.414 (5) |
| C12\_1—H12\_1 | 0.9300 | C12\_2—H12\_2 | 0.9300 |
| C12\_1—C13\_1 | 1.385 (5) | C12\_2—C13\_2 | 1.385 (5) |
| C13\_1—H13\_1 | 0.9300 | C13\_2—H13\_2 | 0.9300 |
| C13\_1—C14\_1 | 1.385 (5) | C13\_2—C14\_2 | 1.386 (5) |
| C14\_1—C15\_1 | 1.386 (5) | C14\_2—C15\_2 | 1.386 (5) |
| C15\_1—H15\_1 | 0.9300 | C15\_2—H15\_2 | 0.9300 |
| C15\_1—C16\_1 | 1.374 (6) | C15\_2—C16\_2 | 1.374 (6) |
| C16\_1—H16\_1 | 0.9300 | C16\_2—H16\_2 | 0.9300 |
|  |  |  |  |
| C3\_1—O2\_1—H2\_1 | 109.5 | C3\_2—O2\_2—H2\_2 | 109.5 |
| C5\_1—O3\_1—C6\_1 | 117.9 (3) | C5\_2—O3\_2—C6\_2 | 118.0 (3) |
| C9\_1—O4\_1—C8\_1 | 119.9 (3) | C9\_2—O4\_2—C8\_2 | 119.7 (3) |
| C14\_1—O5\_1—H5\_1 | 109.5 | C14\_2—O5\_2—H5\_2 | 109.5 |
| O1\_1—C1\_1—C2\_1 | 120.2 (4) | O1\_2—C1\_2—C2\_2 | 120.5 (4) |
| O1\_1—C1\_1—C10\_1 | 124.6 (3) | O1\_2—C1\_2—C10\_2 | 124.4 (3) |
| C10\_1—C1\_1—C2\_1 | 115.2 (3) | C10\_2—C1\_2—C2\_2 | 115.1 (3) |
| C3\_1—C2\_1—C1\_1 | 122.4 (3) | C3\_2—C2\_2—C1\_2 | 122.3 (3) |
| C8\_1—C2\_1—C1\_1 | 119.9 (3) | C8\_2—C2\_2—C1\_2 | 120.0 (3) |
| C8\_1—C2\_1—C3\_1 | 117.8 (3) | C8\_2—C2\_2—C3\_2 | 117.7 (3) |
| O2\_1—C3\_1—C2\_1 | 120.2 (3) | O2\_2—C3\_2—C2\_2 | 120.2 (3) |
| O2\_1—C3\_1—C4\_1 | 119.1 (4) | O2\_2—C3\_2—C4\_2 | 119.2 (4) |
| C4\_1—C3\_1—C2\_1 | 120.7 (4) | C4\_2—C3\_2—C2\_2 | 120.6 (4) |
| C3\_1—C4\_1—H4\_1 | 120.6 | C3\_2—C4\_2—H4\_2 | 120.5 |
| C3\_1—C4\_1—C5\_1 | 118.8 (4) | C3\_2—C4\_2—C5\_2 | 119.0 (4) |
| C5\_1—C4\_1—H4\_1 | 120.6 | C5\_2—C4\_2—H4\_2 | 120.5 |
| O3\_1—C5\_1—C4\_1 | 123.3 (3) | O3\_2—C5\_2—C4\_2 | 123.4 (3) |
| O3\_1—C5\_1—C7\_1 | 114.3 (3) | O3\_2—C5\_2—C7\_2 | 114.2 (3) |
| C7\_1—C5\_1—C4\_1 | 122.4 (3) | C7\_2—C5\_2—C4\_2 | 122.4 (3) |
| O3\_1—C6\_1—H6A\_1 | 109.5 | O3\_2—C6\_2—H6A\_2 | 109.5 |
| O3\_1—C6\_1—H6B\_1 | 109.5 | O3\_2—C6\_2—H6B\_2 | 109.5 |
| O3\_1—C6\_1—H6C\_1 | 109.5 | O3\_2—C6\_2—H6C\_2 | 109.5 |
| H6A\_1—C6\_1—H6B\_1 | 109.5 | H6A\_2—C6\_2—H6B\_2 | 109.5 |
| H6A\_1—C6\_1—H6C\_1 | 109.5 | H6A\_2—C6\_2—H6C\_2 | 109.5 |
| H6B\_1—C6\_1—H6C\_1 | 109.5 | H6B\_2—C6\_2—H6C\_2 | 109.5 |
| C5\_1—C7\_1—H7\_1 | 121.3 | C5\_2—C7\_2—H7\_2 | 121.3 |
| C8\_1—C7\_1—C5\_1 | 117.5 (4) | C8\_2—C7\_2—C5\_2 | 117.4 (4) |
| C8\_1—C7\_1—H7\_1 | 121.3 | C8\_2—C7\_2—H7\_2 | 121.3 |
| O4\_1—C8\_1—C2\_1 | 121.0 (3) | O4\_2—C8\_2—C2\_2 | 121.1 (3) |
| O4\_1—C8\_1—C7\_1 | 116.2 (3) | O4\_2—C8\_2—C7\_2 | 115.9 (3) |
| C7\_1—C8\_1—C2\_1 | 122.8 (4) | C7\_2—C8\_2—C2\_2 | 122.9 (4) |
| O4\_1—C9\_1—C11\_1 | 111.0 (3) | O4\_2—C9\_2—C11\_2 | 110.9 (3) |
| C10\_1—C9\_1—O4\_1 | 121.5 (3) | C10\_2—C9\_2—O4\_2 | 121.6 (3) |
| C10\_1—C9\_1—C11\_1 | 127.5 (3) | C10\_2—C9\_2—C11\_2 | 127.4 (3) |
| C1\_1—C10\_1—H10\_1 | 118.8 | C1\_2—C10\_2—H10\_2 | 118.8 |
| C9\_1—C10\_1—C1\_1 | 122.4 (3) | C9\_2—C10\_2—C1\_2 | 122.5 (3) |
| C9\_1—C10\_1—H10\_1 | 118.8 | C9\_2—C10\_2—H10\_2 | 118.8 |
| C12\_1—C11\_1—C9\_1 | 122.0 (3) | C12\_2—C11\_2—C9\_2 | 122.0 (3) |
| C12\_1—C11\_1—C16\_1 | 117.2 (4) | C12\_2—C11\_2—C16\_2 | 117.4 (4) |
| C16\_1—C11\_1—C9\_1 | 120.8 (4) | C16\_2—C11\_2—C9\_2 | 120.5 (4) |
| C11\_1—C12\_1—H12\_1 | 119.0 | C11\_2—C12\_2—H12\_2 | 119.1 |
| C13\_1—C12\_1—C11\_1 | 122.0 (3) | C13\_2—C12\_2—C11\_2 | 121.8 (3) |
| C13\_1—C12\_1—H12\_1 | 119.0 | C13\_2—C12\_2—H12\_2 | 119.1 |
| C12\_1—C13\_1—H13\_1 | 120.2 | C12\_2—C13\_2—H13\_2 | 120.1 |
| C14\_1—C13\_1—C12\_1 | 119.6 (4) | C12\_2—C13\_2—C14\_2 | 119.7 (4) |
| C14\_1—C13\_1—H13\_1 | 120.2 | C14\_2—C13\_2—H13\_2 | 120.1 |
| O5\_1—C14\_1—C13\_1 | 122.6 (4) | O5\_2—C14\_2—C13\_2 | 122.7 (4) |
| O5\_1—C14\_1—C15\_1 | 117.7 (3) | O5\_2—C14\_2—C15\_2 | 117.6 (3) |
| C13\_1—C14\_1—C15\_1 | 119.7 (4) | C15\_2—C14\_2—C13\_2 | 119.6 (4) |
| C14\_1—C15\_1—H15\_1 | 119.7 | C14\_2—C15\_2—H15\_2 | 119.6 |
| C16\_1—C15\_1—C14\_1 | 120.7 (4) | C16\_2—C15\_2—C14\_2 | 120.7 (4) |
| C16\_1—C15\_1—H15\_1 | 119.7 | C16\_2—C15\_2—H15\_2 | 119.6 |
| C11\_1—C16\_1—H16\_1 | 119.6 | C11\_2—C16\_2—H16\_2 | 119.6 |
| C15\_1—C16\_1—C11\_1 | 120.9 (4) | C15\_2—C16\_2—C11\_2 | 120.8 (4) |
| C15\_1—C16\_1—H16\_1 | 119.6 | C15\_2—C16\_2—H16\_2 | 119.6 |
|  |  |  |  |
| O1\_1—C1\_1—C2\_1—C3\_1 | 1.2 (10) | O1\_2—C1\_2—C2\_2—C3\_2 | -0.1 (9) |
| O1\_1—C1\_1—C2\_1—C8\_1 | -179.5 (6) | O1\_2—C1\_2—C2\_2—C8\_2 | 179.5 (6) |
| O1\_1—C1\_1—C10\_1—C9\_1 | 178.3 (6) | O1\_2—C1\_2—C10\_2—C9\_2 | 178.6 (6) |
| O2\_1—C3\_1—C4\_1—C5\_1 | 177.7 (6) | O2\_2—C3\_2—C4\_2—C5\_2 | -177.6 (5) |
| O3\_1—C5\_1—C7\_1—C8\_1 | 178.9 (6) | O3\_2—C5\_2—C7\_2—C8\_2 | -179.5 (5) |
| O4\_1—C9\_1—C10\_1—C1\_1 | 1.3 (10) | O4\_2—C9\_2—C10\_2—C1\_2 | 2.1 (9) |
| O4\_1—C9\_1—C11\_1—C12\_1 | -2.1 (8) | O4\_2—C9\_2—C11\_2—C12\_2 | 13.1 (8) |
| O4\_1—C9\_1—C11\_1—C16\_1 | 178.0 (6) | O4\_2—C9\_2—C11\_2—C16\_2 | -164.1 (6) |
| O5\_1—C14\_1—C15\_1—C16\_1 | -179.6 (6) | O5\_2—C14\_2—C15\_2—C16\_2 | -179.8 (6) |
| C1\_1—C2\_1—C3\_1—O2\_1 | 0.1 (9) | C1\_2—C2\_2—C3\_2—O2\_2 | -1.4 (9) |
| C1\_1—C2\_1—C3\_1—C4\_1 | 179.5 (6) | C1\_2—C2\_2—C3\_2—C4\_2 | 179.1 (6) |
| C1\_1—C2\_1—C8\_1—O4\_1 | 1.1 (9) | C1\_2—C2\_2—C8\_2—O4\_2 | 1.7 (9) |
| C1\_1—C2\_1—C8\_1—C7\_1 | -178.0 (6) | C1\_2—C2\_2—C8\_2—C7\_2 | -179.8 (6) |
| C2\_1—C1\_1—C10\_1—C9\_1 | -1.5 (9) | C2\_2—C1\_2—C10\_2—C9\_2 | -0.6 (9) |
| C2\_1—C3\_1—C4\_1—C5\_1 | -1.7 (9) | C2\_2—C3\_2—C4\_2—C5\_2 | 2.0 (9) |
| C3\_1—C2\_1—C8\_1—O4\_1 | -179.5 (5) | C3\_2—C2\_2—C8\_2—O4\_2 | -178.7 (5) |
| C3\_1—C2\_1—C8\_1—C7\_1 | 1.3 (10) | C3\_2—C2\_2—C8\_2—C7\_2 | -0.2 (9) |
| C3\_1—C4\_1—C5\_1—O3\_1 | -177.4 (6) | C3\_2—C4\_2—C5\_2—O3\_2 | 178.9 (5) |
| C3\_1—C4\_1—C5\_1—C7\_1 | 1.9 (10) | C3\_2—C4\_2—C5\_2—C7\_2 | -2.8 (9) |
| C4\_1—C5\_1—C7\_1—C8\_1 | -0.5 (9) | C4\_2—C5\_2—C7\_2—C8\_2 | 2.0 (9) |
| C5\_1—C7\_1—C8\_1—O4\_1 | 179.6 (5) | C5\_2—C7\_2—C8\_2—O4\_2 | 178.1 (5) |
| C5\_1—C7\_1—C8\_1—C2\_1 | -1.1 (9) | C5\_2—C7\_2—C8\_2—C2\_2 | -0.5 (9) |
| C6\_1—O3\_1—C5\_1—C4\_1 | 1.2 (9) | C6\_2—O3\_2—C5\_2—C4\_2 | -2.9 (8) |
| C6\_1—O3\_1—C5\_1—C7\_1 | -178.2 (5) | C6\_2—O3\_2—C5\_2—C7\_2 | 178.7 (5) |
| C8\_1—O4\_1—C9\_1—C10\_1 | 0.2 (9) | C8\_2—O4\_2—C9\_2—C10\_2 | -1.6 (8) |
| C8\_1—O4\_1—C9\_1—C11\_1 | -179.4 (5) | C8\_2—O4\_2—C9\_2—C11\_2 | 178.6 (5) |
| C8\_1—C2\_1—C3\_1—O2\_1 | -179.2 (5) | C8\_2—C2\_2—C3\_2—O2\_2 | 179.0 (5) |
| C8\_1—C2\_1—C3\_1—C4\_1 | 0.1 (9) | C8\_2—C2\_2—C3\_2—C4\_2 | -0.6 (9) |
| C9\_1—O4\_1—C8\_1—C2\_1 | -1.4 (9) | C9\_2—O4\_2—C8\_2—C2\_2 | -0.3 (9) |
| C9\_1—O4\_1—C8\_1—C7\_1 | 177.8 (5) | C9\_2—O4\_2—C8\_2—C7\_2 | -178.9 (5) |
| C9\_1—C11\_1—C12\_1—C13\_1 | 178.8 (6) | C9\_2—C11\_2—C12\_2—C13\_2 | -178.0 (6) |
| C9\_1—C11\_1—C16\_1—C15\_1 | -178.6 (6) | C9\_2—C11\_2—C16\_2—C15\_2 | 177.3 (6) |
| C10\_1—C1\_1—C2\_1—C3\_1 | -179.0 (6) | C10\_2—C1\_2—C2\_2—C3\_2 | 179.2 (6) |
| C10\_1—C1\_1—C2\_1—C8\_1 | 0.3 (9) | C10\_2—C1\_2—C2\_2—C8\_2 | -1.2 (8) |
| C10\_1—C9\_1—C11\_1—C12\_1 | 178.3 (6) | C10\_2—C9\_2—C11\_2—C12\_2 | -166.7 (6) |
| C10\_1—C9\_1—C11\_1—C16\_1 | -1.6 (10) | C10\_2—C9\_2—C11\_2—C16\_2 | 16.1 (10) |
| C11\_1—C9\_1—C10\_1—C1\_1 | -179.2 (6) | C11\_2—C9\_2—C10\_2—C1\_2 | -178.1 (6) |
| C11\_1—C12\_1—C13\_1—C14\_1 | 0.2 (10) | C11\_2—C12\_2—C13\_2—C14\_2 | 0.5 (9) |
| C12\_1—C11\_1—C16\_1—C15\_1 | 1.4 (9) | C12\_2—C11\_2—C16\_2—C15\_2 | 0.0 (10) |
| C12\_1—C13\_1—C14\_1—O5\_1 | 179.7 (6) | C12\_2—C13\_2—C14\_2—O5\_2 | 179.1 (5) |
| C12\_1—C13\_1—C14\_1—C15\_1 | 0.8 (10) | C12\_2—C13\_2—C14\_2—C15\_2 | 0.5 (10) |
| C13\_1—C14\_1—C15\_1—C16\_1 | -0.6 (10) | C13\_2—C14\_2—C15\_2—C16\_2 | -1.1 (10) |
| C14\_1—C15\_1—C16\_1—C11\_1 | -0.5 (10) | C14\_2—C15\_2—C16\_2—C11\_2 | 0.9 (11) |
| C16\_1—C11\_1—C12\_1—C13\_1 | -1.3 (9) | C16\_2—C11\_2—C12\_2—C13\_2 | -0.7 (9) |