

5,11,17,23,29-Penta-*tert*-butyl-31,32,33,34,35-pentapropoxycalix[5]-arene dichloromethane hemisolvate

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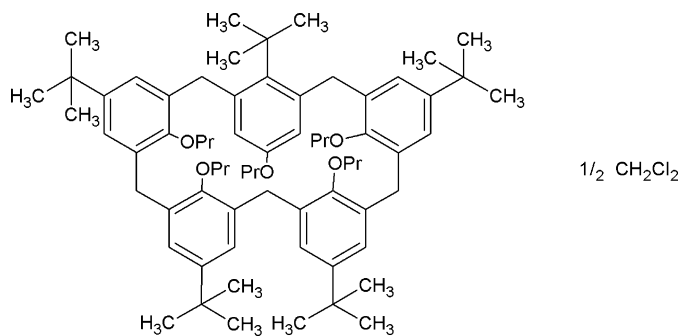
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; disorder in main residue; R factor = 0.074; wR factor = 0.151; data-to-parameter ratio = 13.2.

The title compound, *tert*-butylpropoxycalix[5]arene, $\text{C}_{70}\text{H}_{100}\text{O}_5 \cdot 0.5\text{CH}_2\text{Cl}_2$, crystallizes as a solvate with two molecules of calix[5]arene in 1,2-alternate conformations and one molecule of dichloromethane in the asymmetric unit. One *tert*-butyl group in one of the molecules and two in the other are disordered over two positions with occupancy factors fixed at 0.5917:0.4083, 0.5901:0.4099 and 0.8535:0.1465, respectively, in the final refinement. The C atoms of a propoxy group in each of the molecules are also disordered over two positions with occupancies of 0.7372:0.2628 and 0.5027:0.4973. The molecules form intramolecular hydrogen bonds between propoxy O atoms and an adjacent CH_2 group in a neighbouring propoxy chain. In the crystal, intermolecular $\text{C}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{Cl}$ interactions occur involving the dichloromethane molecule.

Related literature

For the synthesis and NMR analysis of esters of *p-tert*-butylcalix[5]arene, see: Stewart *et al.* (1995). For the weighting scheme used, see: Watkin (1994); Prince (1982).



Experimental

Crystal data

| | |
|---|-----------------------------------|
| $\text{C}_{70}\text{H}_{100}\text{O}_5 \cdot 0.5\text{CH}_2\text{Cl}_2$ | $V = 12911.5$ (3) Å ³ |
| $M_r = 1064.03$ | $Z = 8$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 12.3740$ (2) Å | $\mu = 0.11$ mm ⁻¹ |
| $b = 23.9130$ (2) Å | $T = 150$ K |
| $c = 43.6550$ (5) Å | $0.45 \times 0.23 \times 0.12$ mm |
| $\beta = 91.7460$ (5)° | |

Data collection

| | |
|--------------------------------|---|
| Nonius KappaCCD diffractometer | 13395 reflections with $I > 2\sigma(I)$ |
| 39073 measured reflections | $R_{\text{int}} = 0.043$ |
| 20282 independent reflections | $\theta_{\text{max}} = 24.1^\circ$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.074$ | 220 restraints |
| $wR(F^2) = 0.151$ | H-atom parameters constrained |
| $S = 1.02$ | $\Delta\rho_{\text{max}} = 1.88$ e Å ⁻³ |
| 20282 reflections | $\Delta\rho_{\text{min}} = -1.75$ e Å ⁻³ |
| 1531 parameters | |

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|-----------------------|--------------|---------------------|--------------|-----------------------|
| C71—H711···O7 | 1.03 | 2.36 | 3.363 (8) | 163 |
| C48—H482···O1 | 0.99 | 2.60 | 3.351 (5) | 134 |
| C110—H1101···O8 | 1.00 | 2.57 | 3.361 (5) | 136 |
| C120—H1202···O9 | 1.00 | 2.57 | 3.371 (5) | 136 |
| C14—H142···O3 | 1.01 | 2.47 | 2.869 (5) | 103 |
| C38—H382···Cl1 | 0.97 | 2.92 | 3.795 (5) | 151 |

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *CRYSTALS* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5077).

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supplementary materials

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5,11,17,23,29-Penta-*tert*-butyl-31,32,33,34,35-pentapropoxycalix[5]arene dichloromethane hemisolvate

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Comment

The studied compound was prepared by alkylation of *tert*-butylcalix[5]arene with propyl iodide in a presence of NaH and crystallized from mixture of dichloromethane and methanol. Molecules of dichloromethane are present in the crystal structure. The asymmetric unit contains two molecules of calix[5]arene which are turned to each other in direction of the *b* axis at an angle of 67% (angle between planes formed by the bridging CH₂ groups). This leads to the formation of infinite channels along the *a* axis by half of the molecules. The channels are separated by layers of turned molecules. The solvent molecule forms C—H···O hydrogen bonds. Hydrogen atom (H711) of the CH₂ group in dichloromethane point toward O7, the distance between HC—H···O is 2.36 Å, and the chlorine atom has close contact to the terminal CH₃ group of the propoxy chain (the HC—H···Cl distance is 2.92 Å). In each macrocycle two propoxy chains point above the cavity, while the others are turned out. The orientation toward the cavity is caused by intra-molecular hydrogen bonds between a methylene group of a propoxy chain and a neighbouring oxygen atom (C110-H1101···O8, C120-H1202···O9, C48—H482···O1, the distances are given in Table 1). Two disordered positions were modeled for three *tert*-butyl groups and the C atoms of two propoxy groups. The disorder components were found from difference electron density maps and their occupancy factors were fixed after several cycles of refinement as follows: *tert*-butyl groups with central carbon atoms: C67 - 0.59:0.40; C137 - 0.59:0.41; C138 - 0.85:0.15; propoxy group bound to oxygen atoms: O1 - 0.7372:0.2628 and O6 - 0.5027: 0.4973.

Experimental

To the solution of 250 mg (0.3 mmol) of 1 in 15 ml of dry DMF cooled to 0 °C was added 123 mg (3 mmol) of 60% suspension of NaH in mineral oil and the mixture was stirred for 15 minutes. Then, 0.45 ml of propyl iodide was added and the reaction was stirred at room temperature. After two days, the mixture was poured into 30 ml of 1 M HCl and extracted 3 times 20 ml of dichloromethane. Combined extracts were washed with 20 ml of water and 20 ml of brine and dried over MgSO₄. The drying agent was filtered off and the filtrate was evaporated to dryness. The crude product was dissolved in 10 ml of dichloromethane, 10 ml of MeOH was added and the mixture was slowly evaporated in an open flask. After two days, 235 mg (75%) of the white crystals of product 2 was obtained.

NMR spectra corresponded with data in the literature (Stewart *et al.*, 1995) - on a compound prepared using a different procedure, in acetonitrile with K₂CO₃, yield 83%. MS-ESI+: C₇₀H₁₀₀O₅ required 1020.76; found 1043.71 ([M+Na]⁺; 100%), 1059.70 ([M+K]⁺; 10%)

Refinement

Refinement of F² against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F², conventional *R*-factors *R* are based on F, with F set to zero for negative F². The threshold expression of F² > 2σ(F²) is used only for calculating *R*-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on F² are

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statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger. The position of disordered atoms were located from difference maps of electron density. Disordered fragments were then placed in appropriate positions, and all distances between neighbouring atoms and angles were restrained. Site occupancies were refined for the different parts with the same thermal parameters for the same atoms in the various fragments. At the end of refinement, site occupancies were fixed and hydrogen atoms were placed in calculated positions with the thermal parameters $U_{\text{iso}}(\text{H})$ (in the range 1.2–1.5 times U_{eq} of the parent atom).

Figures

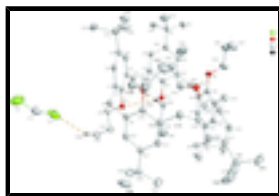


Fig. 1. A view of first molecule of 1 with atom's numbering. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are drawn as dashed lines. Hydrogen atoms not participating in hydrogen bonds are omitted. For clarity only the major disorder component of the disordered *tert*-butyl and propoxy groups are shown.

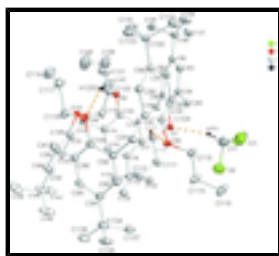


Fig. 2. A view of second molecule of 1 with atom's numbering. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are drawn as dashed lines. Hydrogen atoms not participating in hydrogen bonds are omitted. For clarity only the major disorder component of the disordered *tert*-butyl and propoxy groups are shown.

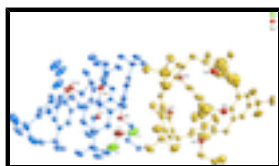


Fig. 3. The asymmetric unit of 1.

5,11,17,23,29-Penta-*tert*-butyl-31,32,33,34,35-pentapropoxycalix[5]arene dichloromethane hemisolvate

Crystal data

$\text{C}_{70}\text{H}_{100}\text{O}_5 \cdot 0.5\text{CH}_2\text{Cl}_2$

$M_r = 1064.03$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.3740$ (2) Å

$b = 23.9130$ (2) Å

$c = 43.6550$ (5) Å

$\beta = 91.7460$ (5)°

$V = 12911.5$ (3) Å³

$Z = 8$

$F(000) = 4648$

$D_x = 1.095$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 390743 reflections

$\theta = 1.0$ – 24.1 °

$\mu = 0.11$ mm⁻¹

$T = 150$ K

Plate, colourless

$0.45 \times 0.23 \times 0.12$ mm

Data collection

Nonius KappaCCD

$R_{\text{int}} = 0.043$

diffractometer
 graphite $\theta_{\max} = 24.1^\circ$, $\theta_{\min} = 1.3^\circ$
 $\omega/2\theta$ scans $h = -14 \rightarrow 14$
 39073 measured reflections $k = -27 \rightarrow 27$
 20282 independent reflections $l = -50 \rightarrow 50$
 13395 reflections with $I > 2\sigma(I)$

Refinement

Refinement on F^2 Primary atom site location: structure-invariant direct methods
 Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.074$ H-atom parameters constrained
 Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982) [weight] = $1.0/[A_0 * T_0(x) + A_1 * T_1(x) \dots + A_{n-1} * T_{n-1}(x)]$
 $wR(F^2) = 0.151$ where A_i are the Chebychev coefficients listed below and $x = F / F_{\max}$ Method = Robust Weighting (Prince, 1982) $W = [\text{weight}] * [1 - (\Delta F / 6 * \text{sigma} - \text{ma} F)^2]^2$ A_i are: 11.5 14.0 3.91
 $S = 1.02$ $(\Delta/\sigma)_{\max} = 0.001$
 20282 reflections $\Delta\rho_{\max} = 1.88 \text{ e } \text{Å}^{-3}$
 1531 parameters $\Delta\rho_{\min} = -1.75 \text{ e } \text{Å}^{-3}$
 220 restraints

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|--------------|--------------|-------------|----------------------------------|-----------|
| C11 | 0.57648 (17) | 0.44344 (8) | 0.53618 (5) | 0.1149 | |
| C12 | 0.75149 (18) | 0.42717 (11) | 0.49435 (7) | 0.1499 | |
| O1 | 0.3168 (2) | 0.36142 (11) | 0.61877 (6) | 0.0385 | |
| O2 | 0.4804 (2) | 0.27551 (11) | 0.70453 (6) | 0.0369 | |
| O3 | 0.2037 (2) | 0.23598 (12) | 0.73657 (7) | 0.0465 | |
| O4 | -0.0814 (2) | 0.19447 (12) | 0.69175 (7) | 0.0446 | |
| O5 | 0.0087 (2) | 0.31590 (12) | 0.62105 (6) | 0.0396 | |
| O7 | 0.4990 (2) | 0.38058 (11) | 0.44291 (6) | 0.0350 | |
| O8 | 0.44330 (19) | 0.26652 (11) | 0.50838 (6) | 0.0313 | |
| O9 | 0.21648 (19) | 0.13254 (11) | 0.46283 (6) | 0.0317 | |
| O10 | 0.2735 (2) | 0.18753 (12) | 0.38854 (6) | 0.0394 | |
| C1 | 0.0976 (3) | 0.23706 (17) | 0.59817 (9) | 0.0331 | |
| C2 | 0.1905 (3) | 0.27406 (17) | 0.58846 (9) | 0.0354 | |
| C3 | 0.2992 (3) | 0.26365 (17) | 0.60504 (9) | 0.0327 | |
| C4 | 0.3457 (3) | 0.21050 (17) | 0.60532 (9) | 0.0344 | |
| C5 | 0.4462 (3) | 0.19915 (17) | 0.61923 (9) | 0.0343 | |
| C6 | 0.4981 (3) | 0.24336 (17) | 0.63415 (9) | 0.0336 | |
| C7 | 0.4556 (3) | 0.29704 (16) | 0.63505 (9) | 0.0324 | |
| C8 | 0.5175 (3) | 0.34373 (17) | 0.65123 (9) | 0.0369 | |
| C9 | 0.4690 (3) | 0.36604 (16) | 0.68048 (9) | 0.0321 | |

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|-----|-------------|--------------|--------------|--------|
| C10 | 0.4440 (3) | 0.42264 (17) | 0.68304 (9) | 0.0366 |
| C11 | 0.3998 (3) | 0.44602 (17) | 0.70921 (9) | 0.0366 |
| C12 | 0.3743 (3) | 0.40857 (17) | 0.73253 (9) | 0.0367 |
| C13 | 0.3977 (3) | 0.35146 (17) | 0.73122 (9) | 0.0331 |
| C14 | 0.3679 (3) | 0.31298 (18) | 0.75739 (9) | 0.0368 |
| C15 | 0.2511 (3) | 0.31707 (17) | 0.76683 (9) | 0.0349 |
| C16 | 0.2218 (3) | 0.35663 (19) | 0.78843 (9) | 0.0410 |
| C17 | 0.1162 (3) | 0.36135 (19) | 0.79821 (9) | 0.0421 |
| C18 | 0.0403 (3) | 0.32465 (19) | 0.78536 (9) | 0.0422 |
| C19 | 0.0651 (3) | 0.28482 (18) | 0.76340 (10) | 0.0379 |
| C20 | -0.0241 (3) | 0.24950 (19) | 0.74867 (10) | 0.0442 |
| C21 | -0.0819 (3) | 0.27921 (17) | 0.72163 (10) | 0.0368 |
| C22 | -0.1100 (3) | 0.33538 (17) | 0.72356 (10) | 0.0390 |
| C23 | -0.1610 (3) | 0.36469 (18) | 0.69960 (9) | 0.0363 |
| C24 | -0.1785 (3) | 0.33557 (17) | 0.67210 (9) | 0.0355 |
| C25 | -0.1519 (3) | 0.27880 (18) | 0.66909 (10) | 0.0376 |
| C26 | -0.1724 (3) | 0.2503 (2) | 0.63880 (10) | 0.0442 |
| C27 | -0.0753 (3) | 0.22581 (18) | 0.62280 (9) | 0.0366 |
| C28 | -0.0759 (3) | 0.17028 (18) | 0.61437 (9) | 0.0382 |
| C29 | 0.0059 (3) | 0.14613 (18) | 0.59739 (9) | 0.0382 |
| C30 | 0.0907 (3) | 0.18102 (17) | 0.58940 (9) | 0.0355 |
| C31 | 0.3570 (3) | 0.30688 (16) | 0.61932 (9) | 0.0313 |
| C32 | 0.4498 (3) | 0.33161 (16) | 0.70573 (9) | 0.0331 |
| C33 | 0.1723 (3) | 0.28035 (17) | 0.75489 (9) | 0.0356 |
| C34 | -0.1069 (3) | 0.25127 (17) | 0.69434 (10) | 0.0373 |
| C35 | 0.0118 (3) | 0.25910 (17) | 0.61450 (9) | 0.0345 |
| C39 | 0.5932 (3) | 0.2661 (2) | 0.71254 (11) | 0.0482 |
| C40 | 0.6153 (4) | 0.2544 (2) | 0.74556 (11) | 0.0555 |
| C41 | 0.5689 (5) | 0.1992 (2) | 0.75635 (14) | 0.0754 |
| C42 | 0.2004 (4) | 0.2471 (2) | 0.70448 (10) | 0.0486 |
| C43 | 0.2555 (6) | 0.2000 (3) | 0.68780 (14) | 0.0846 |
| C44 | 0.2068 (7) | 0.1459 (3) | 0.6895 (2) | 0.1284 |
| C45 | -0.1665 (4) | 0.1582 (2) | 0.70146 (14) | 0.0657 |
| C46 | -0.1239 (5) | 0.0991 (2) | 0.70335 (16) | 0.0791 |
| C47 | -0.0469 (6) | 0.0912 (3) | 0.73034 (18) | 0.1052 |
| C48 | 0.0753 (3) | 0.33122 (17) | 0.64732 (10) | 0.0390 |
| C49 | 0.0738 (4) | 0.39336 (19) | 0.65105 (11) | 0.0499 |
| C50 | 0.1414 (4) | 0.4096 (3) | 0.67903 (15) | 0.0842 |
| C51 | 0.5002 (3) | 0.14147 (18) | 0.61738 (11) | 0.0440 |
| C52 | 0.4236 (4) | 0.09687 (19) | 0.60426 (13) | 0.0609 |
| C53 | 0.5965 (4) | 0.1456 (2) | 0.59599 (13) | 0.0665 |
| C54 | 0.5408 (5) | 0.1230 (2) | 0.64941 (12) | 0.0711 |
| C55 | 0.3829 (4) | 0.50901 (18) | 0.71227 (11) | 0.0441 |
| C56 | 0.4919 (5) | 0.5358 (2) | 0.7190 (2) | 0.1149 |
| C57 | 0.3044 (5) | 0.5239 (2) | 0.73684 (14) | 0.0875 |
| C58 | 0.3378 (6) | 0.5344 (2) | 0.68244 (13) | 0.0828 |
| C59 | 0.0816 (4) | 0.4055 (2) | 0.82133 (10) | 0.0552 |
| C60 | 0.1754 (5) | 0.4432 (3) | 0.83163 (14) | 0.0818 |
| C61 | 0.0371 (6) | 0.3769 (3) | 0.84946 (12) | 0.0914 |

| | | | | |
|------|-------------|--------------|--------------|--------|
| C62 | -0.0046 (4) | 0.4437 (2) | 0.80613 (12) | 0.0727 |
| C63 | -0.1956 (3) | 0.42560 (18) | 0.70422 (10) | 0.0396 |
| C64 | -0.0977 (4) | 0.46152 (19) | 0.71482 (12) | 0.0556 |
| C65 | -0.2798 (4) | 0.4267 (2) | 0.72898 (11) | 0.0547 |
| C66 | -0.2449 (4) | 0.45182 (19) | 0.67507 (10) | 0.0477 |
| C71 | 0.6226 (5) | 0.4543 (3) | 0.49944 (17) | 0.0921 |
| C72 | 0.4129 (3) | 0.18398 (17) | 0.35096 (9) | 0.0337 |
| C73 | 0.3859 (3) | 0.24204 (16) | 0.33889 (9) | 0.0360 |
| C74 | 0.4649 (3) | 0.28711 (16) | 0.35017 (9) | 0.0331 |
| C75 | 0.5754 (3) | 0.27735 (18) | 0.35251 (9) | 0.0368 |
| C76 | 0.6493 (3) | 0.31754 (18) | 0.36326 (9) | 0.0366 |
| C77 | 0.6063 (3) | 0.36744 (18) | 0.37403 (9) | 0.0386 |
| C78 | 0.4954 (3) | 0.37921 (16) | 0.37216 (9) | 0.0325 |
| C79 | 0.4527 (3) | 0.43374 (17) | 0.38472 (10) | 0.0401 |
| C80 | 0.3719 (3) | 0.43022 (16) | 0.41026 (9) | 0.0329 |
| C81 | 0.2732 (3) | 0.45755 (16) | 0.40702 (10) | 0.0377 |
| C82 | 0.1998 (3) | 0.46128 (16) | 0.43037 (9) | 0.0350 |
| C83 | 0.2274 (3) | 0.43444 (16) | 0.45753 (10) | 0.0353 |
| C84 | 0.3232 (3) | 0.40413 (16) | 0.46212 (9) | 0.0305 |
| C85 | 0.3493 (3) | 0.37538 (16) | 0.49267 (9) | 0.0335 |
| C86 | 0.2831 (3) | 0.32317 (16) | 0.49943 (8) | 0.0287 |
| C87 | 0.1695 (3) | 0.32567 (16) | 0.49931 (9) | 0.0318 |
| C88 | 0.1048 (3) | 0.27963 (16) | 0.50487 (9) | 0.0308 |
| C89 | 0.1560 (3) | 0.22889 (16) | 0.51008 (8) | 0.0308 |
| C90 | 0.2691 (3) | 0.22374 (16) | 0.51103 (8) | 0.0285 |
| C91 | 0.3210 (3) | 0.16770 (16) | 0.51910 (9) | 0.0314 |
| C92 | 0.3798 (3) | 0.13757 (15) | 0.49404 (9) | 0.0292 |
| C93 | 0.4877 (3) | 0.12282 (16) | 0.49839 (9) | 0.0328 |
| C94 | 0.5442 (3) | 0.09268 (16) | 0.47680 (10) | 0.0342 |
| C95 | 0.4904 (3) | 0.08084 (16) | 0.44912 (10) | 0.0350 |
| C96 | 0.3819 (3) | 0.09491 (16) | 0.44346 (9) | 0.0335 |
| C97 | 0.3278 (3) | 0.08105 (17) | 0.41269 (9) | 0.0375 |
| C98 | 0.3863 (3) | 0.10652 (17) | 0.38593 (9) | 0.0352 |
| C99 | 0.4666 (3) | 0.07706 (18) | 0.37127 (9) | 0.0394 |
| C100 | 0.5235 (3) | 0.09963 (18) | 0.34715 (9) | 0.0386 |
| C101 | 0.4935 (3) | 0.15263 (17) | 0.33717 (9) | 0.0364 |
| C102 | 0.4273 (3) | 0.33965 (17) | 0.35875 (9) | 0.0338 |
| C103 | 0.3960 (3) | 0.40346 (16) | 0.43806 (9) | 0.0314 |
| C104 | 0.3314 (3) | 0.27171 (16) | 0.50648 (8) | 0.0300 |
| C105 | 0.3270 (3) | 0.12129 (15) | 0.46665 (9) | 0.0295 |
| C106 | 0.3597 (3) | 0.16010 (17) | 0.37535 (9) | 0.0340 |
| C110 | 0.5036 (3) | 0.32053 (16) | 0.43991 (9) | 0.0331 |
| C111 | 0.6159 (3) | 0.30165 (18) | 0.44939 (10) | 0.0429 |
| C112 | 0.6232 (4) | 0.2383 (2) | 0.44767 (13) | 0.0632 |
| C113 | 0.4892 (3) | 0.28464 (18) | 0.53762 (9) | 0.0356 |
| C114 | 0.6099 (3) | 0.2761 (2) | 0.53786 (10) | 0.0507 |
| C115 | 0.6632 (3) | 0.2964 (2) | 0.56753 (10) | 0.0601 |
| C116 | 0.1508 (3) | 0.08509 (18) | 0.46990 (10) | 0.0382 |
| C117 | 0.0337 (3) | 0.1005 (2) | 0.46478 (10) | 0.0458 |

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|------|--------------|--------------|--------------|--------|--------|
| C118 | 0.0045 (4) | 0.1146 (2) | 0.43170 (12) | 0.0660 | |
| C119 | 0.3045 (3) | 0.23067 (17) | 0.41036 (9) | 0.0374 | |
| C120 | 0.2040 (3) | 0.25435 (18) | 0.42402 (10) | 0.0411 | |
| C121 | 0.1302 (4) | 0.2835 (2) | 0.40130 (11) | 0.0589 | |
| C122 | 0.7708 (3) | 0.30570 (19) | 0.36255 (11) | 0.0442 | |
| C123 | 0.8015 (4) | 0.2962 (2) | 0.32900 (12) | 0.0616 | |
| C124 | 0.8383 (4) | 0.3538 (2) | 0.37563 (13) | 0.0609 | |
| C125 | 0.7994 (4) | 0.2530 (2) | 0.38076 (12) | 0.0546 | |
| C126 | 0.0947 (3) | 0.49451 (18) | 0.42547 (11) | 0.0438 | |
| C127 | 0.1222 (4) | 0.55546 (18) | 0.41810 (11) | 0.0509 | |
| C128 | 0.0246 (4) | 0.4942 (2) | 0.45379 (12) | 0.0617 | |
| C129 | 0.0298 (4) | 0.4691 (2) | 0.39812 (13) | 0.0670 | |
| C130 | -0.0185 (3) | 0.28697 (17) | 0.50565 (10) | 0.0370 | |
| C131 | -0.0611 (3) | 0.3027 (2) | 0.47376 (11) | 0.0600 | |
| C132 | -0.0454 (3) | 0.33372 (19) | 0.52823 (11) | 0.0509 | |
| C133 | -0.0763 (3) | 0.23437 (19) | 0.51616 (12) | 0.0532 | |
| C134 | 0.6598 (3) | 0.07164 (18) | 0.48388 (12) | 0.0484 | |
| C135 | 0.6575 (6) | 0.0370 (3) | 0.51548 (18) | 0.0476 | 0.5901 |
| C136 | 0.7090 (7) | 0.0358 (4) | 0.4610 (2) | 0.0596 | 0.5901 |
| C137 | 0.7350 (6) | 0.1218 (3) | 0.4924 (2) | 0.0517 | 0.5901 |
| C335 | 0.6565 (11) | 0.0080 (5) | 0.4800 (4) | 0.0955 | 0.4099 |
| C336 | 0.7242 (10) | 0.0847 (8) | 0.4528 (3) | 0.0975 | 0.4099 |
| C337 | 0.7146 (12) | 0.0991 (9) | 0.5083 (4) | 0.1125 | 0.4099 |
| O6 | 0.3176 (2) | 0.35209 (12) | 0.35529 (7) | 0.0415 | |
| C107 | 0.2872 (16) | 0.3702 (12) | 0.3248 (4) | 0.1249 | 0.5027 |
| C108 | 0.1665 (15) | 0.3862 (7) | 0.3215 (5) | 0.1379 | 0.5027 |
| C109 | 0.1217 (16) | 0.3326 (7) | 0.3150 (4) | 0.1466 | 0.5027 |
| C207 | 0.2826 (8) | 0.3635 (7) | 0.3245 (3) | 0.0407 | 0.4973 |
| C208 | 0.1594 (8) | 0.3581 (5) | 0.3250 (3) | 0.0586 | 0.4973 |
| C209 | 0.1099 (9) | 0.3696 (4) | 0.2938 (2) | 0.0636 | 0.4973 |
| C138 | 0.6146 (8) | 0.0672 (3) | 0.33234 (19) | 0.0577 | 0.8535 |
| C139 | 0.5640 (7) | 0.0173 (3) | 0.3152 (2) | 0.1007 | 0.8535 |
| C140 | 0.6942 (6) | 0.0454 (4) | 0.35689 (16) | 0.0883 | 0.8535 |
| C141 | 0.6763 (7) | 0.1023 (4) | 0.30980 (17) | 0.0876 | 0.8535 |
| C338 | 0.609 (3) | 0.0655 (14) | 0.3296 (8) | 0.0460 | 0.1465 |
| C339 | 0.559 (2) | 0.0436 (12) | 0.2993 (5) | 0.0399 | 0.1465 |
| C340 | 0.648 (3) | 0.0148 (12) | 0.3481 (6) | 0.0422 | 0.1465 |
| C341 | 0.703 (3) | 0.1045 (14) | 0.3230 (7) | 0.0439 | 0.1465 |
| C67 | 0.0038 (8) | 0.0843 (7) | 0.5877 (3) | 0.0350 | 0.5917 |
| C68 | -0.0996 (8) | 0.0536 (5) | 0.5973 (2) | 0.0529 | 0.5917 |
| C69 | 0.0100 (8) | 0.0801 (4) | 0.5524 (2) | 0.0561 | 0.5917 |
| C70 | 0.1009 (8) | 0.0532 (5) | 0.6022 (3) | 0.0657 | 0.5917 |
| C267 | 0.0053 (17) | 0.0842 (12) | 0.5897 (5) | 0.0650 | 0.4083 |
| C268 | -0.1104 (14) | 0.0634 (8) | 0.5840 (4) | 0.0805 | 0.4083 |
| C269 | 0.0613 (15) | 0.0728 (7) | 0.5598 (4) | 0.0850 | 0.4083 |
| C270 | 0.0613 (16) | 0.0525 (7) | 0.6163 (4) | 0.0847 | 0.4083 |
| C36 | 0.3429 (9) | 0.3941 (3) | 0.59245 (19) | 0.0423 | 0.7372 |
| C37 | 0.2926 (7) | 0.4505 (3) | 0.59579 (18) | 0.0539 | 0.7372 |
| C38 | 0.3076 (6) | 0.4872 (3) | 0.56818 (15) | 0.0600 | 0.7372 |

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|------|-------------|-------------|------------|---------|--------|
| C236 | 0.326 (3) | 0.3806 (10) | 0.5872 (5) | 0.0432 | 0.2628 |
| C237 | 0.2568 (16) | 0.4308 (7) | 0.5791 (4) | 0.0514 | 0.2628 |
| C238 | 0.281 (2) | 0.4777 (8) | 0.6015 (5) | 0.0620 | 0.2628 |
| H21 | 0.1701 | 0.3148 | 0.5916 | 0.0471* | |
| H22 | 0.2013 | 0.2685 | 0.5659 | 0.0474* | |
| H41 | 0.3062 | 0.1796 | 0.5959 | 0.0466* | |
| H61 | 0.5684 | 0.2370 | 0.6444 | 0.0453* | |
| H81 | 0.5922 | 0.3297 | 0.6567 | 0.0501* | |
| H82 | 0.5233 | 0.3760 | 0.6366 | 0.0500* | |
| H101 | 0.4579 | 0.4474 | 0.6656 | 0.0494* | |
| H121 | 0.3373 | 0.4227 | 0.7508 | 0.0494* | |
| H141 | 0.4159 | 0.3227 | 0.7756 | 0.0502* | |
| H142 | 0.3839 | 0.2733 | 0.7511 | 0.0504* | |
| H161 | 0.2777 | 0.3824 | 0.7968 | 0.0556* | |
| H181 | -0.0346 | 0.3264 | 0.7922 | 0.0551* | |
| H202 | -0.0793 | 0.2406 | 0.7643 | 0.0595* | |
| H201 | 0.0074 | 0.2130 | 0.7414 | 0.0594* | |
| H221 | -0.0943 | 0.3554 | 0.7430 | 0.0529* | |
| H241 | -0.2099 | 0.3556 | 0.6540 | 0.0495* | |
| H261 | -0.2229 | 0.2180 | 0.6423 | 0.0594* | |
| H262 | -0.2087 | 0.2777 | 0.6249 | 0.0592* | |
| H281 | -0.1373 | 0.1466 | 0.6205 | 0.0522* | |
| H301 | 0.1482 | 0.1654 | 0.5774 | 0.0465* | |
| H392 | 0.6374 | 0.3003 | 0.7063 | 0.0611* | |
| H391 | 0.6167 | 0.2328 | 0.7004 | 0.0615* | |
| H401 | 0.5827 | 0.2860 | 0.7577 | 0.0734* | |
| H402 | 0.6967 | 0.2540 | 0.7498 | 0.0733* | |
| H413 | 0.5874 | 0.1926 | 0.7782 | 0.1181* | |
| H412 | 0.4901 | 0.1984 | 0.7530 | 0.1179* | |
| H411 | 0.6004 | 0.1682 | 0.7440 | 0.1183* | |
| H422 | 0.2395 | 0.2851 | 0.7013 | 0.0648* | |
| H421 | 0.1233 | 0.2516 | 0.6966 | 0.0644* | |
| H431 | 0.3335 | 0.1954 | 0.6964 | 0.1075* | |
| H432 | 0.2590 | 0.2093 | 0.6647 | 0.1077* | |
| H441 | 0.2456 | 0.1187 | 0.6768 | 0.1933* | |
| H443 | 0.2154 | 0.1339 | 0.7120 | 0.1936* | |
| H442 | 0.1308 | 0.1489 | 0.6836 | 0.1932* | |
| H451 | -0.1949 | 0.1702 | 0.7221 | 0.0873* | |
| H452 | -0.2289 | 0.1603 | 0.6859 | 0.0874* | |
| H462 | -0.1853 | 0.0716 | 0.7050 | 0.1030* | |
| H461 | -0.0847 | 0.0905 | 0.6840 | 0.1034* | |
| H471 | -0.0260 | 0.0517 | 0.7324 | 0.1573* | |
| H473 | -0.0833 | 0.1035 | 0.7496 | 0.1573* | |
| H472 | 0.0189 | 0.1144 | 0.7279 | 0.1570* | |
| H481 | 0.0461 | 0.3129 | 0.6664 | 0.0532* | |
| H482 | 0.1509 | 0.3182 | 0.6452 | 0.0526* | |
| H492 | -0.0028 | 0.4068 | 0.6531 | 0.0669* | |
| H491 | 0.1045 | 0.4109 | 0.6323 | 0.0677* | |
| H501 | 0.1380 | 0.4503 | 0.6823 | 0.1272* | |

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|------|---------|--------|--------|---------|
| H502 | 0.1122 | 0.3909 | 0.6976 | 0.1272* |
| H503 | 0.2169 | 0.3976 | 0.6765 | 0.1273* |
| H522 | 0.4595 | 0.0603 | 0.6040 | 0.0990* |
| H521 | 0.3598 | 0.0945 | 0.6172 | 0.0991* |
| H523 | 0.3998 | 0.1067 | 0.5829 | 0.0991* |
| H532 | 0.6319 | 0.1093 | 0.5942 | 0.1030* |
| H531 | 0.6503 | 0.1725 | 0.6043 | 0.1032* |
| H533 | 0.5716 | 0.1584 | 0.5756 | 0.1034* |
| H543 | 0.5774 | 0.0864 | 0.6482 | 0.1111* |
| H542 | 0.5940 | 0.1510 | 0.6580 | 0.1112* |
| H541 | 0.4795 | 0.1202 | 0.6631 | 0.1110* |
| H563 | 0.4835 | 0.5766 | 0.7206 | 0.1702* |
| H562 | 0.5196 | 0.5211 | 0.7389 | 0.1702* |
| H561 | 0.5416 | 0.5262 | 0.7030 | 0.1702* |
| H571 | 0.2898 | 0.5640 | 0.7370 | 0.1418* |
| H572 | 0.3354 | 0.5134 | 0.7571 | 0.1422* |
| H573 | 0.2357 | 0.5037 | 0.7340 | 0.1421* |
| H582 | 0.3274 | 0.5745 | 0.6851 | 0.1289* |
| H581 | 0.2677 | 0.5158 | 0.6766 | 0.1296* |
| H583 | 0.3889 | 0.5277 | 0.6658 | 0.1293* |
| H602 | 0.1477 | 0.4714 | 0.8464 | 0.1233* |
| H601 | 0.2344 | 0.4217 | 0.8419 | 0.1230* |
| H603 | 0.2055 | 0.4639 | 0.8138 | 0.1233* |
| H613 | 0.0185 | 0.4051 | 0.8646 | 0.1412* |
| H612 | 0.0888 | 0.3504 | 0.8580 | 0.1410* |
| H611 | -0.0302 | 0.3561 | 0.8430 | 0.1411* |
| H623 | -0.0245 | 0.4733 | 0.8202 | 0.1209* |
| H622 | -0.0693 | 0.4215 | 0.8000 | 0.1210* |
| H621 | 0.0231 | 0.4616 | 0.7874 | 0.1215* |
| H641 | -0.1237 | 0.4995 | 0.7203 | 0.0921* |
| H642 | -0.0618 | 0.4447 | 0.7330 | 0.0920* |
| H643 | -0.0455 | 0.4649 | 0.6978 | 0.0924* |
| H652 | -0.3016 | 0.4662 | 0.7327 | 0.0903* |
| H651 | -0.2488 | 0.4111 | 0.7485 | 0.0904* |
| H653 | -0.3437 | 0.4053 | 0.7225 | 0.0900* |
| H662 | -0.2643 | 0.4913 | 0.6790 | 0.0779* |
| H661 | -0.3108 | 0.4313 | 0.6683 | 0.0779* |
| H663 | -0.1920 | 0.4508 | 0.6587 | 0.0783* |
| H712 | 0.6226 | 0.4954 | 0.4944 | 0.1125* |
| H711 | 0.5706 | 0.4357 | 0.4836 | 0.1122* |
| H731 | 0.3118 | 0.2524 | 0.3452 | 0.0471* |
| H732 | 0.3849 | 0.2406 | 0.3159 | 0.0472* |
| H751 | 0.6030 | 0.2408 | 0.3464 | 0.0485* |
| H771 | 0.6540 | 0.3954 | 0.3827 | 0.0513* |
| H791 | 0.5152 | 0.4568 | 0.3920 | 0.0545* |
| H792 | 0.4155 | 0.4541 | 0.3669 | 0.0544* |
| H811 | 0.2562 | 0.4752 | 0.3875 | 0.0513* |
| H831 | 0.1790 | 0.4374 | 0.4744 | 0.0475* |
| H851 | 0.3371 | 0.4030 | 0.5096 | 0.0452* |

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|-------|---------|--------|--------|---------|
| H852 | 0.4294 | 0.3653 | 0.4934 | 0.0450* |
| H871 | 0.1345 | 0.3615 | 0.4952 | 0.0425* |
| H891 | 0.1127 | 0.1958 | 0.5130 | 0.0424* |
| H911 | 0.3753 | 0.1735 | 0.5367 | 0.0441* |
| H912 | 0.2643 | 0.1423 | 0.5266 | 0.0440* |
| H931 | 0.5247 | 0.1349 | 0.5174 | 0.0446* |
| H951 | 0.5289 | 0.0616 | 0.4331 | 0.0476* |
| H972 | 0.2515 | 0.0952 | 0.4122 | 0.0492* |
| H971 | 0.3257 | 0.0394 | 0.4099 | 0.0493* |
| H991 | 0.4843 | 0.0389 | 0.3787 | 0.0513* |
| H1011 | 0.5313 | 0.1694 | 0.3198 | 0.0504* |
| H1101 | 0.4484 | 0.3033 | 0.4532 | 0.0450* |
| H1102 | 0.4855 | 0.3097 | 0.4177 | 0.0449* |
| H1112 | 0.6311 | 0.3152 | 0.4710 | 0.0582* |
| H1111 | 0.6696 | 0.3195 | 0.4356 | 0.0582* |
| H1123 | 0.6962 | 0.2252 | 0.4541 | 0.1011* |
| H1122 | 0.5718 | 0.2209 | 0.4616 | 0.1010* |
| H1121 | 0.6063 | 0.2242 | 0.4269 | 0.1009* |
| H1131 | 0.4553 | 0.2636 | 0.5548 | 0.0497* |
| H1132 | 0.4742 | 0.3260 | 0.5406 | 0.0493* |
| H1142 | 0.6257 | 0.2347 | 0.5353 | 0.0667* |
| H1141 | 0.6397 | 0.2965 | 0.5199 | 0.0662* |
| H1153 | 0.7391 | 0.2886 | 0.5680 | 0.0958* |
| H1152 | 0.6300 | 0.2784 | 0.5854 | 0.0962* |
| H1151 | 0.6523 | 0.3377 | 0.5691 | 0.0963* |
| H1161 | 0.1661 | 0.0727 | 0.4925 | 0.0508* |
| H1162 | 0.1695 | 0.0535 | 0.4559 | 0.0503* |
| H1171 | 0.0177 | 0.1339 | 0.4777 | 0.0607* |
| H1172 | -0.0147 | 0.0690 | 0.4718 | 0.0605* |
| H1182 | -0.0724 | 0.1248 | 0.4294 | 0.1040* |
| H1181 | 0.0488 | 0.1459 | 0.4249 | 0.1040* |
| H1183 | 0.0191 | 0.0821 | 0.4188 | 0.1044* |
| H1192 | 0.3539 | 0.2144 | 0.4272 | 0.0504* |
| H1191 | 0.3451 | 0.2609 | 0.3994 | 0.0500* |
| H1201 | 0.2261 | 0.2824 | 0.4408 | 0.0557* |
| H1202 | 0.1647 | 0.2232 | 0.4342 | 0.0554* |
| H1212 | 0.0670 | 0.2991 | 0.4113 | 0.0952* |
| H1211 | 0.1695 | 0.3145 | 0.3916 | 0.0950* |
| H1213 | 0.1071 | 0.2572 | 0.3853 | 0.0952* |
| H1232 | 0.8788 | 0.2879 | 0.3280 | 0.0989* |
| H1231 | 0.7852 | 0.3303 | 0.3169 | 0.0992* |
| H1233 | 0.7585 | 0.2649 | 0.3198 | 0.0994* |
| H1241 | 0.9145 | 0.3453 | 0.3737 | 0.1020* |
| H1243 | 0.8213 | 0.3600 | 0.3970 | 0.1019* |
| H1242 | 0.8214 | 0.3886 | 0.3637 | 0.1020* |
| H1251 | 0.8756 | 0.2442 | 0.3787 | 0.0908* |
| H1253 | 0.7861 | 0.2599 | 0.4025 | 0.0910* |
| H1252 | 0.7551 | 0.2209 | 0.3734 | 0.0911* |
| H1271 | 0.0558 | 0.5783 | 0.4160 | 0.0832* |

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|-------|---------|---------|--------|---------|--------|
| H1272 | 0.1684 | 0.5712 | 0.4350 | 0.0832* | |
| H1273 | 0.1629 | 0.5580 | 0.3990 | 0.0831* | |
| H1282 | -0.0423 | 0.5155 | 0.4497 | 0.0959* | |
| H1281 | 0.0651 | 0.5107 | 0.4716 | 0.0961* | |
| H1283 | 0.0039 | 0.4555 | 0.4588 | 0.0962* | |
| H1292 | -0.0375 | 0.4898 | 0.3948 | 0.1129* | |
| H1291 | 0.0121 | 0.4303 | 0.4028 | 0.1131* | |
| H1293 | 0.0719 | 0.4703 | 0.3793 | 0.1133* | |
| H1311 | -0.1395 | 0.3084 | 0.4733 | 0.0978* | |
| H1313 | -0.0272 | 0.3380 | 0.4671 | 0.0982* | |
| H1312 | -0.0439 | 0.2727 | 0.4592 | 0.0981* | |
| H1321 | -0.1242 | 0.3375 | 0.5305 | 0.0829* | |
| H1323 | -0.0125 | 0.3258 | 0.5489 | 0.0832* | |
| H1322 | -0.0180 | 0.3694 | 0.5208 | 0.0829* | |
| H1331 | -0.1536 | 0.2405 | 0.5171 | 0.0869* | |
| H1332 | -0.0487 | 0.2221 | 0.5367 | 0.0872* | |
| H1333 | -0.0635 | 0.2035 | 0.5015 | 0.0870* | |
| H1352 | 0.7276 | 0.0226 | 0.5209 | 0.0789* | 0.5901 |
| H1351 | 0.6355 | 0.0604 | 0.5314 | 0.0789* | 0.5901 |
| H1353 | 0.6085 | 0.0062 | 0.5133 | 0.0791* | 0.5901 |
| H1362 | 0.7792 | 0.0216 | 0.4684 | 0.0938* | 0.5901 |
| H1361 | 0.6612 | 0.0051 | 0.4555 | 0.0939* | 0.5901 |
| H1363 | 0.7221 | 0.0582 | 0.4422 | 0.0941* | 0.5901 |
| H1371 | 0.8032 | 0.1085 | 0.5017 | 0.0882* | 0.5901 |
| H1373 | 0.6995 | 0.1479 | 0.5061 | 0.0883* | 0.5901 |
| H1372 | 0.7518 | 0.1414 | 0.4734 | 0.0878* | 0.5901 |
| H3351 | 0.7291 | -0.0060 | 0.4769 | 0.1489* | 0.4099 |
| H3353 | 0.6300 | -0.0081 | 0.4988 | 0.1491* | 0.4099 |
| H3352 | 0.6105 | -0.0019 | 0.4632 | 0.1489* | 0.4099 |
| H3361 | 0.7941 | 0.0679 | 0.4532 | 0.1479* | 0.4099 |
| H3362 | 0.7297 | 0.1238 | 0.4493 | 0.1479* | 0.4099 |
| H3363 | 0.6822 | 0.0684 | 0.4349 | 0.1480* | 0.4099 |
| H3372 | 0.7934 | 0.1066 | 0.5021 | 0.1601* | 0.4099 |
| H3371 | 0.7097 | 0.0870 | 0.5269 | 0.1601* | 0.4099 |
| H3373 | 0.6859 | 0.1419 | 0.5072 | 0.1602* | 0.4099 |
| H1072 | 0.3361 | 0.4039 | 0.3196 | 0.1390* | 0.5027 |
| H1071 | 0.3079 | 0.3411 | 0.3092 | 0.1392* | 0.5027 |
| H1081 | 0.1431 | 0.4039 | 0.3405 | 0.1502* | 0.5027 |
| H1082 | 0.1555 | 0.4113 | 0.3041 | 0.1502* | 0.5027 |
| H1093 | 0.0468 | 0.3375 | 0.3115 | 0.1931* | 0.5027 |
| H1092 | 0.1352 | 0.3082 | 0.3333 | 0.1932* | 0.5027 |
| H1091 | 0.1560 | 0.3145 | 0.2977 | 0.1932* | 0.5027 |
| H2072 | 0.3037 | 0.4000 | 0.3179 | 0.0561* | 0.4973 |
| H2071 | 0.3084 | 0.3344 | 0.3099 | 0.0562* | 0.4973 |
| H2081 | 0.1253 | 0.3857 | 0.3396 | 0.0739* | 0.4973 |
| H2082 | 0.1386 | 0.3209 | 0.3324 | 0.0744* | 0.4973 |
| H2093 | 0.0320 | 0.3727 | 0.2951 | 0.1000* | 0.4973 |
| H2092 | 0.1385 | 0.4037 | 0.2859 | 0.0999* | 0.4973 |
| H2091 | 0.1280 | 0.3399 | 0.2803 | 0.1000* | 0.4973 |

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|-------|---------|---------|--------|---------|--------|
| H1393 | 0.6223 | -0.0048 | 0.3063 | 0.1501* | 0.8535 |
| H1392 | 0.5253 | -0.0063 | 0.3295 | 0.1498* | 0.8535 |
| H1391 | 0.5146 | 0.0308 | 0.2987 | 0.1501* | 0.8535 |
| H1401 | 0.7541 | 0.0258 | 0.3474 | 0.1381* | 0.8535 |
| H1402 | 0.7240 | 0.0778 | 0.3687 | 0.1380* | 0.8535 |
| H1403 | 0.6583 | 0.0199 | 0.3706 | 0.1380* | 0.8535 |
| H1412 | 0.7362 | 0.0817 | 0.3017 | 0.1350* | 0.8535 |
| H1411 | 0.7055 | 0.1361 | 0.3205 | 0.1354* | 0.8535 |
| H1413 | 0.6280 | 0.1143 | 0.2926 | 0.1350* | 0.8535 |
| H3392 | 0.6270 | 0.0260 | 0.2862 | 0.0670* | 0.1465 |
| H3391 | 0.4987 | 0.0108 | 0.3058 | 0.0670* | 0.1465 |
| H3393 | 0.5193 | 0.0799 | 0.2872 | 0.0670* | 0.1465 |
| H3403 | 0.7193 | 0.0039 | 0.3397 | 0.0620* | 0.1465 |
| H3402 | 0.6670 | 0.0291 | 0.3689 | 0.0620* | 0.1465 |
| H3401 | 0.6020 | -0.0131 | 0.3481 | 0.0619* | 0.1465 |
| H3413 | 0.7492 | 0.0883 | 0.3077 | 0.0640* | 0.1465 |
| H3412 | 0.7424 | 0.1142 | 0.3406 | 0.0640* | 0.1465 |
| H3411 | 0.6738 | 0.1400 | 0.3132 | 0.0641* | 0.1465 |
| H681 | -0.1012 | 0.0160 | 0.5886 | 0.0809* | 0.5917 |
| H682 | -0.1030 | 0.0514 | 0.6190 | 0.0809* | 0.5917 |
| H683 | -0.1646 | 0.0745 | 0.5892 | 0.0815* | 0.5917 |
| H692 | 0.0125 | 0.0413 | 0.5465 | 0.0860* | 0.5917 |
| H691 | 0.0757 | 0.0995 | 0.5452 | 0.0864* | 0.5917 |
| H693 | -0.0527 | 0.0978 | 0.5431 | 0.0858* | 0.5917 |
| H702 | 0.0910 | 0.0127 | 0.5994 | 0.0950* | 0.5917 |
| H701 | 0.1062 | 0.0607 | 0.6244 | 0.0955* | 0.5917 |
| H703 | 0.1651 | 0.0644 | 0.5931 | 0.0948* | 0.5917 |
| H2683 | -0.1154 | 0.0277 | 0.5763 | 0.1291* | 0.4083 |
| H2682 | -0.1520 | 0.0667 | 0.6037 | 0.1292* | 0.4083 |
| H2681 | -0.1488 | 0.0907 | 0.5695 | 0.1291* | 0.4083 |
| H2693 | 0.0404 | 0.0386 | 0.5512 | 0.1300* | 0.4083 |
| H2692 | 0.1388 | 0.0735 | 0.5647 | 0.1299* | 0.4083 |
| H2691 | 0.0447 | 0.1043 | 0.5455 | 0.1302* | 0.4083 |
| H2701 | 0.0589 | 0.0134 | 0.6139 | 0.1320* | 0.4083 |
| H2702 | 0.0203 | 0.0616 | 0.6357 | 0.1320* | 0.4083 |
| H2703 | 0.1342 | 0.0664 | 0.6196 | 0.1321* | 0.4083 |
| H362 | 0.4224 | 0.3981 | 0.5909 | 0.0560* | 0.7372 |
| H361 | 0.3157 | 0.3759 | 0.5730 | 0.0564* | 0.7372 |
| H372 | 0.3236 | 0.4692 | 0.6148 | 0.0743* | 0.7372 |
| H371 | 0.2138 | 0.4460 | 0.5991 | 0.0742* | 0.7372 |
| H381 | 0.2806 | 0.5253 | 0.5714 | 0.0941* | 0.7372 |
| H382 | 0.3834 | 0.4894 | 0.5634 | 0.0939* | 0.7372 |
| H383 | 0.2679 | 0.4718 | 0.5502 | 0.0941* | 0.7372 |
| H2362 | 0.4007 | 0.3860 | 0.5822 | 0.0560* | 0.2628 |
| H2361 | 0.2975 | 0.3488 | 0.5734 | 0.0561* | 0.2628 |
| H2372 | 0.1831 | 0.4217 | 0.5817 | 0.0740* | 0.2628 |
| H2371 | 0.2724 | 0.4428 | 0.5592 | 0.0740* | 0.2628 |
| H2381 | 0.2407 | 0.5111 | 0.5956 | 0.0960* | 0.2628 |
| H2382 | 0.2671 | 0.4686 | 0.6222 | 0.0959* | 0.2628 |

supplementary materials

H2383 0.3595 0.4885 0.6006 0.0961* 0.2628

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C11 | 0.1092 (15) | 0.0894 (13) | 0.1436 (19) | -0.0272 (11) | -0.0370 (13) | 0.0077 (13) |
| C12 | 0.0935 (15) | 0.1327 (19) | 0.221 (3) | 0.0327 (14) | -0.0447 (16) | -0.0620 (19) |
| O1 | 0.0387 (16) | 0.0324 (16) | 0.0447 (17) | 0.0002 (13) | 0.0078 (13) | 0.0051 (13) |
| O2 | 0.0309 (15) | 0.0334 (16) | 0.0466 (17) | 0.0001 (12) | 0.0045 (13) | 0.0025 (13) |
| O3 | 0.0501 (18) | 0.0413 (18) | 0.0481 (18) | 0.0043 (15) | 0.0009 (15) | -0.0003 (15) |
| O4 | 0.0384 (16) | 0.0338 (16) | 0.062 (2) | 0.0005 (13) | 0.0082 (14) | -0.0016 (14) |
| O5 | 0.0390 (16) | 0.0392 (17) | 0.0405 (16) | 0.0045 (13) | -0.0007 (13) | -0.0036 (13) |
| O7 | 0.0274 (14) | 0.0287 (15) | 0.0490 (17) | 0.0011 (12) | 0.0044 (12) | -0.0006 (13) |
| O8 | 0.0205 (13) | 0.0413 (16) | 0.0322 (14) | 0.0012 (11) | 0.0003 (11) | -0.0006 (12) |
| O9 | 0.0224 (13) | 0.0329 (15) | 0.0396 (16) | 0.0037 (11) | -0.0011 (11) | -0.0002 (12) |
| O10 | 0.0292 (15) | 0.0412 (17) | 0.0479 (17) | 0.0023 (13) | 0.0032 (13) | -0.0113 (14) |
| C1 | 0.030 (2) | 0.041 (2) | 0.028 (2) | 0.0029 (18) | -0.0029 (16) | 0.0001 (18) |
| C2 | 0.036 (2) | 0.037 (2) | 0.033 (2) | 0.0038 (18) | -0.0005 (18) | -0.0018 (18) |
| C3 | 0.030 (2) | 0.036 (2) | 0.032 (2) | 0.0023 (18) | 0.0068 (17) | 0.0053 (18) |
| C4 | 0.033 (2) | 0.035 (2) | 0.035 (2) | -0.0040 (18) | 0.0012 (17) | -0.0018 (18) |
| C5 | 0.033 (2) | 0.032 (2) | 0.038 (2) | -0.0001 (18) | 0.0041 (18) | 0.0030 (18) |
| C6 | 0.025 (2) | 0.043 (2) | 0.033 (2) | -0.0012 (18) | 0.0042 (17) | 0.0017 (18) |
| C7 | 0.031 (2) | 0.035 (2) | 0.031 (2) | -0.0034 (18) | 0.0099 (17) | 0.0005 (17) |
| C8 | 0.032 (2) | 0.037 (2) | 0.043 (2) | -0.0042 (18) | 0.0081 (18) | 0.0001 (19) |
| C9 | 0.028 (2) | 0.033 (2) | 0.035 (2) | -0.0044 (17) | 0.0032 (17) | 0.0000 (18) |
| C10 | 0.034 (2) | 0.038 (2) | 0.039 (2) | -0.0049 (18) | 0.0049 (18) | 0.0045 (19) |
| C11 | 0.035 (2) | 0.036 (2) | 0.039 (2) | -0.0004 (18) | 0.0013 (18) | -0.0018 (19) |
| C12 | 0.034 (2) | 0.040 (2) | 0.037 (2) | 0.0018 (19) | 0.0048 (18) | 0.0012 (19) |
| C13 | 0.026 (2) | 0.035 (2) | 0.038 (2) | -0.0036 (17) | 0.0012 (17) | 0.0027 (18) |
| C14 | 0.033 (2) | 0.046 (3) | 0.032 (2) | -0.0020 (19) | 0.0019 (17) | 0.0035 (19) |
| C15 | 0.035 (2) | 0.039 (2) | 0.031 (2) | 0.0003 (19) | 0.0007 (17) | 0.0081 (18) |
| C16 | 0.040 (2) | 0.044 (3) | 0.039 (2) | 0.003 (2) | 0.0010 (19) | 0.003 (2) |
| C17 | 0.041 (2) | 0.054 (3) | 0.031 (2) | 0.011 (2) | 0.0028 (19) | 0.004 (2) |
| C18 | 0.036 (2) | 0.055 (3) | 0.036 (2) | 0.006 (2) | 0.0056 (19) | 0.007 (2) |
| C19 | 0.033 (2) | 0.038 (2) | 0.042 (2) | -0.0002 (19) | 0.0030 (19) | 0.009 (2) |
| C20 | 0.042 (3) | 0.044 (3) | 0.047 (3) | -0.001 (2) | -0.001 (2) | 0.012 (2) |
| C21 | 0.027 (2) | 0.037 (2) | 0.046 (3) | -0.0027 (18) | 0.0021 (18) | 0.001 (2) |
| C22 | 0.036 (2) | 0.036 (2) | 0.044 (3) | -0.0050 (19) | 0.0028 (19) | 0.003 (2) |
| C23 | 0.032 (2) | 0.041 (2) | 0.036 (2) | -0.0050 (18) | 0.0014 (18) | 0.0014 (19) |
| C24 | 0.024 (2) | 0.043 (2) | 0.039 (2) | -0.0006 (18) | 0.0011 (17) | 0.0037 (19) |
| C25 | 0.025 (2) | 0.044 (3) | 0.044 (2) | -0.0025 (18) | 0.0043 (18) | -0.003 (2) |
| C26 | 0.032 (2) | 0.052 (3) | 0.049 (3) | 0.003 (2) | 0.003 (2) | -0.007 (2) |
| C27 | 0.026 (2) | 0.046 (3) | 0.038 (2) | 0.0047 (19) | -0.0004 (17) | -0.002 (2) |
| C28 | 0.029 (2) | 0.044 (3) | 0.042 (2) | 0.0006 (19) | 0.0000 (18) | -0.002 (2) |
| C29 | 0.034 (2) | 0.043 (2) | 0.037 (2) | -0.0002 (19) | -0.0024 (18) | -0.002 (2) |
| C30 | 0.027 (2) | 0.042 (2) | 0.037 (2) | 0.0035 (18) | 0.0019 (17) | -0.0028 (19) |
| C31 | 0.032 (2) | 0.031 (2) | 0.031 (2) | 0.0010 (17) | 0.0087 (17) | 0.0021 (17) |
| C32 | 0.027 (2) | 0.032 (2) | 0.040 (2) | -0.0016 (17) | 0.0012 (17) | -0.0008 (18) |

| | | | | | | |
|-----|-----------|-----------|-----------|--------------|--------------|--------------|
| C33 | 0.039 (2) | 0.036 (2) | 0.032 (2) | 0.0056 (19) | 0.0045 (18) | 0.0074 (18) |
| C34 | 0.024 (2) | 0.032 (2) | 0.056 (3) | -0.0026 (17) | 0.0074 (19) | 0.002 (2) |
| C35 | 0.033 (2) | 0.036 (2) | 0.033 (2) | 0.0063 (18) | -0.0060 (17) | -0.0020 (18) |
| C39 | 0.033 (2) | 0.047 (3) | 0.064 (3) | 0.005 (2) | 0.002 (2) | 0.003 (2) |
| C40 | 0.042 (3) | 0.065 (3) | 0.060 (3) | 0.005 (2) | 0.002 (2) | 0.004 (3) |
| C41 | 0.072 (4) | 0.070 (4) | 0.085 (4) | 0.015 (3) | 0.009 (3) | 0.032 (3) |
| C42 | 0.049 (3) | 0.052 (3) | 0.045 (3) | -0.001 (2) | 0.004 (2) | 0.000 (2) |
| C43 | 0.107 (5) | 0.076 (4) | 0.071 (4) | -0.003 (4) | 0.022 (4) | -0.024 (3) |
| C44 | 0.130 (7) | 0.089 (6) | 0.169 (8) | -0.014 (5) | 0.048 (6) | -0.058 (6) |
| C45 | 0.050 (3) | 0.042 (3) | 0.106 (5) | -0.009 (2) | 0.006 (3) | 0.000 (3) |
| C46 | 0.089 (5) | 0.045 (3) | 0.104 (5) | -0.006 (3) | 0.015 (4) | 0.002 (3) |
| C47 | 0.104 (6) | 0.053 (4) | 0.158 (7) | 0.007 (4) | 0.004 (5) | 0.024 (4) |
| C48 | 0.031 (2) | 0.042 (3) | 0.044 (2) | -0.0002 (19) | 0.0057 (19) | -0.003 (2) |
| C49 | 0.037 (2) | 0.045 (3) | 0.069 (3) | -0.006 (2) | 0.007 (2) | -0.008 (2) |
| C50 | 0.044 (3) | 0.082 (4) | 0.127 (6) | -0.001 (3) | -0.005 (3) | -0.049 (4) |
| C51 | 0.040 (2) | 0.038 (2) | 0.053 (3) | 0.007 (2) | -0.007 (2) | -0.005 (2) |
| C52 | 0.056 (3) | 0.033 (3) | 0.093 (4) | 0.003 (2) | -0.013 (3) | -0.005 (3) |
| C53 | 0.047 (3) | 0.050 (3) | 0.104 (5) | 0.010 (2) | 0.017 (3) | -0.018 (3) |
| C54 | 0.087 (4) | 0.050 (3) | 0.075 (4) | 0.018 (3) | -0.022 (3) | 0.004 (3) |
| C55 | 0.045 (3) | 0.034 (2) | 0.054 (3) | 0.000 (2) | 0.009 (2) | -0.002 (2) |
| C56 | 0.074 (4) | 0.043 (4) | 0.227 (9) | -0.003 (3) | -0.004 (5) | -0.035 (5) |
| C57 | 0.126 (6) | 0.047 (3) | 0.093 (5) | 0.027 (3) | 0.055 (4) | 0.005 (3) |
| C58 | 0.137 (6) | 0.039 (3) | 0.073 (4) | 0.016 (3) | 0.020 (4) | 0.014 (3) |
| C59 | 0.055 (3) | 0.075 (4) | 0.035 (3) | 0.022 (3) | -0.005 (2) | -0.009 (2) |
| C60 | 0.076 (4) | 0.088 (4) | 0.080 (4) | 0.034 (3) | -0.026 (3) | -0.045 (4) |
| C61 | 0.123 (6) | 0.112 (5) | 0.040 (3) | 0.041 (5) | 0.023 (3) | -0.002 (3) |
| C62 | 0.070 (4) | 0.084 (4) | 0.063 (4) | 0.039 (3) | -0.004 (3) | -0.013 (3) |
| C63 | 0.042 (2) | 0.038 (2) | 0.038 (2) | 0.002 (2) | 0.0002 (19) | 0.0030 (19) |
| C64 | 0.059 (3) | 0.037 (3) | 0.070 (3) | -0.001 (2) | -0.009 (3) | -0.001 (2) |
| C65 | 0.058 (3) | 0.052 (3) | 0.055 (3) | 0.012 (2) | 0.012 (2) | 0.000 (2) |
| C66 | 0.055 (3) | 0.042 (3) | 0.046 (3) | 0.006 (2) | 0.002 (2) | 0.006 (2) |
| C71 | 0.065 (4) | 0.067 (4) | 0.144 (7) | -0.001 (3) | -0.014 (4) | -0.006 (4) |
| C72 | 0.032 (2) | 0.036 (2) | 0.034 (2) | 0.0034 (18) | -0.0007 (17) | -0.0058 (18) |
| C73 | 0.034 (2) | 0.035 (2) | 0.038 (2) | 0.0033 (18) | -0.0012 (18) | -0.0015 (19) |
| C74 | 0.035 (2) | 0.033 (2) | 0.031 (2) | 0.0009 (18) | 0.0052 (17) | 0.0052 (18) |
| C75 | 0.034 (2) | 0.038 (2) | 0.039 (2) | 0.0061 (19) | 0.0022 (18) | -0.0002 (19) |
| C76 | 0.030 (2) | 0.042 (2) | 0.038 (2) | -0.0001 (19) | 0.0016 (18) | 0.0031 (19) |
| C77 | 0.039 (2) | 0.038 (2) | 0.039 (2) | -0.0038 (19) | 0.0042 (19) | 0.0030 (19) |
| C78 | 0.038 (2) | 0.032 (2) | 0.028 (2) | 0.0006 (18) | 0.0038 (17) | 0.0029 (17) |
| C79 | 0.046 (3) | 0.030 (2) | 0.045 (3) | 0.0020 (19) | 0.011 (2) | 0.0043 (19) |
| C80 | 0.037 (2) | 0.027 (2) | 0.034 (2) | -0.0016 (18) | 0.0049 (18) | -0.0012 (17) |
| C81 | 0.041 (2) | 0.029 (2) | 0.043 (2) | 0.0024 (19) | 0.0002 (19) | 0.0014 (19) |
| C82 | 0.034 (2) | 0.028 (2) | 0.043 (2) | 0.0016 (17) | 0.0018 (19) | -0.0005 (18) |
| C83 | 0.032 (2) | 0.029 (2) | 0.045 (2) | -0.0021 (18) | 0.0045 (18) | -0.0027 (19) |
| C84 | 0.029 (2) | 0.028 (2) | 0.034 (2) | -0.0016 (17) | -0.0022 (17) | 0.0001 (17) |
| C85 | 0.029 (2) | 0.032 (2) | 0.040 (2) | -0.0011 (17) | 0.0003 (17) | -0.0047 (18) |
| C86 | 0.028 (2) | 0.030 (2) | 0.028 (2) | -0.0014 (16) | 0.0008 (16) | -0.0031 (16) |
| C87 | 0.028 (2) | 0.032 (2) | 0.036 (2) | 0.0042 (17) | 0.0019 (17) | -0.0036 (18) |
| C88 | 0.025 (2) | 0.036 (2) | 0.031 (2) | 0.0031 (17) | 0.0042 (16) | -0.0058 (17) |

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|------|-------------|------------|------------|--------------|--------------|--------------|
| C89 | 0.026 (2) | 0.034 (2) | 0.033 (2) | -0.0015 (17) | 0.0030 (16) | -0.0034 (18) |
| C90 | 0.0247 (19) | 0.033 (2) | 0.028 (2) | 0.0019 (16) | 0.0007 (15) | -0.0045 (17) |
| C91 | 0.028 (2) | 0.033 (2) | 0.034 (2) | 0.0016 (17) | 0.0038 (17) | 0.0025 (17) |
| C92 | 0.026 (2) | 0.027 (2) | 0.035 (2) | 0.0015 (16) | 0.0042 (16) | 0.0043 (17) |
| C93 | 0.031 (2) | 0.032 (2) | 0.034 (2) | 0.0012 (17) | 0.0001 (17) | 0.0037 (18) |
| C94 | 0.023 (2) | 0.031 (2) | 0.049 (3) | -0.0007 (17) | 0.0051 (18) | 0.0054 (19) |
| C95 | 0.030 (2) | 0.030 (2) | 0.046 (3) | 0.0012 (17) | 0.0121 (19) | 0.0007 (19) |
| C96 | 0.031 (2) | 0.030 (2) | 0.039 (2) | -0.0020 (17) | 0.0026 (18) | 0.0029 (18) |
| C97 | 0.036 (2) | 0.037 (2) | 0.040 (2) | -0.0034 (19) | 0.0060 (19) | -0.0026 (19) |
| C98 | 0.037 (2) | 0.034 (2) | 0.035 (2) | 0.0007 (18) | 0.0035 (18) | -0.0034 (18) |
| C99 | 0.045 (3) | 0.036 (2) | 0.038 (2) | 0.007 (2) | 0.010 (2) | -0.0018 (19) |
| C100 | 0.038 (2) | 0.041 (2) | 0.037 (2) | 0.0096 (19) | 0.0062 (19) | -0.0026 (19) |
| C101 | 0.040 (2) | 0.039 (2) | 0.031 (2) | 0.0028 (19) | 0.0043 (18) | -0.0022 (18) |
| C102 | 0.030 (2) | 0.035 (2) | 0.037 (2) | 0.0044 (18) | 0.0063 (17) | 0.0063 (18) |
| C103 | 0.028 (2) | 0.025 (2) | 0.041 (2) | 0.0015 (16) | 0.0029 (17) | -0.0020 (18) |
| C104 | 0.0235 (19) | 0.037 (2) | 0.030 (2) | -0.0004 (17) | 0.0044 (16) | -0.0028 (17) |
| C105 | 0.0235 (19) | 0.027 (2) | 0.038 (2) | 0.0030 (16) | 0.0074 (17) | 0.0069 (17) |
| C106 | 0.025 (2) | 0.037 (2) | 0.040 (2) | 0.0011 (17) | 0.0017 (17) | -0.0086 (19) |
| C110 | 0.034 (2) | 0.031 (2) | 0.035 (2) | 0.0038 (17) | 0.0062 (17) | 0.0032 (18) |
| C111 | 0.040 (2) | 0.044 (3) | 0.046 (3) | 0.007 (2) | 0.006 (2) | 0.008 (2) |
| C112 | 0.055 (3) | 0.047 (3) | 0.089 (4) | 0.020 (2) | 0.023 (3) | 0.022 (3) |
| C113 | 0.026 (2) | 0.048 (3) | 0.033 (2) | -0.0027 (18) | -0.0020 (17) | 0.0011 (19) |
| C114 | 0.029 (2) | 0.089 (4) | 0.033 (2) | -0.004 (2) | -0.0002 (18) | 0.004 (2) |
| C115 | 0.032 (2) | 0.107 (5) | 0.041 (3) | -0.012 (3) | -0.005 (2) | 0.006 (3) |
| C116 | 0.029 (2) | 0.041 (2) | 0.044 (3) | -0.0063 (18) | 0.0038 (18) | 0.001 (2) |
| C117 | 0.029 (2) | 0.060 (3) | 0.048 (3) | -0.005 (2) | 0.003 (2) | -0.009 (2) |
| C118 | 0.047 (3) | 0.078 (4) | 0.072 (4) | -0.006 (3) | -0.013 (3) | 0.008 (3) |
| C119 | 0.037 (2) | 0.034 (2) | 0.041 (2) | 0.0024 (18) | 0.0041 (19) | -0.0083 (19) |
| C120 | 0.040 (2) | 0.038 (2) | 0.045 (3) | 0.008 (2) | 0.007 (2) | 0.001 (2) |
| C121 | 0.046 (3) | 0.070 (4) | 0.062 (3) | 0.022 (3) | 0.011 (2) | 0.013 (3) |
| C122 | 0.031 (2) | 0.048 (3) | 0.054 (3) | 0.002 (2) | 0.005 (2) | 0.002 (2) |
| C123 | 0.038 (3) | 0.078 (4) | 0.069 (3) | 0.006 (3) | 0.012 (2) | -0.002 (3) |
| C124 | 0.032 (3) | 0.059 (3) | 0.091 (4) | -0.002 (2) | -0.005 (3) | -0.007 (3) |
| C125 | 0.040 (3) | 0.055 (3) | 0.069 (3) | 0.007 (2) | 0.001 (2) | 0.004 (3) |
| C126 | 0.036 (2) | 0.041 (3) | 0.054 (3) | 0.008 (2) | -0.003 (2) | 0.000 (2) |
| C127 | 0.060 (3) | 0.039 (3) | 0.054 (3) | 0.016 (2) | 0.001 (2) | 0.002 (2) |
| C128 | 0.044 (3) | 0.065 (3) | 0.077 (4) | 0.023 (3) | 0.012 (3) | 0.013 (3) |
| C129 | 0.049 (3) | 0.057 (3) | 0.093 (4) | 0.011 (3) | -0.023 (3) | -0.018 (3) |
| C130 | 0.023 (2) | 0.038 (2) | 0.049 (3) | 0.0046 (18) | 0.0018 (18) | -0.002 (2) |
| C131 | 0.029 (2) | 0.088 (4) | 0.062 (3) | 0.009 (3) | -0.005 (2) | 0.002 (3) |
| C132 | 0.033 (2) | 0.048 (3) | 0.073 (3) | 0.004 (2) | 0.015 (2) | -0.013 (2) |
| C133 | 0.025 (2) | 0.046 (3) | 0.090 (4) | 0.000 (2) | 0.011 (2) | -0.005 (3) |
| C134 | 0.024 (2) | 0.040 (3) | 0.082 (4) | 0.0045 (19) | 0.005 (2) | 0.004 (2) |
| C135 | 0.028 (4) | 0.046 (4) | 0.069 (5) | 0.012 (3) | 0.005 (3) | 0.023 (4) |
| C136 | 0.036 (4) | 0.068 (5) | 0.074 (5) | 0.022 (4) | 0.007 (4) | -0.005 (4) |
| C137 | 0.025 (4) | 0.046 (4) | 0.084 (6) | 0.005 (3) | -0.005 (4) | 0.013 (4) |
| C335 | 0.040 (7) | 0.106 (10) | 0.140 (11) | 0.024 (7) | -0.005 (7) | 0.024 (9) |
| C336 | 0.030 (6) | 0.132 (10) | 0.131 (10) | 0.030 (7) | 0.002 (6) | 0.012 (9) |
| C337 | 0.044 (7) | 0.160 (13) | 0.132 (12) | 0.038 (8) | -0.018 (8) | -0.006 (11) |

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|------|-------------|-------------|-------------|-------------|-------------|-------------|
| O6 | 0.0312 (15) | 0.0400 (17) | 0.0535 (19) | 0.0062 (13) | 0.0019 (13) | 0.0040 (14) |
| C107 | 0.158 (15) | 0.108 (12) | 0.104 (11) | 0.000 (11) | -0.074 (10) | 0.035 (10) |
| C108 | 0.182 (13) | 0.114 (11) | 0.112 (9) | -0.012 (10) | -0.085 (9) | 0.024 (9) |
| C109 | 0.187 (14) | 0.132 (12) | 0.116 (10) | -0.014 (11) | -0.079 (10) | 0.012 (10) |
| C207 | 0.021 (5) | 0.040 (6) | 0.060 (7) | 0.016 (4) | -0.003 (5) | 0.006 (5) |
| C208 | 0.043 (5) | 0.058 (6) | 0.073 (6) | 0.010 (5) | -0.031 (4) | 0.007 (5) |
| C209 | 0.068 (6) | 0.054 (6) | 0.067 (6) | 0.006 (5) | -0.033 (5) | 0.006 (5) |
| C138 | 0.066 (4) | 0.054 (3) | 0.054 (4) | 0.023 (3) | 0.025 (3) | 0.003 (3) |
| C139 | 0.109 (5) | 0.089 (5) | 0.106 (5) | 0.033 (4) | 0.031 (4) | -0.025 (4) |
| C140 | 0.079 (4) | 0.110 (5) | 0.078 (4) | 0.057 (4) | 0.038 (4) | 0.033 (4) |
| C141 | 0.086 (5) | 0.109 (6) | 0.071 (5) | 0.053 (5) | 0.050 (4) | 0.035 (5) |
| C338 | 0.058 (8) | 0.047 (8) | 0.034 (8) | 0.024 (8) | 0.016 (7) | 0.001 (7) |
| C339 | 0.054 (9) | 0.045 (9) | 0.020 (8) | 0.028 (8) | 0.010 (8) | -0.006 (8) |
| C340 | 0.053 (11) | 0.045 (10) | 0.030 (10) | 0.029 (9) | 0.005 (9) | -0.005 (9) |
| C341 | 0.051 (13) | 0.044 (12) | 0.038 (12) | 0.026 (11) | 0.007 (11) | -0.001 (11) |
| C67 | 0.024 (5) | 0.040 (7) | 0.041 (6) | -0.004 (5) | 0.008 (4) | 0.004 (5) |
| C68 | 0.052 (5) | 0.048 (5) | 0.060 (5) | -0.014 (4) | 0.013 (4) | -0.001 (4) |
| C69 | 0.067 (5) | 0.046 (5) | 0.055 (5) | -0.008 (4) | 0.004 (4) | -0.016 (4) |
| C70 | 0.065 (6) | 0.052 (5) | 0.079 (7) | 0.012 (5) | -0.017 (5) | -0.013 (5) |
| C267 | 0.082 (13) | 0.040 (10) | 0.073 (11) | 0.002 (10) | -0.006 (10) | -0.029 (9) |
| C268 | 0.098 (10) | 0.051 (8) | 0.092 (10) | -0.002 (7) | -0.004 (8) | -0.030 (7) |
| C269 | 0.116 (10) | 0.044 (7) | 0.096 (9) | -0.003 (7) | 0.016 (8) | -0.025 (6) |
| C270 | 0.122 (12) | 0.037 (7) | 0.094 (10) | 0.006 (8) | -0.007 (9) | -0.014 (8) |
| C36 | 0.041 (5) | 0.035 (5) | 0.052 (4) | -0.012 (4) | 0.009 (3) | 0.012 (3) |
| C37 | 0.078 (5) | 0.034 (4) | 0.051 (5) | 0.004 (4) | 0.013 (4) | 0.005 (4) |
| C38 | 0.079 (5) | 0.044 (4) | 0.058 (4) | -0.001 (3) | 0.005 (4) | 0.008 (3) |
| C236 | 0.033 (9) | 0.031 (9) | 0.067 (9) | -0.011 (9) | 0.013 (8) | 0.015 (8) |
| C237 | 0.072 (9) | 0.037 (8) | 0.046 (9) | -0.002 (7) | 0.017 (8) | 0.006 (7) |
| C238 | 0.072 (9) | 0.042 (9) | 0.072 (9) | -0.005 (8) | -0.001 (8) | -0.004 (8) |

Geometric parameters (Å, °)

| | | | |
|---------|------------|----------|-----------|
| Cl1—C71 | 1.738 (7) | C89—C90 | 1.404 (5) |
| Cl2—C71 | 1.742 (6) | C89—H891 | 0.967 |
| O1—C31 | 1.396 (5) | C90—C91 | 1.523 (5) |
| O1—C36 | 1.435 (8) | C90—C104 | 1.400 (5) |
| O1—C31 | 1.396 (5) | C91—C92 | 1.514 (5) |
| O1—C236 | 1.459 (18) | C91—H911 | 1.015 |
| O2—C32 | 1.395 (5) | C91—H912 | 0.992 |
| O2—C39 | 1.446 (5) | C92—C93 | 1.389 (5) |
| O3—C33 | 1.391 (5) | C92—C105 | 1.400 (5) |
| O3—C42 | 1.426 (5) | C93—C94 | 1.391 (5) |
| O4—C34 | 1.400 (5) | C93—H931 | 0.978 |
| O4—C45 | 1.439 (5) | C94—C95 | 1.391 (6) |
| O5—C35 | 1.389 (5) | C94—C134 | 1.539 (5) |
| O5—C48 | 1.439 (5) | C95—C96 | 1.398 (5) |
| O7—C103 | 1.398 (4) | C95—H951 | 0.974 |
| O7—C110 | 1.443 (4) | C96—C97 | 1.519 (5) |
| O8—C104 | 1.391 (4) | C96—C105 | 1.388 (5) |

supplementary materials

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|----------|-----------|------------|------------|
| O8—C113 | 1.448 (4) | C97—C98 | 1.521 (5) |
| O9—C105 | 1.399 (4) | C97—H972 | 1.003 |
| O9—C116 | 1.435 (5) | C97—H971 | 1.004 |
| O10—C106 | 1.392 (4) | C98—C99 | 1.390 (5) |
| O10—C119 | 1.448 (5) | C98—C106 | 1.398 (6) |
| C1—C2 | 1.520 (5) | C99—C100 | 1.393 (6) |
| C1—C30 | 1.396 (6) | C99—H991 | 0.991 |
| C1—C35 | 1.400 (5) | C100—C101 | 1.387 (6) |
| C2—C3 | 1.529 (5) | C100—C138 | 1.529 (11) |
| C2—H21 | 1.016 | C100—C101 | 1.387 (6) |
| C2—H22 | 1.007 | C100—C338 | 1.56 (5) |
| C3—C4 | 1.395 (5) | C101—H1011 | 0.987 |
| C3—C31 | 1.393 (5) | C102—O6 | 1.393 (4) |
| C4—C5 | 1.394 (5) | C110—C111 | 1.506 (5) |
| C4—H41 | 0.970 | C110—H1101 | 0.999 |
| C5—C6 | 1.389 (5) | C110—H1102 | 1.024 |
| C5—C51 | 1.536 (6) | C111—C112 | 1.519 (6) |
| C6—C7 | 1.388 (5) | C111—H1112 | 1.010 |
| C6—H61 | 0.977 | C111—H1111 | 1.005 |
| C7—C8 | 1.516 (5) | C112—H1123 | 0.989 |
| C7—C31 | 1.402 (5) | C112—H1122 | 0.984 |
| C8—C9 | 1.524 (5) | C112—H1121 | 0.984 |
| C8—H81 | 1.005 | C113—C114 | 1.506 (5) |
| C8—H82 | 1.007 | C113—H1131 | 1.007 |
| C9—C10 | 1.394 (6) | C113—H1132 | 1.015 |
| C9—C32 | 1.402 (5) | C114—C115 | 1.515 (6) |
| C10—C11 | 1.398 (6) | C114—H1142 | 1.016 |
| C10—H101 | 0.984 | C114—H1141 | 1.002 |
| C11—C12 | 1.399 (6) | C115—H1153 | 0.956 |
| C11—C55 | 1.527 (6) | C115—H1152 | 0.992 |
| C12—C13 | 1.398 (6) | C115—H1151 | 1.000 |
| C12—H121 | 0.990 | C116—C117 | 1.505 (5) |
| C13—C14 | 1.521 (5) | C116—H1161 | 1.041 |
| C13—C32 | 1.387 (5) | C116—H1162 | 1.002 |
| C14—C15 | 1.518 (5) | C117—C118 | 1.516 (6) |
| C14—H141 | 1.006 | C117—H1171 | 1.001 |
| C14—H142 | 1.009 | C117—H1172 | 1.017 |
| C15—C16 | 1.392 (6) | C118—H1182 | 0.985 |
| C15—C33 | 1.401 (6) | C118—H1181 | 0.980 |
| C16—C17 | 1.392 (6) | C118—H1183 | 0.979 |
| C16—H161 | 0.988 | C119—C120 | 1.506 (5) |
| C17—C18 | 1.391 (6) | C119—H1192 | 1.018 |
| C17—C59 | 1.531 (6) | C119—H1191 | 1.008 |
| C18—C19 | 1.392 (6) | C120—C121 | 1.500 (6) |
| C18—H181 | 0.983 | C120—H1201 | 1.023 |
| C19—C20 | 1.517 (6) | C120—H1202 | 1.002 |
| C19—C33 | 1.392 (5) | C121—H1212 | 0.981 |
| C20—C21 | 1.536 (6) | C121—H1211 | 0.988 |
| C20—H202 | 1.003 | C121—H1213 | 0.976 |

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| C20—H201 | 1.012 | C122—C123 | 1.541 (6) |
| C21—C22 | 1.391 (6) | C122—C124 | 1.522 (6) |
| C21—C34 | 1.393 (6) | C122—C125 | 1.525 (6) |
| C22—C23 | 1.395 (6) | C123—H1232 | 0.979 |
| C22—H221 | 0.987 | C123—H1231 | 0.990 |
| C23—C24 | 1.399 (6) | C123—H1233 | 0.997 |
| C23—C63 | 1.533 (6) | C124—H1241 | 0.970 |
| C24—C25 | 1.404 (6) | C124—H1243 | 0.975 |
| C24—H241 | 0.993 | C124—H1242 | 1.001 |
| C25—C26 | 1.503 (6) | C125—H1251 | 0.973 |
| C25—C34 | 1.386 (6) | C125—H1253 | 0.982 |
| C26—C27 | 1.525 (5) | C125—H1252 | 0.991 |
| C26—H261 | 1.007 | C126—C127 | 1.533 (6) |
| C26—H262 | 0.991 | C126—C128 | 1.532 (6) |
| C27—C28 | 1.378 (6) | C126—C129 | 1.544 (6) |
| C27—C35 | 1.397 (6) | C127—H1271 | 0.988 |
| C28—C29 | 1.398 (6) | C127—H1272 | 0.995 |
| C28—H281 | 0.990 | C127—H1273 | 0.988 |
| C29—C30 | 1.393 (6) | C128—H1282 | 0.985 |
| C29—C267 | 1.52 (3) | C128—H1281 | 0.995 |
| C29—C30 | 1.393 (6) | C128—H1283 | 0.986 |
| C29—C67 | 1.537 (18) | C129—H1292 | 0.976 |
| C30—H301 | 0.971 | C129—H1291 | 0.977 |
| C39—C40 | 1.485 (6) | C129—H1293 | 0.987 |
| C39—H392 | 1.025 | C130—C131 | 1.521 (6) |
| C39—H391 | 1.006 | C130—C132 | 1.533 (6) |
| C40—C41 | 1.521 (7) | C130—C133 | 1.525 (6) |
| C40—H401 | 1.014 | C131—H1311 | 0.980 |
| C40—H402 | 1.018 | C131—H1313 | 0.991 |
| C41—H413 | 0.985 | C131—H1312 | 0.986 |
| C41—H412 | 0.982 | C132—H1321 | 0.987 |
| C41—H411 | 1.002 | C132—H1323 | 0.999 |
| C42—C43 | 1.515 (7) | C132—H1322 | 0.976 |
| C42—H422 | 1.040 | C133—H1331 | 0.970 |
| C42—H421 | 1.009 | C133—H1332 | 0.994 |
| C43—C44 | 1.430 (9) | C133—H1333 | 0.993 |
| C43—H431 | 1.031 | C134—C135 | 1.611 (8) |
| C43—H432 | 1.036 | C134—C136 | 1.464 (8) |
| C44—H441 | 0.987 | C134—C137 | 1.555 (8) |
| C44—H443 | 1.029 | C134—C335 | 1.531 (12) |
| C44—H442 | 0.969 | C134—C336 | 1.626 (12) |
| C45—C46 | 1.510 (7) | C134—C337 | 1.407 (13) |
| C45—H451 | 1.016 | C135—H1352 | 0.955 |
| C45—H452 | 1.014 | C135—H1351 | 0.940 |
| C46—C47 | 1.504 (9) | C135—H1353 | 0.957 |
| C46—H462 | 1.010 | C136—H1362 | 0.979 |
| C46—H461 | 1.008 | C136—H1361 | 0.968 |
| C47—H471 | 0.983 | C136—H1363 | 0.996 |
| C47—H473 | 1.011 | C137—H1371 | 0.978 |

supplementary materials

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| C47—H472 | 0.993 | C137—H1373 | 0.977 |
| C48—C49 | 1.495 (6) | C137—H1372 | 0.982 |
| C48—H481 | 1.018 | C335—H3351 | 0.973 |
| C48—H482 | 0.993 | C335—H3353 | 0.971 |
| C49—C50 | 1.511 (7) | C335—H3352 | 0.944 |
| C49—H492 | 1.008 | C336—H3361 | 0.953 |
| C49—H491 | 1.005 | C336—H3362 | 0.950 |
| C50—H501 | 0.985 | C336—H3363 | 1.003 |
| C50—H502 | 1.003 | C337—H3372 | 1.035 |
| C50—H503 | 0.986 | C337—H3371 | 0.866 |
| C51—C52 | 1.527 (6) | C337—H3373 | 1.085 |
| C51—C53 | 1.539 (6) | O6—C107 | 1.439 (15) |
| C51—C54 | 1.536 (6) | O6—C207 | 1.426 (11) |
| C52—H522 | 0.981 | C107—C108 | 1.544 (16) |
| C52—H521 | 0.985 | C107—H1072 | 1.037 |
| C52—H523 | 0.996 | C107—H1071 | 1.013 |
| C53—H532 | 0.976 | C108—C109 | 1.422 (15) |
| C53—H531 | 0.987 | C108—H1081 | 0.980 |
| C53—H533 | 0.983 | C108—H1082 | 0.975 |
| C54—H543 | 0.988 | C109—H1093 | 0.942 |
| C54—H542 | 1.002 | C109—H1092 | 1.002 |
| C54—H541 | 0.982 | C109—H1091 | 0.979 |
| C55—C56 | 1.515 (7) | C207—C208 | 1.532 (12) |
| C55—C57 | 1.511 (6) | C207—H2072 | 0.957 |
| C55—C58 | 1.527 (7) | C207—H2071 | 1.002 |
| C56—H563 | 0.984 | C208—C209 | 1.500 (12) |
| C56—H562 | 0.988 | C208—H2081 | 1.018 |
| C56—H561 | 0.973 | C208—H2082 | 0.983 |
| C57—H571 | 0.977 | C209—H2093 | 0.970 |
| C57—H572 | 0.984 | C209—H2092 | 0.958 |
| C57—H573 | 0.982 | C209—H2091 | 0.955 |
| C58—H582 | 0.975 | C138—C139 | 1.532 (9) |
| C58—H581 | 1.001 | C138—C140 | 1.524 (9) |
| C58—H583 | 0.990 | C138—C141 | 1.517 (9) |
| C59—C60 | 1.526 (7) | C139—H1393 | 0.983 |
| C59—C61 | 1.523 (7) | C139—H1392 | 0.977 |
| C59—C62 | 1.539 (6) | C139—H1391 | 0.986 |
| C60—H602 | 1.000 | C140—H1401 | 0.981 |
| C60—H601 | 0.988 | C140—H1402 | 0.995 |
| C60—H603 | 1.002 | C140—H1403 | 0.971 |
| C61—H613 | 0.976 | C141—H1412 | 0.967 |
| C61—H612 | 0.968 | C141—H1411 | 0.995 |
| C61—H611 | 1.003 | C141—H1413 | 0.989 |
| C62—H623 | 0.975 | C338—C339 | 1.53 (2) |
| C62—H622 | 0.991 | C338—C340 | 1.53 (2) |
| C62—H621 | 0.993 | C338—C341 | 1.53 (2) |
| C63—C64 | 1.544 (6) | C339—H3392 | 1.110 |
| C63—C65 | 1.524 (6) | C339—H3391 | 1.129 |
| C63—C66 | 1.529 (6) | C339—H3393 | 1.123 |

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| C64—H641 | 0.994 | C340—H3403 | 0.997 |
| C64—H642 | 0.984 | C340—H3402 | 0.993 |
| C64—H643 | 1.003 | C340—H3401 | 0.879 |
| C65—H652 | 0.997 | C341—H3413 | 0.971 |
| C65—H651 | 0.998 | C341—H3412 | 0.926 |
| C65—H653 | 0.977 | C341—H3411 | 1.012 |
| C66—H662 | 0.990 | C67—C68 | 1.545 (11) |
| C66—H661 | 0.989 | C67—C69 | 1.548 (12) |
| C66—H663 | 0.983 | C67—C70 | 1.533 (12) |
| C71—H712 | 1.009 | C68—H681 | 0.977 |
| C71—H711 | 1.031 | C68—H682 | 0.950 |
| C72—C73 | 1.518 (5) | C68—H683 | 1.004 |
| C72—C101 | 1.399 (5) | C69—H692 | 0.966 |
| C72—C106 | 1.391 (5) | C69—H691 | 0.995 |
| C73—C74 | 1.527 (5) | C69—H693 | 0.963 |
| C73—H731 | 0.997 | C70—H702 | 0.983 |
| C73—H732 | 1.006 | C70—H701 | 0.984 |
| C74—C75 | 1.388 (5) | C70—H703 | 0.937 |
| C74—C102 | 1.395 (5) | C267—C268 | 1.529 (17) |
| C75—C76 | 1.397 (6) | C267—C269 | 1.520 (17) |
| C75—H751 | 0.978 | C267—C270 | 1.533 (17) |
| C76—C77 | 1.394 (6) | C268—H2683 | 0.919 |
| C76—C122 | 1.531 (5) | C268—H2682 | 1.018 |
| C77—C78 | 1.400 (5) | C268—H2681 | 1.018 |
| C77—H771 | 0.962 | C269—H2693 | 0.934 |
| C78—C79 | 1.516 (5) | C269—H2692 | 0.976 |
| C78—C102 | 1.385 (5) | C269—H2691 | 0.995 |
| C79—C80 | 1.523 (5) | C270—H2701 | 0.942 |
| C79—H791 | 0.993 | C270—H2702 | 1.026 |
| C79—H792 | 1.016 | C270—H2703 | 0.968 |
| C80—C81 | 1.388 (5) | C36—C37 | 1.494 (10) |
| C80—C103 | 1.396 (5) | C36—H362 | 0.992 |
| C81—C82 | 1.389 (6) | C36—H361 | 1.002 |
| C81—H811 | 0.968 | C37—C38 | 1.506 (8) |
| C82—C83 | 1.382 (6) | C37—H372 | 1.006 |
| C82—C126 | 1.533 (5) | C37—H371 | 0.996 |
| C83—C84 | 1.399 (5) | C38—H381 | 0.982 |
| C83—H831 | 0.964 | C38—H382 | 0.969 |
| C84—C85 | 1.526 (5) | C38—H383 | 0.983 |
| C84—C103 | 1.404 (5) | C236—C237 | 1.509 (18) |
| C85—C86 | 1.527 (5) | C236—H2362 | 0.970 |
| C85—H851 | 1.007 | C236—H2361 | 1.024 |
| C85—H852 | 1.019 | C237—C238 | 1.512 (16) |
| C86—C87 | 1.407 (5) | C237—H2372 | 0.948 |
| C86—C104 | 1.398 (5) | C237—H2371 | 0.940 |
| C87—C88 | 1.387 (5) | C238—H2381 | 0.972 |
| C87—H871 | 0.973 | C238—H2382 | 0.955 |
| C88—C89 | 1.384 (5) | C238—H2383 | 1.003 |
| C88—C130 | 1.537 (5) | | |

supplementary materials

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| C31—O1—C36 | 115.7 (4) | C98—C97—H972 | 108.5 |
| C31—O1—C236 | 105.8 (9) | C96—C97—H971 | 109.5 |
| C32—O2—C39 | 113.6 (3) | C98—C97—H971 | 108.4 |
| C33—O3—C42 | 115.0 (3) | H972—C97—H971 | 108.1 |
| C34—O4—C45 | 113.1 (3) | C97—C98—C99 | 121.0 (4) |
| C35—O5—C48 | 113.2 (3) | C97—C98—C106 | 120.6 (4) |
| C103—O7—C110 | 114.5 (3) | C99—C98—C106 | 118.5 (4) |
| C104—O8—C113 | 112.9 (3) | C98—C99—C100 | 122.4 (4) |
| C105—O9—C116 | 112.3 (3) | C98—C99—H991 | 118.0 |
| C106—O10—C119 | 114.7 (3) | C100—C99—H991 | 119.6 |
| C2—C1—C30 | 121.5 (4) | C99—C100—C101 | 117.1 (4) |
| C2—C1—C35 | 120.9 (4) | C99—C100—C138 | 121.3 (4) |
| C30—C1—C35 | 117.4 (4) | C101—C100—C138 | 121.7 (4) |
| C1—C2—C3 | 115.8 (3) | C99—C100—C101 | 117.1 (4) |
| C1—C2—H21 | 109.1 | C99—C100—C338 | 122.4 (12) |
| C3—C2—H21 | 108.1 | C101—C100—C338 | 120.2 (11) |
| C1—C2—H22 | 108.7 | C72—C101—C100 | 122.8 (4) |
| C3—C2—H22 | 107.5 | C72—C101—H1011 | 118.2 |
| H21—C2—H22 | 107.4 | C100—C101—H1011 | 119.0 |
| C2—C3—C4 | 120.6 (4) | C74—C102—C78 | 121.6 (4) |
| C2—C3—C31 | 121.5 (4) | C74—C102—O6 | 119.7 (4) |
| C4—C3—C31 | 117.8 (4) | C78—C102—O6 | 118.6 (3) |
| C3—C4—C5 | 122.9 (4) | C84—C103—O7 | 119.6 (3) |
| C3—C4—H41 | 119.2 | C84—C103—C80 | 121.4 (3) |
| C5—C4—H41 | 117.9 | O7—C103—C80 | 118.7 (3) |
| C4—C5—C6 | 116.7 (4) | C90—C104—C86 | 121.3 (3) |
| C4—C5—C51 | 122.4 (4) | C90—C104—O8 | 118.0 (3) |
| C6—C5—C51 | 120.8 (4) | C86—C104—O8 | 120.7 (3) |
| C5—C6—C7 | 123.2 (4) | C92—C105—O9 | 118.5 (3) |
| C5—C6—H61 | 119.1 | C92—C105—C96 | 121.6 (3) |
| C7—C6—H61 | 117.7 | O9—C105—C96 | 119.9 (3) |
| C6—C7—C8 | 120.5 (4) | C98—C106—O10 | 118.1 (4) |
| C6—C7—C31 | 117.8 (4) | C98—C106—C72 | 121.2 (4) |
| C8—C7—C31 | 121.6 (4) | O10—C106—C72 | 120.6 (4) |
| C7—C8—C9 | 116.3 (3) | O7—C110—C111 | 108.2 (3) |
| C7—C8—H81 | 108.2 | O7—C110—H1101 | 109.2 |
| C9—C8—H81 | 107.4 | C111—C110—H1101 | 111.0 |
| C7—C8—H82 | 108.3 | O7—C110—H1102 | 109.2 |
| C9—C8—H82 | 107.5 | C111—C110—H1102 | 111.0 |
| H81—C8—H82 | 108.9 | H1101—C110—H1102 | 108.2 |
| C8—C9—C10 | 120.1 (4) | C110—C111—C112 | 109.9 (4) |
| C8—C9—C32 | 122.2 (4) | C110—C111—H1112 | 107.7 |
| C10—C9—C32 | 117.7 (4) | C112—C111—H1112 | 110.9 |
| C9—C10—C11 | 123.2 (4) | C110—C111—H1111 | 109.2 |
| C9—C10—H101 | 118.5 | C112—C111—H1111 | 110.7 |
| C11—C10—H101 | 118.3 | H1112—C111—H1111 | 108.3 |
| C10—C11—C12 | 116.2 (4) | C111—C112—H1123 | 110.9 |
| C10—C11—C55 | 121.6 (4) | C111—C112—H1122 | 110.5 |
| C12—C11—C55 | 122.2 (4) | H1123—C112—H1122 | 107.0 |

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| C11—C12—C13 | 122.9 (4) | C111—C112—H1121 | 112.1 |
| C11—C12—H121 | 119.2 | H1123—C112—H1121 | 108.8 |
| C13—C12—H121 | 117.9 | H1122—C112—H1121 | 107.4 |
| C12—C13—C14 | 120.3 (4) | O8—C113—C114 | 109.1 (3) |
| C12—C13—C32 | 118.0 (4) | O8—C113—H1131 | 110.4 |
| C14—C13—C32 | 121.7 (4) | C114—C113—H1131 | 111.2 |
| C13—C14—C15 | 114.8 (3) | O8—C113—H1132 | 109.7 |
| C13—C14—H141 | 107.7 | C114—C113—H1132 | 108.5 |
| C15—C14—H141 | 108.3 | H1131—C113—H1132 | 107.8 |
| C13—C14—H142 | 108.2 | C113—C114—C115 | 111.6 (4) |
| C15—C14—H142 | 109.3 | C113—C114—H1142 | 109.0 |
| H141—C14—H142 | 108.4 | C115—C114—H1142 | 109.0 |
| C14—C15—C16 | 119.9 (4) | C113—C114—H1141 | 108.5 |
| C14—C15—C33 | 121.1 (4) | C115—C114—H1141 | 110.5 |
| C16—C15—C33 | 119.1 (4) | H1142—C114—H1141 | 108.1 |
| C15—C16—C17 | 122.0 (4) | C114—C115—H1153 | 111.1 |
| C15—C16—H161 | 118.7 | C114—C115—H1152 | 110.8 |
| C17—C16—H161 | 119.3 | H1153—C115—H1152 | 109.2 |
| C16—C17—C18 | 117.0 (4) | C114—C115—H1151 | 108.6 |
| C16—C17—C59 | 122.8 (4) | H1153—C115—H1151 | 108.8 |
| C18—C17—C59 | 120.2 (4) | H1152—C115—H1151 | 108.4 |
| C17—C18—C19 | 123.3 (4) | O9—C116—C117 | 108.9 (3) |
| C17—C18—H181 | 118.8 | O9—C116—H1161 | 110.0 |
| C19—C18—H181 | 118.0 | C117—C116—H1161 | 110.9 |
| C18—C19—C20 | 119.9 (4) | O9—C116—H1162 | 108.8 |
| C18—C19—C33 | 118.0 (4) | C117—C116—H1162 | 109.5 |
| C20—C19—C33 | 122.1 (4) | H1161—C116—H1162 | 108.8 |
| C19—C20—C21 | 112.6 (3) | C116—C117—C118 | 113.4 (4) |
| C19—C20—H202 | 109.3 | C116—C117—H1171 | 108.6 |
| C21—C20—H202 | 108.1 | C118—C117—H1171 | 108.2 |
| C19—C20—H201 | 109.3 | C116—C117—H1172 | 110.3 |
| C21—C20—H201 | 109.4 | C118—C117—H1172 | 109.1 |
| H202—C20—H201 | 108.0 | H1171—C117—H1172 | 107.0 |
| C20—C21—C22 | 120.8 (4) | C117—C118—H1182 | 110.7 |
| C20—C21—C34 | 121.5 (4) | C117—C118—H1181 | 109.9 |
| C22—C21—C34 | 117.8 (4) | H1182—C118—H1181 | 109.1 |
| C21—C22—C23 | 123.3 (4) | C117—C118—H1183 | 109.2 |
| C21—C22—H221 | 118.5 | H1182—C118—H1183 | 109.5 |
| C23—C22—H221 | 118.3 | H1181—C118—H1183 | 108.4 |
| C22—C23—C24 | 116.6 (4) | O10—C119—C120 | 108.9 (3) |
| C22—C23—C63 | 120.0 (4) | O10—C119—H1192 | 110.0 |
| C24—C23—C63 | 123.3 (4) | C120—C119—H1192 | 110.1 |
| C23—C24—C25 | 122.1 (4) | O10—C119—H1191 | 109.0 |
| C23—C24—H241 | 119.4 | C120—C119—H1191 | 110.3 |
| C25—C24—H241 | 118.5 | H1192—C119—H1191 | 108.5 |
| C24—C25—C26 | 119.2 (4) | C119—C120—C121 | 114.0 (4) |
| C24—C25—C34 | 118.3 (4) | C119—C120—H1201 | 108.9 |
| C26—C25—C34 | 122.5 (4) | C121—C120—H1201 | 108.2 |
| C25—C26—C27 | 117.6 (3) | C119—C120—H1202 | 108.3 |

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| C25—C26—H261 | 107.6 | C121—C120—H1202 | 110.2 |
| C27—C26—H261 | 106.1 | H1201—C120—H1202 | 107.1 |
| C25—C26—H262 | 107.3 | C120—C121—H1212 | 111.1 |
| C27—C26—H262 | 108.9 | C120—C121—H1211 | 109.4 |
| H261—C26—H262 | 109.0 | H1212—C121—H1211 | 108.4 |
| C26—C27—C28 | 119.6 (4) | C120—C121—H1213 | 109.3 |
| C26—C27—C35 | 121.7 (4) | H1212—C121—H1213 | 110.1 |
| C28—C27—C35 | 118.6 (4) | H1211—C121—H1213 | 108.4 |
| C27—C28—C29 | 122.8 (4) | C76—C122—C123 | 108.5 (4) |
| C27—C28—H281 | 118.6 | C76—C122—C124 | 112.4 (4) |
| C29—C28—H281 | 118.6 | C123—C122—C124 | 108.6 (4) |
| C28—C29—C30 | 116.7 (4) | C76—C122—C125 | 110.8 (4) |
| C28—C29—C267 | 121.4 (8) | C123—C122—C125 | 108.3 (4) |
| C30—C29—C267 | 121.8 (8) | C124—C122—C125 | 108.2 (4) |
| C28—C29—C30 | 116.7 (4) | C122—C123—H1232 | 110.0 |
| C28—C29—C67 | 122.5 (5) | C122—C123—H1231 | 109.5 |
| C30—C29—C67 | 120.9 (5) | H1232—C123—H1231 | 109.0 |
| C1—C30—C29 | 123.1 (4) | C122—C123—H1233 | 110.5 |
| C1—C30—H301 | 118.5 | H1232—C123—H1233 | 109.9 |
| C29—C30—H301 | 118.3 | H1231—C123—H1233 | 107.9 |
| C7—C31—O1 | 118.0 (3) | C122—C124—H1241 | 109.5 |
| C7—C31—C3 | 121.5 (4) | C122—C124—H1243 | 110.0 |
| O1—C31—C3 | 120.5 (3) | H1241—C124—H1243 | 110.7 |
| C9—C32—O2 | 118.9 (3) | C122—C124—H1242 | 109.3 |
| C9—C32—C13 | 121.6 (4) | H1241—C124—H1242 | 108.4 |
| O2—C32—C13 | 119.5 (4) | H1243—C124—H1242 | 108.9 |
| C15—C33—C19 | 120.7 (4) | C122—C125—H1251 | 110.0 |
| C15—C33—O3 | 119.2 (4) | C122—C125—H1253 | 108.8 |
| C19—C33—O3 | 119.8 (4) | H1251—C125—H1253 | 108.4 |
| O4—C34—C21 | 119.3 (4) | C122—C125—H1252 | 110.7 |
| O4—C34—C25 | 118.9 (4) | H1251—C125—H1252 | 109.2 |
| C21—C34—C25 | 121.7 (4) | H1253—C125—H1252 | 109.6 |
| C1—C35—C27 | 121.4 (4) | C82—C126—C127 | 109.2 (4) |
| C1—C35—O5 | 120.0 (4) | C82—C126—C128 | 112.5 (4) |
| C27—C35—O5 | 118.5 (4) | C127—C126—C128 | 108.0 (4) |
| O2—C39—C40 | 114.3 (4) | C82—C126—C129 | 108.8 (4) |
| O2—C39—H392 | 109.3 | C127—C126—C129 | 109.0 (4) |
| C40—C39—H392 | 109.0 | C128—C126—C129 | 109.2 (4) |
| O2—C39—H391 | 106.7 | C126—C127—H1271 | 110.8 |
| C40—C39—H391 | 108.3 | C126—C127—H1272 | 109.3 |
| H392—C39—H391 | 109.0 | H1271—C127—H1272 | 108.6 |
| C39—C40—C41 | 113.8 (5) | C126—C127—H1273 | 111.0 |
| C39—C40—H401 | 107.6 | H1271—C127—H1273 | 109.3 |
| C41—C40—H401 | 108.9 | H1272—C127—H1273 | 107.8 |
| C39—C40—H402 | 109.2 | C126—C128—H1282 | 110.2 |
| C41—C40—H402 | 108.5 | C126—C128—H1281 | 110.2 |
| H401—C40—H402 | 108.7 | H1282—C128—H1281 | 109.7 |
| C40—C41—H413 | 111.0 | C126—C128—H1283 | 109.9 |
| C40—C41—H412 | 110.7 | H1282—C128—H1283 | 107.6 |

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| H413—C41—H412 | 110.1 | H1281—C128—H1283 | 109.2 |
| C40—C41—H411 | 108.5 | C126—C129—H1292 | 109.5 |
| H413—C41—H411 | 108.6 | C126—C129—H1291 | 109.0 |
| H412—C41—H411 | 107.8 | H1292—C129—H1291 | 108.6 |
| O3—C42—C43 | 109.5 (4) | C126—C129—H1293 | 111.0 |
| O3—C42—H422 | 107.0 | H1292—C129—H1293 | 109.4 |
| C43—C42—H422 | 111.6 | H1291—C129—H1293 | 109.3 |
| O3—C42—H421 | 110.6 | C88—C130—C131 | 108.9 (3) |
| C43—C42—H421 | 110.5 | C88—C130—C132 | 109.4 (3) |
| H422—C42—H421 | 107.6 | C131—C130—C132 | 109.4 (4) |
| C42—C43—C44 | 116.9 (6) | C88—C130—C133 | 112.8 (3) |
| C42—C43—H431 | 109.6 | C131—C130—C133 | 109.0 (4) |
| C44—C43—H431 | 106.0 | C132—C130—C133 | 107.1 (4) |
| C42—C43—H432 | 109.9 | C130—C131—H1311 | 111.8 |
| C44—C43—H432 | 105.9 | C130—C131—H1313 | 109.8 |
| H431—C43—H432 | 108.1 | H1311—C131—H1313 | 107.6 |
| C43—C44—H441 | 110.8 | C130—C131—H1312 | 109.6 |
| C43—C44—H443 | 105.6 | H1311—C131—H1312 | 108.7 |
| H441—C44—H443 | 108.1 | H1313—C131—H1312 | 109.3 |
| C43—C44—H442 | 109.1 | C130—C132—H1321 | 111.4 |
| H441—C44—H442 | 112.7 | C130—C132—H1323 | 110.7 |
| H443—C44—H442 | 110.2 | H1321—C132—H1323 | 107.7 |
| O4—C45—C46 | 108.8 (4) | C130—C132—H1322 | 109.8 |
| O4—C45—H451 | 111.5 | H1321—C132—H1322 | 107.9 |
| C46—C45—H451 | 110.2 | H1323—C132—H1322 | 109.3 |
| O4—C45—H452 | 108.7 | C130—C133—H1331 | 111.1 |
| C46—C45—H452 | 110.0 | C130—C133—H1332 | 111.3 |
| H451—C45—H452 | 107.7 | H1331—C133—H1332 | 108.6 |
| C45—C46—C47 | 111.8 (5) | C130—C133—H1333 | 109.5 |
| C45—C46—H462 | 110.5 | H1331—C133—H1333 | 108.4 |
| C47—C46—H462 | 108.7 | H1332—C133—H1333 | 107.8 |
| C45—C46—H461 | 108.8 | C94—C134—C135 | 107.4 (4) |
| C47—C46—H461 | 108.8 | C94—C134—C136 | 117.2 (5) |
| H462—C46—H461 | 108.1 | C135—C134—C136 | 107.6 (6) |
| C46—C47—H471 | 110.6 | C94—C134—C137 | 110.0 (4) |
| C46—C47—H473 | 109.2 | C135—C134—C137 | 102.6 (5) |
| H471—C47—H473 | 108.9 | C136—C134—C137 | 110.9 (6) |
| C46—C47—H472 | 110.4 | C94—C134—C335 | 106.3 (6) |
| H471—C47—H472 | 109.4 | C94—C134—C336 | 104.2 (6) |
| H473—C47—H472 | 108.3 | C335—C134—C336 | 96.3 (9) |
| O5—C48—C49 | 109.3 (4) | C94—C134—C337 | 115.0 (7) |
| O5—C48—H481 | 109.5 | C335—C134—C337 | 123.9 (11) |
| C49—C48—H481 | 109.4 | C336—C134—C337 | 107.8 (10) |
| O5—C48—H482 | 111.4 | C134—C135—H1352 | 110.9 |
| C49—C48—H482 | 109.7 | C134—C135—H1351 | 109.9 |
| H481—C48—H482 | 107.5 | H1352—C135—H1351 | 108.2 |
| C48—C49—C50 | 109.6 (4) | C134—C135—H1353 | 109.9 |
| C48—C49—H492 | 110.0 | H1352—C135—H1353 | 108.5 |
| C50—C49—H492 | 110.2 | H1351—C135—H1353 | 109.4 |

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| C48—C49—H491 | 108.7 | C134—C136—H1362 | 111.2 |
| C50—C49—H491 | 109.8 | C134—C136—H1361 | 110.4 |
| H492—C49—H491 | 108.6 | H1362—C136—H1361 | 110.3 |
| C49—C50—H501 | 110.3 | C134—C136—H1363 | 109.2 |
| C49—C50—H502 | 109.6 | H1362—C136—H1363 | 107.1 |
| H501—C50—H502 | 107.8 | H1361—C136—H1363 | 108.5 |
| C49—C50—H503 | 109.7 | C134—C137—H1371 | 110.6 |
| H501—C50—H503 | 110.5 | C134—C137—H1373 | 111.3 |
| H502—C50—H503 | 109.0 | H1371—C137—H1373 | 110.5 |
| C5—C51—C52 | 112.4 (3) | C134—C137—H1372 | 107.9 |
| C5—C51—C53 | 108.7 (4) | H1371—C137—H1372 | 107.7 |
| C52—C51—C53 | 107.5 (4) | H1373—C137—H1372 | 108.7 |
| C5—C51—C54 | 109.9 (4) | C134—C335—H3351 | 109.7 |
| C52—C51—C54 | 108.9 (4) | C134—C335—H3353 | 108.0 |
| C53—C51—C54 | 109.4 (4) | H3351—C335—H3353 | 108.4 |
| C51—C52—H522 | 110.5 | C134—C335—H3352 | 110.5 |
| C51—C52—H521 | 109.0 | H3351—C335—H3352 | 110.1 |
| H522—C52—H521 | 109.0 | H3353—C335—H3352 | 110.1 |
| C51—C52—H523 | 110.4 | C134—C336—H3361 | 111.6 |
| H522—C52—H523 | 108.7 | C134—C336—H3362 | 111.2 |
| H521—C52—H523 | 109.2 | H3361—C336—H3362 | 110.4 |
| C51—C53—H532 | 110.4 | C134—C336—H3363 | 108.6 |
| C51—C53—H531 | 110.2 | H3361—C336—H3363 | 107.6 |
| H532—C53—H531 | 108.1 | H3362—C336—H3363 | 107.2 |
| C51—C53—H533 | 110.0 | C134—C337—H3372 | 108.6 |
| H532—C53—H533 | 109.6 | C134—C337—H3371 | 120.5 |
| H531—C53—H533 | 108.5 | H3372—C337—H3371 | 113.4 |
| C51—C54—H543 | 109.9 | C134—C337—H3373 | 105.0 |
| C51—C54—H542 | 110.0 | H3372—C337—H3373 | 97.7 |
| H543—C54—H542 | 108.4 | H3371—C337—H3373 | 108.7 |
| C51—C54—H541 | 109.6 | C102—O6—C107 | 113.0 (9) |
| H543—C54—H541 | 109.7 | C102—O6—C207 | 114.2 (5) |
| H542—C54—H541 | 109.2 | O6—C107—C108 | 112.6 (15) |
| C11—C55—C56 | 108.1 (4) | O6—C107—H1072 | 107.3 |
| C11—C55—C57 | 112.8 (4) | C108—C107—H1072 | 110.9 |
| C56—C55—C57 | 110.5 (5) | O6—C107—H1071 | 110.6 |
| C11—C55—C58 | 111.4 (4) | C108—C107—H1071 | 111.9 |
| C56—C55—C58 | 107.3 (5) | H1072—C107—H1071 | 103.1 |
| C57—C55—C58 | 106.6 (4) | C107—C108—C109 | 99.5 (17) |
| C55—C56—H563 | 109.8 | C107—C108—H1081 | 109.8 |
| C55—C56—H562 | 107.7 | C109—C108—H1081 | 115.8 |
| H563—C56—H562 | 108.9 | C107—C108—H1082 | 109.7 |
| C55—C56—H561 | 109.8 | C109—C108—H1082 | 110.6 |
| H563—C56—H561 | 110.9 | H1081—C108—H1082 | 110.9 |
| H562—C56—H561 | 109.7 | C108—C109—H1093 | 107.2 |
| C55—C57—H571 | 111.0 | C108—C109—H1092 | 108.1 |
| C55—C57—H572 | 109.7 | H1093—C109—H1092 | 110.0 |
| H571—C57—H572 | 108.2 | C108—C109—H1091 | 112.2 |
| C55—C57—H573 | 111.6 | H1093—C109—H1091 | 112.2 |

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| H571—C57—H573 | 108.9 | H1092—C109—H1091 | 107.1 |
| H572—C57—H573 | 107.3 | O6—C207—C208 | 104.1 (8) |
| C55—C58—H582 | 109.5 | O6—C207—H2072 | 112.4 |
| C55—C58—H581 | 109.4 | C208—C207—H2072 | 111.3 |
| H582—C58—H581 | 110.6 | O6—C207—H2071 | 111.9 |
| C55—C58—H583 | 109.7 | C208—C207—H2071 | 106.6 |
| H582—C58—H583 | 109.6 | H2072—C207—H2071 | 110.3 |
| H581—C58—H583 | 108.0 | C207—C208—C209 | 110.5 (10) |
| C17—C59—C60 | 112.1 (4) | C207—C208—H2081 | 112.6 |
| C17—C59—C61 | 109.7 (5) | C209—C208—H2081 | 106.4 |
| C60—C59—C61 | 108.5 (5) | C207—C208—H2082 | 110.6 |
| C17—C59—C62 | 109.2 (4) | C209—C208—H2082 | 111.2 |
| C60—C59—C62 | 106.7 (5) | H2081—C208—H2082 | 105.3 |
| C61—C59—C62 | 110.5 (4) | C208—C209—H2093 | 110.0 |
| C59—C60—H602 | 108.4 | C208—C209—H2092 | 109.9 |
| C59—C60—H601 | 111.8 | H2093—C209—H2092 | 109.6 |
| H602—C60—H601 | 108.8 | C208—C209—H2091 | 109.0 |
| C59—C60—H603 | 111.1 | H2093—C209—H2091 | 110.0 |
| H602—C60—H603 | 108.1 | H2092—C209—H2091 | 108.4 |
| H601—C60—H603 | 108.6 | C100—C138—C139 | 107.9 (6) |
| C59—C61—H613 | 109.6 | C100—C138—C140 | 110.2 (6) |
| C59—C61—H612 | 110.7 | C139—C138—C140 | 108.9 (7) |
| H613—C61—H612 | 110.8 | C100—C138—C141 | 112.7 (6) |
| C59—C61—H611 | 108.3 | C139—C138—C141 | 108.7 (8) |
| H613—C61—H611 | 108.8 | C140—C138—C141 | 108.5 (7) |
| H612—C61—H611 | 108.5 | C138—C139—H1393 | 108.5 |
| C59—C62—H623 | 110.1 | C138—C139—H1392 | 109.7 |
| C59—C62—H622 | 110.0 | H1393—C139—H1392 | 109.0 |
| H623—C62—H622 | 110.0 | C138—C139—H1391 | 109.7 |
| C59—C62—H621 | 111.0 | H1393—C139—H1391 | 109.4 |
| H623—C62—H621 | 107.9 | H1392—C139—H1391 | 110.5 |
| H622—C62—H621 | 107.8 | C138—C140—H1401 | 110.2 |
| C23—C63—C64 | 110.4 (3) | C138—C140—H1402 | 108.6 |
| C23—C63—C65 | 108.1 (4) | H1401—C140—H1402 | 108.7 |
| C64—C63—C65 | 108.9 (4) | C138—C140—H1403 | 110.4 |
| C23—C63—C66 | 112.7 (4) | H1401—C140—H1403 | 108.9 |
| C64—C63—C66 | 108.1 (4) | H1402—C140—H1403 | 110.0 |
| C65—C63—C66 | 108.6 (4) | C138—C141—H1412 | 111.3 |
| C63—C64—H641 | 108.9 | C138—C141—H1411 | 109.1 |
| C63—C64—H642 | 110.2 | H1412—C141—H1411 | 108.3 |
| H641—C64—H642 | 108.7 | C138—C141—H1413 | 110.4 |
| C63—C64—H643 | 109.9 | H1412—C141—H1413 | 108.8 |
| H641—C64—H643 | 109.0 | H1411—C141—H1413 | 108.8 |
| H642—C64—H643 | 110.2 | C100—C338—C339 | 110 (2) |
| C63—C65—H652 | 109.1 | C100—C338—C340 | 111 (2) |
| C63—C65—H651 | 110.3 | C339—C338—C340 | 107 (2) |
| H652—C65—H651 | 108.2 | C100—C338—C341 | 108 (2) |
| C63—C65—H653 | 110.4 | C339—C338—C341 | 109 (3) |
| H652—C65—H653 | 109.0 | C340—C338—C341 | 111 (3) |

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| H651—C65—H653 | 109.8 | C338—C339—H3392 | 106.5 |
| C63—C66—H662 | 109.8 | C338—C339—H3391 | 105.7 |
| C63—C66—H661 | 110.5 | H3392—C339—H3391 | 112.6 |
| H662—C66—H661 | 109.0 | C338—C339—H3393 | 107.6 |
| C63—C66—H663 | 109.7 | H3392—C339—H3393 | 112.3 |
| H662—C66—H663 | 108.7 | H3391—C339—H3393 | 111.5 |
| H661—C66—H663 | 109.3 | C338—C340—H3403 | 106.4 |
| Cl2—C71—Cl1 | 113.0 (4) | C338—C340—H3402 | 105.9 |
| Cl2—C71—H712 | 109.2 | H3403—C340—H3402 | 104.1 |
| Cl1—C71—H712 | 110.4 | C338—C340—H3401 | 114.0 |
| Cl2—C71—H711 | 108.0 | H3403—C340—H3401 | 112.6 |
| Cl1—C71—H711 | 109.8 | H3402—C340—H3401 | 113.1 |
| H712—C71—H711 | 106.1 | C338—C341—H3413 | 110.7 |
| C73—C72—C101 | 119.5 (4) | C338—C341—H3412 | 112.5 |
| C73—C72—C106 | 122.5 (4) | H3413—C341—H3412 | 111.6 |
| C101—C72—C106 | 118.0 (4) | C338—C341—H3411 | 109.0 |
| C72—C73—C74 | 113.7 (3) | H3413—C341—H3411 | 104.8 |
| C72—C73—H731 | 109.0 | H3412—C341—H3411 | 107.9 |
| C74—C73—H731 | 108.8 | C29—C67—C68 | 112.9 (9) |
| C72—C73—H732 | 108.2 | C29—C67—C69 | 109.6 (9) |
| C74—C73—H732 | 109.6 | C68—C67—C69 | 107.8 (10) |
| H731—C73—H732 | 107.4 | C29—C67—C70 | 110.3 (9) |
| C73—C74—C75 | 121.7 (4) | C68—C67—C70 | 107.6 (10) |
| C73—C74—C102 | 120.4 (3) | C69—C67—C70 | 108.5 (9) |
| C75—C74—C102 | 117.9 (4) | C67—C68—H681 | 109.8 |
| C74—C75—C76 | 122.8 (4) | C67—C68—H682 | 111.1 |
| C74—C75—H751 | 118.7 | H681—C68—H682 | 109.7 |
| C76—C75—H751 | 118.4 | C67—C68—H683 | 109.1 |
| C75—C76—C77 | 116.7 (4) | H681—C68—H683 | 108.3 |
| C75—C76—C122 | 119.9 (4) | H682—C68—H683 | 108.7 |
| C77—C76—C122 | 123.4 (4) | C67—C69—H692 | 109.4 |
| C76—C77—C78 | 122.4 (4) | C67—C69—H691 | 110.5 |
| C76—C77—H771 | 119.4 | H692—C69—H691 | 109.3 |
| C78—C77—H771 | 118.2 | C67—C69—H693 | 109.2 |
| C77—C78—C79 | 120.2 (4) | H692—C69—H693 | 109.9 |
| C77—C78—C102 | 118.0 (4) | H691—C69—H693 | 108.6 |
| C79—C78—C102 | 121.7 (4) | C67—C70—H702 | 109.5 |
| C78—C79—C80 | 117.5 (3) | C67—C70—H701 | 110.2 |
| C78—C79—H791 | 108.5 | H702—C70—H701 | 107.6 |
| C80—C79—H791 | 108.6 | C67—C70—H703 | 110.6 |
| C78—C79—H792 | 106.8 | H702—C70—H703 | 109.5 |
| C80—C79—H792 | 107.2 | H701—C70—H703 | 109.4 |
| H791—C79—H792 | 107.9 | C29—C267—C268 | 110.5 (16) |
| C79—C80—C81 | 119.7 (4) | C29—C267—C269 | 111.4 (16) |
| C79—C80—C103 | 122.3 (4) | C268—C267—C269 | 104.5 (17) |
| C81—C80—C103 | 117.9 (4) | C29—C267—C270 | 108.4 (15) |
| C80—C81—C82 | 123.3 (4) | C268—C267—C270 | 111.2 (18) |
| C80—C81—H811 | 117.5 | C269—C267—C270 | 110.7 (17) |
| C82—C81—H811 | 119.2 | C267—C268—H2683 | 114.4 |

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|---------------|-----------|------------------|------------|
| C81—C82—C83 | 116.8 (4) | C267—C268—H2682 | 109.4 |
| C81—C82—C126 | 120.1 (4) | H2683—C268—H2682 | 110.6 |
| C83—C82—C126 | 123.1 (4) | C267—C268—H2681 | 108.0 |
| C82—C83—C84 | 123.3 (4) | H2683—C268—H2681 | 110.1 |
| C82—C83—H831 | 118.5 | H2682—C268—H2681 | 103.7 |
| C84—C83—H831 | 118.2 | C267—C269—H2693 | 112.0 |
| C83—C84—C85 | 121.0 (3) | C267—C269—H2692 | 106.3 |
| C83—C84—C103 | 117.3 (4) | H2693—C269—H2692 | 111.2 |
| C85—C84—C103 | 121.7 (3) | C267—C269—H2691 | 108.2 |
| C84—C85—C86 | 115.9 (3) | H2693—C269—H2691 | 111.2 |
| C84—C85—H851 | 108.3 | H2692—C269—H2691 | 107.7 |
| C86—C85—H851 | 107.5 | C267—C270—H2701 | 113.4 |
| C84—C85—H852 | 108.4 | C267—C270—H2702 | 107.4 |
| C86—C85—H852 | 109.1 | H2701—C270—H2702 | 106.6 |
| H851—C85—H852 | 107.3 | C267—C270—H2703 | 109.9 |
| C85—C86—C87 | 120.4 (3) | H2701—C270—H2703 | 112.5 |
| C85—C86—C104 | 122.3 (3) | H2702—C270—H2703 | 106.6 |
| C87—C86—C104 | 117.3 (3) | O1—C36—C37 | 108.0 (7) |
| C86—C87—C88 | 123.2 (4) | O1—C36—H362 | 110.7 |
| C86—C87—H871 | 118.4 | C37—C36—H362 | 109.7 |
| C88—C87—H871 | 118.4 | O1—C36—H361 | 111.3 |
| C87—C88—C89 | 117.5 (3) | C37—C36—H361 | 110.2 |
| C87—C88—C130 | 119.4 (3) | H362—C36—H361 | 106.9 |
| C89—C88—C130 | 123.1 (4) | C36—C37—C38 | 112.6 (6) |
| C88—C89—C90 | 122.2 (4) | C36—C37—H372 | 109.3 |
| C88—C89—H891 | 119.1 | C38—C37—H372 | 110.4 |
| C90—C89—H891 | 118.7 | C36—C37—H371 | 109.2 |
| C89—C90—C91 | 119.8 (3) | C38—C37—H371 | 109.0 |
| C89—C90—C104 | 118.4 (3) | H372—C37—H371 | 106.2 |
| C91—C90—C104 | 121.6 (3) | C37—C38—H381 | 111.9 |
| C90—C91—C92 | 117.4 (3) | C37—C38—H382 | 110.3 |
| C90—C91—H911 | 108.6 | H381—C38—H382 | 108.4 |
| C92—C91—H911 | 107.0 | C37—C38—H383 | 110.5 |
| C90—C91—H912 | 108.5 | H381—C38—H383 | 107.4 |
| C92—C91—H912 | 108.0 | H382—C38—H383 | 108.2 |
| H911—C91—H912 | 106.9 | O1—C236—C237 | 114.4 (17) |
| C91—C92—C93 | 120.2 (3) | O1—C236—H2362 | 110.8 |
| C91—C92—C105 | 121.8 (3) | C237—C236—H2362 | 112.2 |
| C93—C92—C105 | 117.9 (3) | O1—C236—H2361 | 106.8 |
| C92—C93—C94 | 122.7 (4) | C237—C236—H2361 | 105.9 |
| C92—C93—H931 | 117.6 | H2362—C236—H2361 | 106.1 |
| C94—C93—H931 | 119.7 | C236—C237—C238 | 109.8 (17) |
| C93—C94—C95 | 117.2 (3) | C236—C237—H2372 | 109.1 |
| C93—C94—C134 | 121.1 (4) | C238—C237—H2372 | 105.5 |
| C95—C94—C134 | 121.7 (4) | C236—C237—H2371 | 109.2 |
| C94—C95—C96 | 122.4 (4) | C238—C237—H2371 | 109.1 |
| C94—C95—H951 | 119.2 | H2372—C237—H2371 | 113.9 |
| C96—C95—H951 | 118.4 | C237—C238—H2381 | 110.3 |
| C95—C96—C97 | 119.9 (4) | C237—C238—H2382 | 113.9 |

supplementary materials

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| C95—C96—C105 | 118.0 (4) | H2381—C238—H2382 | 109.2 |
| C97—C96—C105 | 122.1 (3) | C237—C238—H2383 | 109.9 |
| C96—C97—C98 | 112.6 (3) | H2381—C238—H2383 | 105.8 |
| C96—C97—H972 | 109.6 | H2382—C238—H2383 | 107.4 |

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|-----------------|------------|--------------|--------------|----------------|
| C71—H711...O7 | 1.03 | 2.36 | 3.363 (8) | 163 |
| C48—H482...O1 | 0.99 | 2.60 | 3.351 (5) | 134 |
| C110—H1101...O8 | 1.00 | 2.57 | 3.361 (5) | 136 |
| C14—H142...O2 | 1.01 | 2.39 | 2.874 (5) | 109 |
| C120—H1202...O9 | 1.00 | 2.57 | 3.371 (5) | 136 |
| C14—H142...O3 | 1.01 | 2.47 | 2.869 (5) | 103 |
| C73—H731...O6 | 1.00 | 2.42 | 2.862 (5) | 106 |
| C73—H731...O10 | 1.00 | 2.50 | 2.918 (5) | 105 |
| C85—H852...O7 | 1.02 | 2.42 | 2.900 (5) | 108 |
| C85—H852...O8 | 1.02 | 2.46 | 2.924 (5) | 107 |
| C97—H972...O9 | 1.00 | 2.43 | 2.896 (5) | 107 |
| C97—H972...O10 | 1.00 | 2.46 | 2.829 (5) | 101 |
| C38—H382...C11 | 0.97 | 2.92 | 3.795 (5) | 151 |

Fig. 1

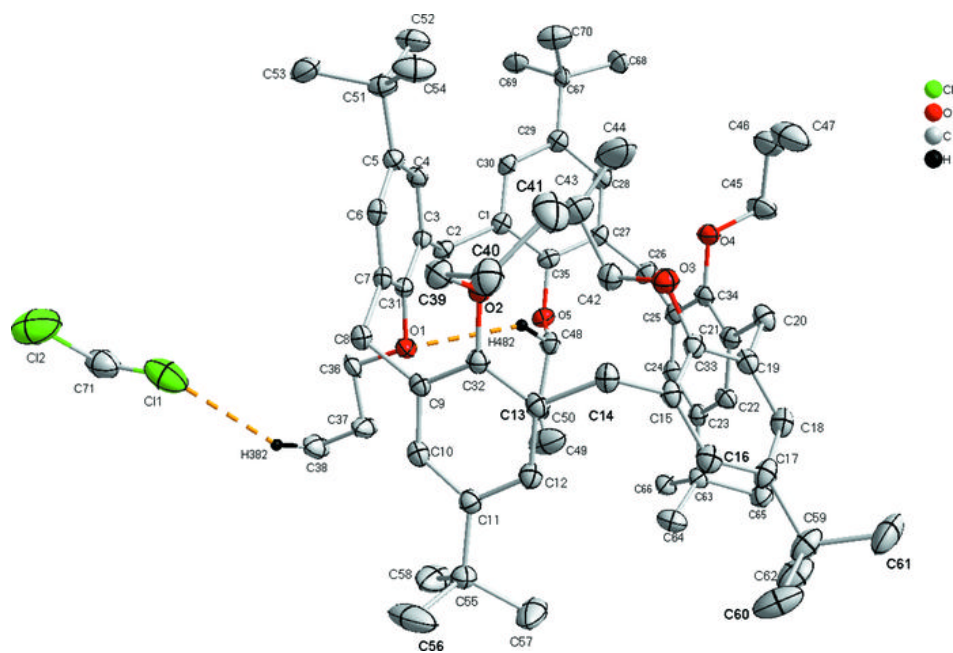


Fig. 2

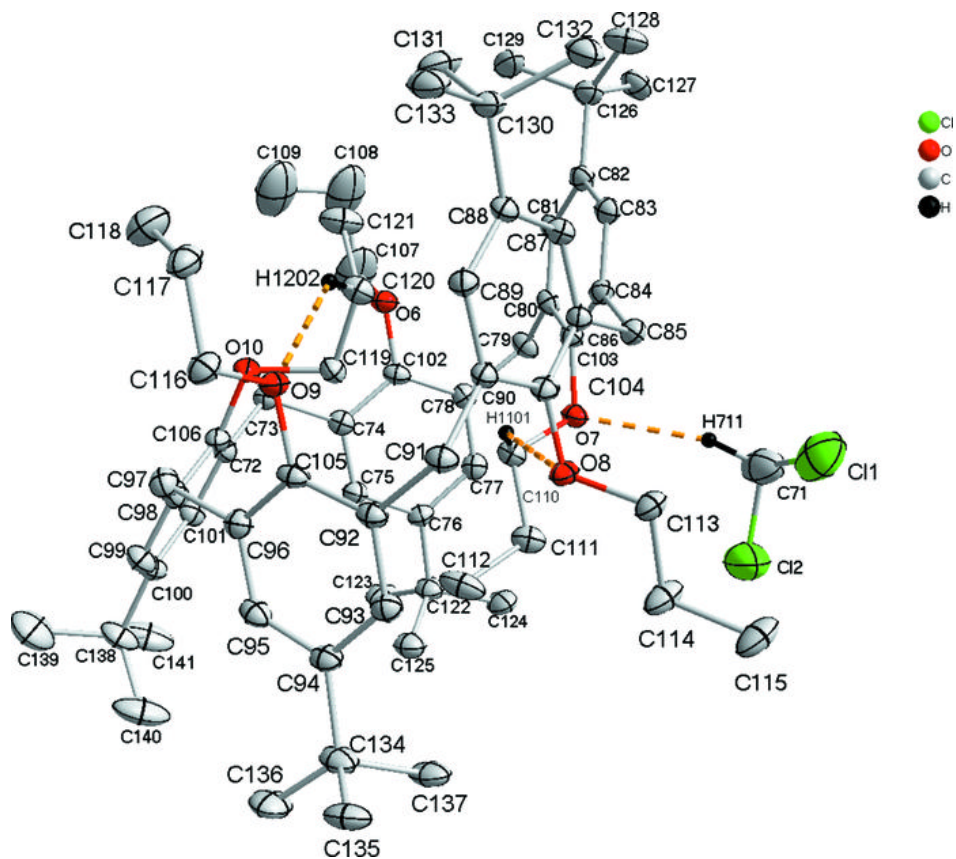


Fig. 3

