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1,3-Alternate conformer 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis(4-methylsulfanylbenzyloxy)-2,8,14,20-tetrathiacalix[4]arene

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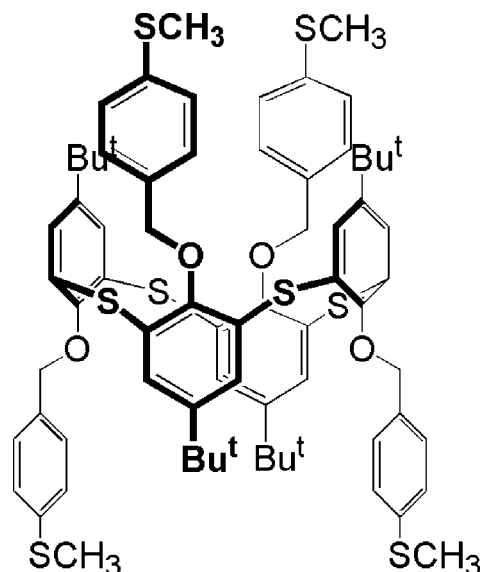
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.059; wR factor = 0.172; data-to-parameter ratio = 15.3.

The title thiacalix[4]arene derivative, $\text{C}_{72}\text{H}_{80}\text{O}_4\text{S}_8$, adopts a 1,3-alternate conformation, where the four 4-methylsulfanylbenzyl groups are located alternately at the two sides of a virtual plane defined by the four bridging S atoms. In the crystal, there are no significant intermolecular interactions present. Some of the peripheral *tert*-butyl and methylsulfanyl groups are disordered over two positions. A region of disordered electron density, occupying voids of ca 700 Å³ for an electron count of 124, was treated using the SQUEEZE routine in *PLATON* [Spek (2009)]. *Acta Cryst.* **D65**, 148–155).

Related literature

For a similar compound adopting a 1,3-alternate conformation, see: Xu *et al.* (2008). For background to thiacalix[4]arene derivatives, see: Kumagai *et al.* (1997); Morohashi *et al.* (2006); Yamato *et al.* (2006). For background to multidentate methylthioethers, see: Maye *et al.* (2005); Lim *et al.* (2007); Yan *et al.* (2010). For the synthesis, see: Morohashi *et al.* (2003).



Experimental

Crystal data

 $\text{C}_{72}\text{H}_{80}\text{O}_4\text{S}_8$
 $M_r = 1265.84$

 Triclinic, $P\bar{1}$
 $a = 15.1863$ (10) Å

 $b = 15.5795$ (11) Å

 $c = 16.9774$ (12) Å

 $\alpha = 75.473$ (2)°

 $\beta = 85.686$ (2)°

 $\gamma = 84.762$ (2)°

 $V = 3866.4$ (5) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 0.27$ mm⁻¹
 $T = 293$ K

 $0.26 \times 0.21 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan

 (*SADABS*; Bruker, 2007)

 $T_{\min} = 0.434$, $T_{\max} = 1.000$

14394 measured reflections

14394 independent reflections

 9034 reflections with $I > 2\sigma(I)$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.059$
 $wR(F^2) = 0.172$
 $S = 0.96$

14394 reflections

939 parameters

244 restraints

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.40$ e Å⁻³
 $\Delta\rho_{\min} = -0.29$ e Å⁻³

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2608).

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supplementary materials

Acta Cryst. (2013). E69, o1009–o1010 [doi:10.1107/S1600536813014827]

1,3-Alternate conformer 5,11,17,23-tetra-*tert*-butyl-25,26,27,28-tetrakis(4-methylsulfanylbenzyloxy)-2,8,14,20-tetrathiacalix[4]arene

Qingsong Gao, Dexun Xie and Delie An

Comment

Thiacalix[4]arenes are macrocyclic molecules made up of *p*-substituted phenolic units linked by sulfur atoms *ortho* to the OH functions (Kumagai *et al.*, 1997). The ability of the parent phenolic thiacalix[4]arenes, as well as of their chemically modified derivatives obtained by the substitution of the phenolic H atoms with various types of ligating groups, to bind metal ions is well established (Morohashi *et al.*, 2006). With thiacalix[4]arenes, the substituents frequently immobilize the molecule in a single conformation: cone, partial cone, 1,2- or 1,3-alternate. The ability to control inter-particle spatial properties of nanoparticle assemblies is one of the major challenges for the design and understanding of functional nanostructures. As a molecular linker, multidentate thioethers have been exploited for such control (Maye *et al.*, 2005). The viability of inter-particle linkages *via* coordination of the methylthio groups of aryethynes to gold surfaces was demonstrated recently in our laboratory (Lim *et al.*, 2007; Yan *et al.*, 2010). Multi-functional groups is the common characteristic of these molecular linkers. The 1,3-alternate conformer thiacalixarene derivative is an ideal molecular linker for assembling nanoparticle clusters. With this in mind, we synthesized the title compound, the first example of a thiacalix[4]arene derivative containing multidentate methylthioethers, and we report herein on its crystal structure.

The molecular structure of the title molecule is shown in Fig 1. The macrocycle adopts a 1,3-alternate conformation in which four substituent groups are located alternately above and below the virtual plane defined by four bridging sulfur atoms, S1–S4. The 1,3-alternate conformation thus appears to be regular and two pairs of opposite phenolic units are almost parallel to each other, but the substituent groups are inclined to one another. Comparable conformations were found in methyl ester derivatives (Xu *et al.*, 2008), whereas the title tetra-benzyl ether derivative is much more distorted as a result of increased steric hindrance.

The plane defined by the substitutional aromatic ring on O4 atom (r.m.s. deviation 0.0177 Å) was chosen as a reference plane. The plane defined by the other substitutional aromatic rings on O atoms (O1, O2 and O3) make dihedral angles of 87.83 (11), 76.84 (11) and 71.78 (13) °, respectively, with this reference plane, whereas the four aromatic rings on the skeleton make dihedral angles of 83.52 (8), 76.20 (8), 84.47 (8) and 83.09 (8) °, respectively, with this reference plane. The conformations of the benzyl ether chains are extended and deviate from the plane defined by four bridging sulfur atoms. Atoms C41, C49, C57 and C65 point towards the exterior of the macrocycle and the torsion angles around the O1—C41, C49—O2, C57—O3 and C65—O4 bonds deviate from ideal *syn* or *anti* values by more than 70°.

In the crystal, there are no significant intermolecular interactions present.

Experimental

A mixture of *p*-tetra-*tert*-butylthiacalix[4]arene (360 mg, 0.50 mmol) and Cs₂CO₃ (1.30 g, 4.00 mmol) in anhydrous acetone (50 ml) was heated at refluxed for 30 min. Then a solution of 4-methylthiobenzyl bromide (864 mg, 4.00 mmol) in acetone (10 ml) was added and the mixture heated at reflux for 2 h. After cooling the reaction mixture, it was filtered.

The filtrate was concentrated and the residue was purified by column chromatography from petroleum ether/dichloromethane (4:1, v/v) to give 410 mg (65%) of compound I as a white solid: M.p. 513~516 K; MS(ESI) m/z: 1283.1 $[M+H_2O]^+$. Spectroscopic data for the title compound is available in the archived CIF. Colourless crystals of the title compound, suitable for X-ray diffraction analysis, were obtained by slow diffusion of petroleum ether into a chloroform solution at 298 K.

Refinement

Some of the peripheral -SCH₃ and *t*-butyl groups are disordered over two positions. These include the S-CH₃ groups involving atoms S5-C48, S6-C56, S7-C64 and S8-C72, and the *t*-butyl groups involving atoms C18-C20, C28-C30 and C38-C40; details are available in the archived CIF. A region of disordered electron density occupying voids of ca. 700 Å³, for an electron count of 124, was treated using the SQUEEZE routine in PLATON (Spek, 2009). It was not taken into consideration during refinement. The C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms: C—H = 0.93–0.97 Å with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and = $1.2U_{eq}(C)$ for other H atoms.

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

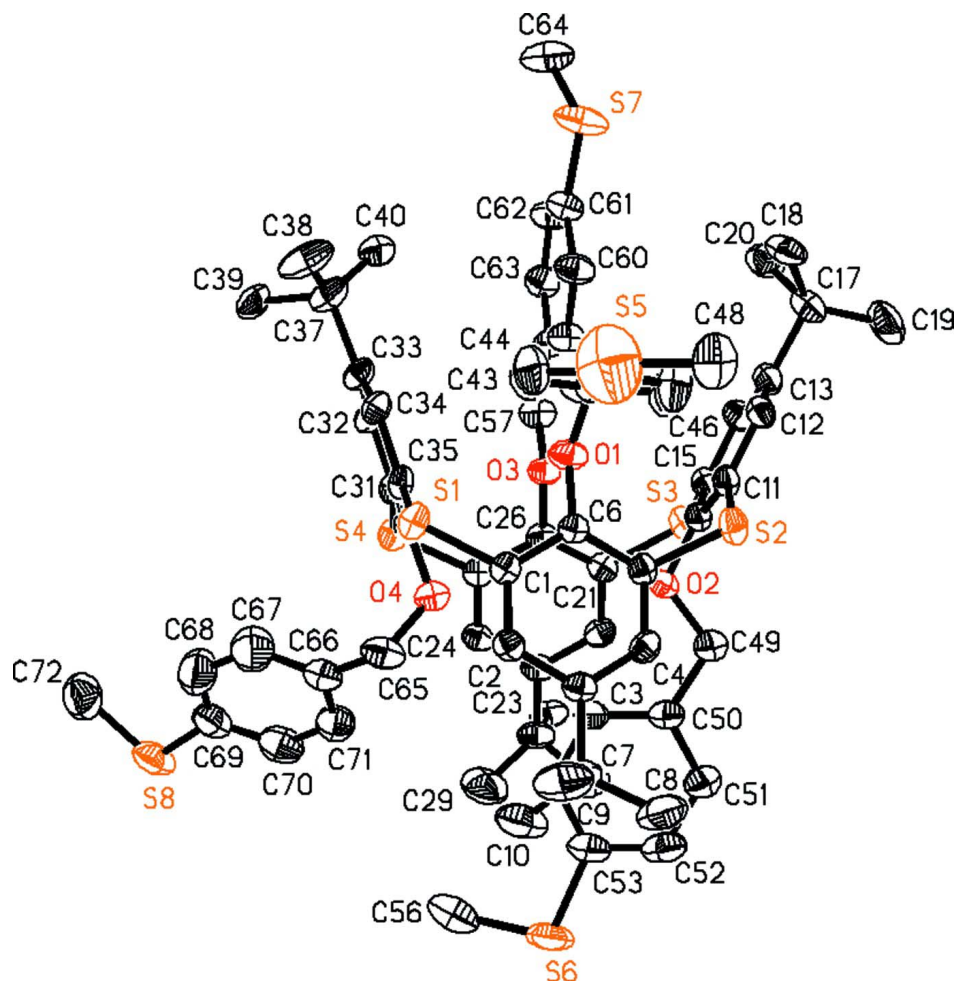


Figure 1

A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. Only the major components of the disordered peripheral groups are shown.

5,11,17,23-Tetra-*tert*-butyl-25,26,27,28-tetrakis(4-methylsulfonylbenzyloxy)-2,8,14,20-tetrathiacalix[4]arene

Crystal data

$C_{72}H_{80}O_4S_8$

$M_r = 1265.84$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 15.1863$ (10) Å

$b = 15.5795$ (11) Å

$c = 16.9774$ (12) Å

$\alpha = 75.473$ (2)°

$\beta = 85.686$ (2)°

$\gamma = 84.762$ (2)°

$V = 3866.4$ (5) Å³

$Z = 2$

$F(000) = 1344$

$D_x = 1.087$ Mg m⁻³

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

Cell parameters from 4356 reflections

$\theta = 4.4\text{--}45.1$ °

$\mu = 0.27$ mm⁻¹

$T = 293$ K

Prismatic, colourless

$0.26 \times 0.21 \times 0.15$ mm

Data collection

| | |
|--|--|
| Bruker SMART CCD area-detector diffractometer | 14394 measured reflections |
| Radiation source: fine-focus sealed tube | 14394 independent reflections |
| Graphite monochromator | 9034 reflections with $I > 2\sigma(I)$ |
| phi and ω scans | $R_{\text{int}} = 0.000$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2007) | $\theta_{\text{max}} = 25.5^\circ$, $\theta_{\text{min}} = 1.4^\circ$ |
| $T_{\text{min}} = 0.434$, $T_{\text{max}} = 1.000$ | $h = -18 \rightarrow 18$ |
| | $k = -18 \rightarrow 18$ |
| | $l = 0 \rightarrow 20$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.059$ | H-atom parameters constrained |
| $wR(F^2) = 0.172$ | $w = 1/[\sigma^2(F_o^2) + (0.1009P)^2]$ |
| $S = 0.96$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 14394 reflections | $(\Delta/\sigma)_{\text{max}} = 0.004$ |
| 939 parameters | $\Delta\rho_{\text{max}} = 0.40 \text{ e } \text{\AA}^{-3}$ |
| 244 restraints | $\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

Special details

Experimental. Spectroscopic data for the title compound:

^1H NMR (400 MHz, CDCl_3): 7.12 (s, 8H), 7.05 (d, $J = 8.4$ Hz, 8H), 6.92 (d, $J = 8.4$ Hz, 8H), 5.04 (s, 8H), 2.48 (s, 12H, SCH_3), 0.86 (s, 36H); ^{13}C NMR (100 MHz, CDCl_3): 156.89 (C), 146.15 (C), 136.67 (C), 134.87 (C), 129.26 (CH), 128.57 (C), 127.69 (CH), 126.95 (CH), 70.65 (CH_2), 33.86 (C), 30.73 (CH_3), 16.31 (SCH_3).

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|-------------|-------------|-------------|----------------------------------|-----------|
| S1 | 0.94198 (4) | 0.90174 (4) | 0.09861 (4) | 0.05036 (19) | |
| S2 | 0.92245 (5) | 0.55348 (5) | 0.07790 (5) | 0.0582 (2) | |
| S3 | 0.55404 (5) | 0.59267 (5) | 0.09846 (5) | 0.0631 (2) | |
| S4 | 0.57286 (4) | 0.93527 (5) | 0.13515 (4) | 0.0541 (2) | |
| S5 | 1.3408 (4) | 0.7583 (4) | -0.0886 (7) | 0.1079 (15) | 0.70 |
| S6 | 0.7412 (5) | 0.5926 (7) | 0.5541 (5) | 0.1038 (18) | 0.50 |
| S7 | 0.7645 (7) | 0.8754 (7) | -0.3436 (5) | 0.101 (2) | 0.50 |
| S8 | 0.5403 (5) | 1.1277 (5) | 0.4157 (3) | 0.0949 (13) | 0.55 |
| C48 | 1.3875 (3) | 0.6516 (4) | -0.0944 (5) | 0.0867 (19) | 0.65 |
| H48A | 1.3728 | 0.6089 | -0.0448 | 0.130* | 0.65 |
| H48B | 1.4507 | 0.6526 | -0.1023 | 0.130* | 0.65 |
| H48C | 1.3644 | 0.6355 | -0.1394 | 0.130* | 0.65 |
| C56 | 0.7113 (9) | 0.7107 (9) | 0.5414 (10) | 0.122 (4) | 0.50 |

| | | | | | |
|------|--------------|--------------|--------------|-------------|------|
| H56A | 0.7601 | 0.7438 | 0.5151 | 0.184* | 0.50 |
| H56B | 0.6971 | 0.7227 | 0.5939 | 0.184* | 0.50 |
| H56C | 0.6608 | 0.7279 | 0.5087 | 0.184* | 0.50 |
| C64 | 0.6894 (8) | 0.9425 (8) | -0.4157 (6) | 0.118 (4) | 0.50 |
| H64A | 0.6667 | 0.9941 | -0.3974 | 0.177* | 0.50 |
| H64B | 0.6413 | 0.9084 | -0.4203 | 0.177* | 0.50 |
| H64C | 0.7203 | 0.9606 | -0.4679 | 0.177* | 0.50 |
| C72 | 0.5345 (9) | 1.2383 (7) | 0.3516 (8) | 0.119 (3) | 0.60 |
| H72D | 0.5930 | 1.2584 | 0.3398 | 0.179* | 0.60 |
| H72E | 0.4987 | 1.2772 | 0.3789 | 0.179* | 0.60 |
| H72F | 0.5086 | 1.2385 | 0.3016 | 0.179* | 0.60 |
| S5' | 1.3463 (11) | 0.7406 (12) | -0.0752 (17) | 0.1084 (16) | 0.30 |
| S6' | 0.7109 (6) | 0.6042 (8) | 0.5530 (6) | 0.122 (3) | 0.50 |
| S7' | 0.7480 (8) | 0.8905 (8) | -0.3466 (5) | 0.117 (3) | 0.50 |
| S8' | 0.5571 (8) | 1.1460 (8) | 0.4075 (6) | 0.140 (4) | 0.45 |
| C48' | 1.3332 (13) | 0.6556 (10) | -0.1267 (10) | 0.138 (5) | 0.35 |
| H48D | 1.3409 | 0.5983 | -0.0894 | 0.207* | 0.35 |
| H48E | 1.3766 | 0.6597 | -0.1714 | 0.207* | 0.35 |
| H48F | 1.2749 | 0.6635 | -0.1470 | 0.207* | 0.35 |
| C56' | 0.7588 (10) | 0.7043 (10) | 0.5410 (10) | 0.138 (5) | 0.50 |
| H56D | 0.7428 | 0.7439 | 0.4901 | 0.208* | 0.50 |
| H56E | 0.8220 | 0.6935 | 0.5412 | 0.208* | 0.50 |
| H56F | 0.7379 | 0.7307 | 0.5850 | 0.208* | 0.50 |
| C64' | 0.6973 (10) | 0.9922 (8) | -0.4005 (8) | 0.143 (5) | 0.50 |
| H64D | 0.6341 | 0.9911 | -0.3922 | 0.215* | 0.50 |
| H64E | 0.7136 | 1.0011 | -0.4576 | 0.215* | 0.50 |
| H64F | 0.7164 | 1.0399 | -0.3812 | 0.215* | 0.50 |
| C72' | 0.5716 (15) | 1.2563 (14) | 0.3432 (17) | 0.174 (11) | 0.40 |
| H72A | 0.6305 | 1.2720 | 0.3472 | 0.260* | 0.40 |
| H72B | 0.5294 | 1.2984 | 0.3607 | 0.260* | 0.40 |
| H72C | 0.5627 | 1.2568 | 0.2877 | 0.260* | 0.40 |
| O1 | 0.89430 (12) | 0.76024 (13) | 0.01849 (11) | 0.0584 (5) | |
| O2 | 0.74105 (12) | 0.60108 (12) | 0.15708 (10) | 0.0515 (4) | |
| O3 | 0.61701 (11) | 0.78218 (12) | 0.04810 (10) | 0.0482 (4) | |
| O4 | 0.75495 (12) | 0.85942 (12) | 0.18907 (11) | 0.0554 (5) | |
| C1 | 0.94462 (15) | 0.78558 (16) | 0.14019 (15) | 0.0422 (6) | |
| C2 | 0.97394 (16) | 0.75315 (17) | 0.21775 (15) | 0.0475 (6) | |
| H2 | 0.9865 | 0.7933 | 0.2470 | 0.057* | |
| C3 | 0.98546 (16) | 0.66224 (18) | 0.25391 (15) | 0.0478 (6) | |
| C4 | 0.96376 (16) | 0.60604 (17) | 0.20888 (16) | 0.0486 (6) | |
| H4 | 0.9686 | 0.5451 | 0.2319 | 0.058* | |
| C5 | 0.93484 (15) | 0.63659 (16) | 0.13047 (15) | 0.0433 (6) | |
| C6 | 0.92664 (15) | 0.72676 (16) | 0.09419 (14) | 0.0410 (6) | |
| C7 | 1.01959 (18) | 0.6293 (2) | 0.34044 (16) | 0.0604 (8) | |
| C8 | 1.0129 (3) | 0.5297 (3) | 0.3732 (2) | 0.1042 (13) | |
| H8A | 0.9520 | 0.5165 | 0.3766 | 0.156* | |
| H8B | 1.0361 | 0.5110 | 0.4264 | 0.156* | |
| H8C | 1.0465 | 0.4987 | 0.3372 | 0.156* | |
| C9 | 1.1168 (2) | 0.6489 (3) | 0.3363 (2) | 0.1014 (13) | |

| | | | | | |
|------|--------------|--------------|---------------|-------------|------|
| H9A | 1.1506 | 0.6166 | 0.3016 | 0.152* | |
| H9B | 1.1387 | 0.6309 | 0.3900 | 0.152* | |
| H9C | 1.1220 | 0.7115 | 0.3148 | 0.152* | |
| C10 | 0.9657 (3) | 0.6748 (3) | 0.3990 (2) | 0.1032 (13) | |
| H10A | 0.9707 | 0.7378 | 0.3814 | 0.155* | |
| H10B | 0.9876 | 0.6529 | 0.4526 | 0.155* | |
| H10C | 0.9048 | 0.6625 | 0.4004 | 0.155* | |
| C11 | 0.81713 (17) | 0.57302 (16) | 0.03584 (16) | 0.0468 (6) | |
| C12 | 0.81386 (18) | 0.56067 (17) | -0.04176 (16) | 0.0513 (7) | |
| H12 | 0.8667 | 0.5513 | -0.0709 | 0.062* | |
| C13 | 0.73439 (19) | 0.56175 (18) | -0.07774 (16) | 0.0536 (7) | |
| C14 | 0.65774 (18) | 0.57739 (19) | -0.03304 (16) | 0.0545 (7) | |
| H14 | 0.6035 | 0.5799 | -0.0559 | 0.065* | |
| C15 | 0.65889 (17) | 0.58959 (17) | 0.04548 (16) | 0.0494 (6) | |
| C16 | 0.73887 (17) | 0.58747 (16) | 0.08053 (15) | 0.0455 (6) | |
| C17 | 0.7309 (2) | 0.5441 (2) | -0.16228 (19) | 0.0693 (9) | |
| C18 | 0.8077 (14) | 0.5946 (9) | -0.2193 (10) | 0.079 (3) | 0.50 |
| H18A | 0.8642 | 0.5692 | -0.1993 | 0.119* | 0.50 |
| H18B | 0.8012 | 0.6565 | -0.2193 | 0.119* | 0.50 |
| H18C | 0.8042 | 0.5885 | -0.2739 | 0.119* | 0.50 |
| C19 | 0.7130 (6) | 0.4463 (7) | -0.1505 (7) | 0.099 (3) | 0.60 |
| H19A | 0.7058 | 0.4348 | -0.2026 | 0.148* | 0.60 |
| H19B | 0.6599 | 0.4340 | -0.1166 | 0.148* | 0.60 |
| H19C | 0.7619 | 0.4089 | -0.1251 | 0.148* | 0.60 |
| C20 | 0.6510 (10) | 0.6081 (7) | -0.2097 (9) | 0.081 (3) | 0.50 |
| H20A | 0.6626 | 0.6692 | -0.2167 | 0.121* | 0.50 |
| H20B | 0.5962 | 0.5966 | -0.1784 | 0.121* | 0.50 |
| H20C | 0.6471 | 0.5962 | -0.2621 | 0.121* | 0.50 |
| C18' | 0.8117 (15) | 0.5609 (9) | -0.2147 (12) | 0.095 (5) | 0.50 |
| H18D | 0.8041 | 0.5475 | -0.2659 | 0.143* | 0.50 |
| H18E | 0.8606 | 0.5239 | -0.1887 | 0.143* | 0.50 |
| H18F | 0.8235 | 0.6222 | -0.2240 | 0.143* | 0.50 |
| C19' | 0.7610 (10) | 0.4428 (12) | -0.1482 (11) | 0.112 (5) | 0.40 |
| H19D | 0.7581 | 0.4249 | -0.1981 | 0.169* | 0.40 |
| H19E | 0.7226 | 0.4089 | -0.1068 | 0.169* | 0.40 |
| H19F | 0.8207 | 0.4325 | -0.1312 | 0.169* | 0.40 |
| C20' | 0.6462 (10) | 0.5704 (7) | -0.1996 (9) | 0.087 (3) | 0.50 |
| H20D | 0.6358 | 0.6339 | -0.2119 | 0.131* | 0.50 |
| H20E | 0.5997 | 0.5438 | -0.1625 | 0.131* | 0.50 |
| H20F | 0.6471 | 0.5507 | -0.2489 | 0.131* | 0.50 |
| C21 | 0.55120 (16) | 0.67324 (18) | 0.15619 (15) | 0.0480 (6) | |
| C22 | 0.51071 (17) | 0.64880 (19) | 0.23451 (16) | 0.0524 (7) | |
| H22 | 0.4942 | 0.5910 | 0.2547 | 0.063* | |
| C23 | 0.49475 (16) | 0.70917 (19) | 0.28255 (15) | 0.0506 (7) | |
| C24 | 0.52130 (16) | 0.79369 (19) | 0.25020 (15) | 0.0485 (6) | |
| H24 | 0.5121 | 0.8350 | 0.2817 | 0.058* | |
| C25 | 0.56121 (15) | 0.81970 (17) | 0.17237 (15) | 0.0448 (6) | |
| C26 | 0.57623 (15) | 0.75879 (17) | 0.12452 (14) | 0.0432 (6) | |
| C27 | 0.4468 (2) | 0.6825 (2) | 0.36633 (17) | 0.0648 (8) | |

| | | | | | |
|------|--------------|--------------|---------------|-------------|------|
| C28 | 0.4834 (8) | 0.5980 (8) | 0.4150 (7) | 0.078 (3) | 0.55 |
| H28A | 0.4491 | 0.5821 | 0.4657 | 0.118* | 0.55 |
| H28B | 0.5436 | 0.6033 | 0.4257 | 0.118* | 0.55 |
| H28C | 0.4817 | 0.5528 | 0.3859 | 0.118* | 0.55 |
| C29 | 0.4863 (8) | 0.7236 (9) | 0.4259 (8) | 0.120 (4) | 0.50 |
| H29A | 0.4622 | 0.6988 | 0.4800 | 0.180* | 0.50 |
| H29B | 0.4723 | 0.7867 | 0.4117 | 0.180* | 0.50 |
| H29C | 0.5494 | 0.7113 | 0.4240 | 0.180* | 0.50 |
| C30 | 0.3469 (7) | 0.6736 (6) | 0.3514 (6) | 0.063 (2) | 0.55 |
| H30A | 0.3438 | 0.6265 | 0.3247 | 0.095* | 0.55 |
| H30B | 0.3228 | 0.7284 | 0.3176 | 0.095* | 0.55 |
| H30C | 0.3135 | 0.6604 | 0.4027 | 0.095* | 0.55 |
| C28' | 0.4615 (12) | 0.5716 (11) | 0.4032 (12) | 0.107 (6) | 0.45 |
| H28D | 0.5218 | 0.5519 | 0.3921 | 0.161* | 0.45 |
| H28E | 0.4227 | 0.5428 | 0.3776 | 0.161* | 0.45 |
| H28F | 0.4482 | 0.5569 | 0.4610 | 0.161* | 0.45 |
| C29' | 0.4421 (7) | 0.7589 (7) | 0.4124 (7) | 0.096 (3) | 0.50 |
| H29D | 0.4133 | 0.7393 | 0.4654 | 0.144* | 0.50 |
| H29E | 0.4092 | 0.8105 | 0.3818 | 0.144* | 0.50 |
| H29F | 0.5010 | 0.7735 | 0.4180 | 0.144* | 0.50 |
| C30' | 0.3535 (11) | 0.7105 (9) | 0.3632 (10) | 0.100 (5) | 0.45 |
| H30D | 0.3283 | 0.6887 | 0.3225 | 0.150* | 0.45 |
| H30E | 0.3459 | 0.7743 | 0.3498 | 0.150* | 0.45 |
| H30F | 0.3242 | 0.6872 | 0.4154 | 0.150* | 0.45 |
| C31 | 0.67539 (16) | 0.94933 (16) | 0.07791 (16) | 0.0457 (6) | |
| C32 | 0.67360 (17) | 1.00449 (17) | 0.00043 (17) | 0.0520 (7) | |
| H32 | 0.6191 | 1.0264 | -0.0209 | 0.062* | |
| C33 | 0.75021 (17) | 1.02849 (17) | -0.04684 (16) | 0.0506 (7) | |
| C34 | 0.82966 (16) | 0.99078 (16) | -0.01344 (16) | 0.0465 (6) | |
| H34 | 0.8823 | 1.0034 | -0.0443 | 0.056* | |
| C35 | 0.83338 (15) | 0.93503 (15) | 0.06423 (16) | 0.0424 (6) | |
| C36 | 0.75657 (16) | 0.91547 (15) | 0.11223 (15) | 0.0424 (6) | |
| C37 | 0.7462 (2) | 1.0937 (2) | -0.13094 (19) | 0.0690 (9) | |
| C38 | 0.8285 (5) | 1.1254 (7) | -0.1654 (6) | 0.100 (3) | 0.50 |
| H38A | 0.8696 | 1.0759 | -0.1697 | 0.151* | 0.50 |
| H38B | 0.8513 | 1.1579 | -0.1313 | 0.151* | 0.50 |
| H38C | 0.8203 | 1.1637 | -0.2187 | 0.151* | 0.50 |
| C39 | 0.6820 (5) | 1.1826 (4) | -0.1164 (4) | 0.0743 (19) | 0.50 |
| H39A | 0.6760 | 1.2258 | -0.1675 | 0.112* | 0.50 |
| H39B | 0.7086 | 1.2082 | -0.0790 | 0.112* | 0.50 |
| H39C | 0.6245 | 1.1645 | -0.0944 | 0.112* | 0.50 |
| C40 | 0.6885 (7) | 1.0612 (6) | -0.1841 (6) | 0.077 (3) | 0.60 |
| H40A | 0.6291 | 1.0590 | -0.1605 | 0.116* | 0.60 |
| H40B | 0.7109 | 1.0028 | -0.1884 | 0.116* | 0.60 |
| H40C | 0.6888 | 1.1010 | -0.2374 | 0.116* | 0.60 |
| C38' | 0.8304 (6) | 1.0565 (6) | -0.1917 (4) | 0.092 (2) | 0.50 |
| H38D | 0.8247 | 0.9951 | -0.1898 | 0.138* | 0.50 |
| H38E | 0.8867 | 1.0626 | -0.1722 | 0.138* | 0.50 |
| H38F | 0.8266 | 1.0912 | -0.2469 | 0.138* | 0.50 |

| | | | | | |
|------|--------------|--------------|---------------|-------------|------|
| C39' | 0.7743 (8) | 1.1786 (5) | -0.1287 (5) | 0.110 (3) | 0.50 |
| H39D | 0.7749 | 1.2171 | -0.1826 | 0.166* | 0.50 |
| H39E | 0.8327 | 1.1709 | -0.1087 | 0.166* | 0.50 |
| H39F | 0.7339 | 1.2046 | -0.0933 | 0.166* | 0.50 |
| C40' | 0.6673 (10) | 1.0938 (10) | -0.1712 (10) | 0.093 (5) | 0.40 |
| H40D | 0.6777 | 1.1173 | -0.2288 | 0.140* | 0.40 |
| H40E | 0.6210 | 1.1301 | -0.1509 | 0.140* | 0.40 |
| H40F | 0.6500 | 1.0341 | -0.1611 | 0.140* | 0.40 |
| C41 | 0.9429 (2) | 0.7617 (3) | -0.05348 (19) | 0.0923 (12) | |
| H41A | 0.9234 | 0.8159 | -0.0924 | 0.111* | |
| H41B | 0.9263 | 0.7125 | -0.0733 | 0.111* | |
| C42 | 1.04093 (19) | 0.7569 (2) | -0.05638 (16) | 0.0562 (7) | |
| C43 | 1.0881 (2) | 0.8287 (2) | -0.0609 (2) | 0.0734 (9) | |
| H43 | 1.0571 | 0.8819 | -0.0570 | 0.088* | |
| C44 | 1.1777 (2) | 0.8264 (2) | -0.0708 (2) | 0.0770 (9) | |
| H44 | 1.2062 | 0.8780 | -0.0755 | 0.092* | |
| C45 | 1.2255 (2) | 0.7502 (2) | -0.07393 (19) | 0.0663 (8) | |
| C46 | 1.1828 (2) | 0.6758 (2) | -0.0680 (2) | 0.0847 (11) | |
| H46 | 1.2149 | 0.6226 | -0.0702 | 0.102* | |
| C47 | 1.0911 (2) | 0.6795 (2) | -0.0585 (2) | 0.0836 (10) | |
| H47 | 1.0627 | 0.6278 | -0.0534 | 0.100* | |
| C49 | 0.7374 (2) | 0.5227 (2) | 0.22128 (18) | 0.0722 (9) | |
| H49A | 0.7884 | 0.4819 | 0.2158 | 0.087* | |
| H49B | 0.6844 | 0.4935 | 0.2185 | 0.087* | |
| C50 | 0.73654 (19) | 0.5463 (2) | 0.30111 (16) | 0.0590 (7) | |
| C51 | 0.7421 (2) | 0.4787 (2) | 0.3715 (2) | 0.0797 (10) | |
| H51 | 0.7469 | 0.4199 | 0.3679 | 0.096* | |
| C52 | 0.7408 (3) | 0.4970 (3) | 0.4467 (2) | 0.0885 (11) | |
| H52 | 0.7463 | 0.4504 | 0.4929 | 0.106* | |
| C53 | 0.7316 (2) | 0.5822 (3) | 0.45457 (18) | 0.0762 (10) | |
| C54 | 0.7265 (2) | 0.6505 (2) | 0.38446 (18) | 0.0738 (9) | |
| H54 | 0.7215 | 0.7093 | 0.3884 | 0.089* | |
| C55 | 0.7288 (2) | 0.6322 (2) | 0.30871 (17) | 0.0635 (8) | |
| H55 | 0.7250 | 0.6789 | 0.2623 | 0.076* | |
| C57 | 0.55681 (18) | 0.8144 (2) | -0.01567 (16) | 0.0621 (8) | |
| H57A | 0.5263 | 0.8702 | -0.0101 | 0.074* | |
| H57B | 0.5129 | 0.7718 | -0.0119 | 0.074* | |
| C58 | 0.60755 (17) | 0.82777 (18) | -0.09687 (15) | 0.0498 (6) | |
| C59 | 0.69751 (18) | 0.8091 (2) | -0.10537 (17) | 0.0595 (8) | |
| H59 | 0.7297 | 0.7851 | -0.0594 | 0.071* | |
| C60 | 0.7401 (2) | 0.8257 (2) | -0.18123 (18) | 0.0677 (9) | |
| H60 | 0.8009 | 0.8121 | -0.1860 | 0.081* | |
| C61 | 0.6942 (2) | 0.8625 (2) | -0.25093 (17) | 0.0671 (8) | |
| C62 | 0.6036 (2) | 0.8789 (2) | -0.24219 (18) | 0.0712 (9) | |
| H62 | 0.5710 | 0.9016 | -0.2881 | 0.085* | |
| C63 | 0.56160 (19) | 0.8621 (2) | -0.16682 (18) | 0.0613 (8) | |
| H63 | 0.5005 | 0.8739 | -0.1621 | 0.074* | |
| C65 | 0.7901 (2) | 0.8914 (2) | 0.25194 (18) | 0.0726 (9) | |
| H65A | 0.8429 | 0.9217 | 0.2296 | 0.087* | |

| | | | | |
|------|------------|------------|--------------|-------------|
| H65B | 0.8078 | 0.8408 | 0.2955 | 0.087* |
| C66 | 0.7271 (2) | 0.9535 (2) | 0.28716 (18) | 0.0674 (8) |
| C67 | 0.7308 (4) | 1.0429 (3) | 0.2639 (3) | 0.1251 (17) |
| H67 | 0.7725 | 1.0668 | 0.2233 | 0.150* |
| C68 | 0.6738 (4) | 1.1006 (3) | 0.2991 (3) | 0.1278 (18) |
| H68 | 0.6770 | 1.1617 | 0.2802 | 0.153* |
| C69 | 0.6153 (3) | 1.0692 (3) | 0.3591 (2) | 0.0833 (10) |
| C70 | 0.6075 (3) | 0.9797 (3) | 0.3810 (2) | 0.0950 (12) |
| H70 | 0.5643 | 0.9567 | 0.4204 | 0.114* |
| C71 | 0.6625 (3) | 0.9227 (3) | 0.3458 (2) | 0.0841 (10) |
| H71 | 0.6556 | 0.8620 | 0.3623 | 0.101* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| S1 | 0.0351 (3) | 0.0425 (4) | 0.0712 (5) | -0.0045 (3) | -0.0091 (3) | -0.0073 (3) |
| S2 | 0.0531 (4) | 0.0521 (4) | 0.0765 (5) | 0.0083 (3) | -0.0126 (4) | -0.0308 (4) |
| S3 | 0.0511 (4) | 0.0731 (5) | 0.0756 (5) | -0.0196 (4) | 0.0114 (4) | -0.0365 (4) |
| S4 | 0.0399 (4) | 0.0493 (4) | 0.0695 (5) | 0.0021 (3) | 0.0070 (3) | -0.0126 (3) |
| S5 | 0.0590 (11) | 0.091 (3) | 0.175 (4) | -0.0079 (15) | 0.0024 (14) | -0.037 (3) |
| S6 | 0.135 (5) | 0.135 (3) | 0.0394 (16) | 0.007 (3) | -0.019 (3) | -0.0198 (15) |
| S7 | 0.095 (3) | 0.167 (5) | 0.043 (2) | -0.012 (4) | 0.0104 (16) | -0.031 (3) |
| S8 | 0.108 (2) | 0.119 (3) | 0.0641 (16) | 0.021 (3) | -0.0073 (16) | -0.0442 (16) |
| C48 | 0.039 (3) | 0.095 (4) | 0.123 (5) | 0.021 (3) | -0.015 (3) | -0.029 (3) |
| C56 | 0.137 (9) | 0.165 (9) | 0.080 (6) | -0.016 (7) | -0.008 (7) | -0.057 (6) |
| C64 | 0.134 (7) | 0.149 (8) | 0.054 (5) | -0.018 (7) | -0.003 (5) | 0.008 (5) |
| C72 | 0.137 (7) | 0.102 (6) | 0.127 (6) | -0.001 (5) | 0.010 (6) | -0.049 (5) |
| S5' | 0.0595 (13) | 0.092 (3) | 0.175 (4) | -0.0095 (18) | 0.0015 (16) | -0.037 (3) |
| S6' | 0.135 (5) | 0.177 (6) | 0.056 (2) | -0.021 (4) | 0.000 (3) | -0.029 (3) |
| S7' | 0.122 (5) | 0.152 (4) | 0.057 (2) | 0.019 (3) | 0.024 (2) | -0.005 (2) |
| S8' | 0.159 (6) | 0.146 (6) | 0.137 (5) | -0.001 (4) | 0.007 (3) | -0.083 (4) |
| C48' | 0.182 (10) | 0.106 (8) | 0.129 (9) | -0.016 (8) | 0.038 (8) | -0.048 (7) |
| C56' | 0.163 (10) | 0.179 (9) | 0.089 (7) | -0.013 (8) | -0.005 (8) | -0.064 (6) |
| C64' | 0.173 (9) | 0.127 (8) | 0.106 (8) | -0.023 (7) | 0.009 (6) | 0.013 (6) |
| C72' | 0.178 (14) | 0.166 (13) | 0.180 (13) | 0.000 (9) | -0.003 (9) | -0.056 (9) |
| O1 | 0.0476 (11) | 0.0799 (14) | 0.0445 (11) | 0.0093 (9) | -0.0129 (9) | -0.0113 (9) |
| O2 | 0.0602 (11) | 0.0554 (11) | 0.0418 (10) | -0.0062 (9) | -0.0020 (8) | -0.0172 (8) |
| O3 | 0.0394 (9) | 0.0626 (11) | 0.0409 (10) | -0.0054 (8) | 0.0035 (8) | -0.0106 (8) |
| O4 | 0.0515 (11) | 0.0623 (12) | 0.0476 (11) | -0.0014 (9) | -0.0024 (9) | -0.0056 (9) |
| C1 | 0.0311 (12) | 0.0451 (14) | 0.0496 (15) | -0.0011 (10) | -0.0043 (11) | -0.0101 (11) |
| C2 | 0.0410 (14) | 0.0534 (16) | 0.0506 (16) | -0.0024 (12) | -0.0082 (12) | -0.0160 (12) |
| C3 | 0.0381 (14) | 0.0607 (17) | 0.0433 (14) | 0.0025 (12) | -0.0055 (11) | -0.0117 (13) |
| C4 | 0.0439 (14) | 0.0442 (15) | 0.0536 (16) | 0.0030 (12) | -0.0050 (12) | -0.0059 (12) |
| C5 | 0.0381 (13) | 0.0429 (14) | 0.0500 (15) | 0.0031 (11) | -0.0071 (11) | -0.0143 (12) |
| C6 | 0.0313 (12) | 0.0483 (15) | 0.0429 (14) | 0.0001 (11) | -0.0041 (10) | -0.0110 (11) |
| C7 | 0.0507 (16) | 0.079 (2) | 0.0449 (16) | 0.0031 (15) | -0.0125 (13) | -0.0036 (14) |
| C8 | 0.126 (3) | 0.105 (3) | 0.066 (2) | -0.009 (2) | -0.021 (2) | 0.012 (2) |
| C9 | 0.066 (2) | 0.150 (4) | 0.078 (2) | -0.014 (2) | -0.0329 (19) | 0.004 (2) |
| C10 | 0.107 (3) | 0.147 (4) | 0.055 (2) | 0.019 (3) | -0.009 (2) | -0.033 (2) |
| C11 | 0.0506 (15) | 0.0406 (14) | 0.0527 (16) | -0.0048 (12) | -0.0048 (13) | -0.0171 (12) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C12 | 0.0526 (16) | 0.0503 (16) | 0.0545 (16) | -0.0058 (13) | 0.0058 (13) | -0.0213 (13) |
| C13 | 0.0592 (17) | 0.0534 (16) | 0.0524 (16) | -0.0065 (13) | -0.0007 (14) | -0.0210 (13) |
| C14 | 0.0511 (16) | 0.0656 (18) | 0.0531 (16) | -0.0071 (14) | -0.0069 (13) | -0.0242 (14) |
| C15 | 0.0513 (16) | 0.0484 (15) | 0.0513 (16) | -0.0064 (12) | 0.0015 (13) | -0.0178 (12) |
| C16 | 0.0523 (16) | 0.0412 (14) | 0.0448 (15) | -0.0061 (12) | -0.0003 (12) | -0.0138 (11) |
| C17 | 0.074 (2) | 0.085 (2) | 0.0605 (19) | -0.0099 (18) | -0.0001 (17) | -0.0375 (17) |
| C18 | 0.094 (6) | 0.100 (8) | 0.046 (4) | -0.006 (7) | 0.012 (4) | -0.030 (5) |
| C19 | 0.118 (6) | 0.102 (5) | 0.100 (5) | -0.004 (5) | -0.028 (5) | -0.065 (4) |
| C20 | 0.093 (5) | 0.095 (6) | 0.061 (5) | -0.002 (5) | -0.017 (4) | -0.029 (5) |
| C18' | 0.102 (7) | 0.110 (9) | 0.083 (7) | -0.019 (7) | 0.007 (5) | -0.041 (7) |
| C19' | 0.143 (10) | 0.117 (8) | 0.101 (8) | -0.020 (8) | 0.001 (8) | -0.071 (6) |
| C20' | 0.096 (6) | 0.108 (7) | 0.069 (5) | -0.015 (6) | -0.019 (4) | -0.038 (5) |
| C21 | 0.0399 (14) | 0.0571 (17) | 0.0487 (15) | -0.0077 (12) | 0.0011 (12) | -0.0156 (12) |
| C22 | 0.0465 (15) | 0.0551 (17) | 0.0519 (16) | -0.0114 (13) | 0.0041 (13) | -0.0057 (13) |
| C23 | 0.0389 (14) | 0.0682 (19) | 0.0425 (14) | -0.0038 (13) | 0.0006 (11) | -0.0105 (13) |
| C24 | 0.0389 (14) | 0.0627 (18) | 0.0449 (15) | 0.0000 (12) | 0.0012 (12) | -0.0172 (13) |
| C25 | 0.0329 (13) | 0.0538 (16) | 0.0464 (15) | -0.0013 (11) | -0.0017 (11) | -0.0107 (12) |
| C26 | 0.0306 (12) | 0.0554 (16) | 0.0407 (14) | -0.0043 (11) | 0.0049 (11) | -0.0083 (12) |
| C27 | 0.0577 (18) | 0.088 (2) | 0.0436 (16) | -0.0090 (16) | 0.0098 (14) | -0.0090 (15) |
| C28 | 0.075 (5) | 0.090 (6) | 0.051 (4) | -0.001 (5) | 0.007 (4) | 0.015 (4) |
| C29 | 0.143 (8) | 0.148 (9) | 0.070 (6) | -0.033 (7) | 0.037 (6) | -0.033 (6) |
| C30 | 0.042 (3) | 0.087 (6) | 0.049 (4) | -0.005 (4) | 0.010 (3) | 0.003 (4) |
| C28' | 0.118 (10) | 0.100 (9) | 0.084 (8) | -0.001 (7) | 0.015 (7) | 0.005 (6) |
| C29' | 0.110 (7) | 0.120 (7) | 0.064 (5) | -0.028 (5) | 0.030 (5) | -0.038 (5) |
| C30' | 0.083 (7) | 0.112 (9) | 0.085 (7) | 0.008 (7) | 0.018 (5) | 0.001 (6) |
| C31 | 0.0368 (13) | 0.0401 (14) | 0.0599 (17) | -0.0021 (11) | -0.0015 (12) | -0.0123 (12) |
| C32 | 0.0381 (14) | 0.0443 (15) | 0.0677 (18) | -0.0015 (12) | -0.0080 (13) | -0.0021 (13) |
| C33 | 0.0462 (15) | 0.0424 (15) | 0.0587 (17) | -0.0123 (12) | -0.0104 (13) | 0.0012 (12) |
| C34 | 0.0380 (13) | 0.0410 (14) | 0.0570 (16) | -0.0083 (11) | 0.0004 (12) | -0.0045 (12) |
| C35 | 0.0350 (13) | 0.0339 (13) | 0.0593 (16) | -0.0024 (10) | -0.0071 (12) | -0.0119 (12) |
| C36 | 0.0434 (14) | 0.0355 (13) | 0.0477 (15) | -0.0004 (11) | -0.0055 (12) | -0.0093 (11) |
| C37 | 0.0621 (19) | 0.065 (2) | 0.069 (2) | -0.0211 (16) | -0.0154 (16) | 0.0133 (16) |
| C38 | 0.061 (4) | 0.118 (6) | 0.089 (5) | -0.018 (5) | 0.000 (4) | 0.039 (5) |
| C39 | 0.093 (5) | 0.048 (3) | 0.071 (4) | 0.007 (3) | -0.021 (4) | 0.007 (3) |
| C40 | 0.107 (7) | 0.067 (4) | 0.054 (4) | -0.006 (4) | -0.016 (4) | -0.004 (3) |
| C38' | 0.095 (5) | 0.107 (6) | 0.061 (4) | 0.005 (5) | -0.013 (4) | 0.001 (4) |
| C39' | 0.161 (7) | 0.070 (5) | 0.085 (5) | -0.021 (5) | 0.000 (5) | 0.012 (4) |
| C40' | 0.065 (6) | 0.108 (9) | 0.089 (8) | -0.010 (6) | -0.021 (5) | 0.015 (7) |
| C41 | 0.062 (2) | 0.162 (4) | 0.0470 (19) | -0.015 (2) | -0.0070 (16) | -0.011 (2) |
| C42 | 0.0555 (17) | 0.071 (2) | 0.0429 (15) | -0.0130 (15) | -0.0041 (13) | -0.0116 (14) |
| C43 | 0.071 (2) | 0.069 (2) | 0.083 (2) | 0.0003 (18) | 0.0100 (18) | -0.0301 (17) |
| C44 | 0.067 (2) | 0.067 (2) | 0.106 (3) | -0.0133 (17) | 0.0039 (19) | -0.0374 (19) |
| C45 | 0.0644 (19) | 0.0563 (19) | 0.076 (2) | -0.0111 (16) | 0.0012 (16) | -0.0114 (15) |
| C46 | 0.070 (2) | 0.054 (2) | 0.132 (3) | -0.0011 (17) | 0.004 (2) | -0.030 (2) |
| C47 | 0.084 (3) | 0.060 (2) | 0.110 (3) | -0.0286 (19) | 0.007 (2) | -0.0222 (19) |
| C49 | 0.099 (3) | 0.061 (2) | 0.0546 (18) | -0.0098 (17) | -0.0013 (17) | -0.0103 (15) |
| C50 | 0.0586 (17) | 0.071 (2) | 0.0445 (16) | -0.0104 (15) | -0.0009 (13) | -0.0068 (14) |
| C51 | 0.104 (3) | 0.069 (2) | 0.060 (2) | -0.0149 (19) | -0.0018 (19) | -0.0024 (17) |
| C52 | 0.101 (3) | 0.103 (3) | 0.050 (2) | -0.021 (2) | -0.0058 (18) | 0.008 (2) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C53 | 0.076 (2) | 0.107 (3) | 0.0442 (18) | -0.013 (2) | -0.0002 (15) | -0.0153 (18) |
| C54 | 0.086 (2) | 0.083 (2) | 0.0519 (19) | -0.0030 (18) | -0.0057 (16) | -0.0177 (17) |
| C55 | 0.074 (2) | 0.070 (2) | 0.0438 (16) | 0.0010 (16) | -0.0058 (14) | -0.0099 (14) |
| C57 | 0.0465 (16) | 0.082 (2) | 0.0534 (17) | 0.0003 (15) | -0.0019 (13) | -0.0102 (15) |
| C58 | 0.0492 (16) | 0.0563 (16) | 0.0424 (15) | -0.0047 (13) | -0.0014 (12) | -0.0094 (12) |
| C59 | 0.0503 (17) | 0.077 (2) | 0.0464 (16) | 0.0027 (14) | -0.0018 (13) | -0.0093 (14) |
| C60 | 0.0531 (17) | 0.096 (2) | 0.0527 (18) | 0.0003 (16) | 0.0019 (14) | -0.0193 (16) |
| C61 | 0.075 (2) | 0.083 (2) | 0.0451 (17) | -0.0056 (17) | -0.0005 (15) | -0.0204 (15) |
| C62 | 0.078 (2) | 0.091 (2) | 0.0457 (17) | -0.0085 (18) | -0.0139 (16) | -0.0142 (16) |
| C63 | 0.0510 (16) | 0.074 (2) | 0.0609 (19) | -0.0034 (14) | -0.0106 (14) | -0.0180 (15) |
| C65 | 0.0573 (18) | 0.108 (3) | 0.0528 (18) | 0.0022 (18) | -0.0069 (15) | -0.0219 (17) |
| C66 | 0.066 (2) | 0.087 (2) | 0.0519 (18) | -0.0102 (18) | -0.0030 (15) | -0.0192 (17) |
| C67 | 0.159 (5) | 0.109 (4) | 0.104 (3) | -0.037 (3) | 0.060 (3) | -0.031 (3) |
| C68 | 0.178 (5) | 0.085 (3) | 0.115 (4) | -0.014 (3) | 0.039 (4) | -0.028 (3) |
| C69 | 0.092 (3) | 0.099 (3) | 0.066 (2) | 0.002 (2) | -0.009 (2) | -0.036 (2) |
| C70 | 0.087 (3) | 0.128 (4) | 0.071 (2) | -0.010 (3) | 0.018 (2) | -0.033 (2) |
| C71 | 0.093 (3) | 0.085 (2) | 0.072 (2) | -0.008 (2) | 0.011 (2) | -0.0201 (19) |

Geometric parameters (Å, °)

| | | | |
|----------|------------|-----------|------------|
| S1—C1 | 1.768 (3) | C23—C24 | 1.378 (4) |
| S1—C35 | 1.779 (2) | C23—C27 | 1.526 (4) |
| S2—C11 | 1.770 (3) | C24—C25 | 1.390 (3) |
| S2—C5 | 1.777 (3) | C24—H24 | 0.9300 |
| S3—C15 | 1.772 (3) | C25—C26 | 1.390 (4) |
| S3—C21 | 1.772 (3) | C27—C30' | 1.445 (16) |
| S4—C25 | 1.773 (3) | C27—C28 | 1.454 (12) |
| S4—C31 | 1.773 (3) | C27—C29 | 1.510 (14) |
| S5—C45 | 1.762 (8) | C27—C29' | 1.574 (12) |
| S5—C48 | 1.769 (8) | C27—C30 | 1.580 (10) |
| S6—C53 | 1.756 (9) | C27—C28' | 1.683 (17) |
| S6—C56 | 1.816 (14) | C28—H28A | 0.9600 |
| S7—C64 | 1.800 (12) | C28—H28B | 0.9600 |
| S7—C61 | 1.811 (9) | C28—H28C | 0.9600 |
| S8—C69 | 1.773 (7) | C29—H29A | 0.9600 |
| S8—C72 | 1.791 (11) | C29—H29B | 0.9600 |
| C48—H48A | 0.9600 | C29—H29C | 0.9600 |
| C48—H48B | 0.9600 | C30—H30A | 0.9600 |
| C48—H48C | 0.9600 | C30—H30B | 0.9600 |
| C56—H56A | 0.9600 | C30—H30C | 0.9600 |
| C56—H56B | 0.9600 | C28'—H28D | 0.9600 |
| C56—H56C | 0.9600 | C28'—H28E | 0.9600 |
| C64—H64A | 0.9600 | C28'—H28F | 0.9600 |
| C64—H64B | 0.9600 | C29'—H29D | 0.9600 |
| C64—H64C | 0.9600 | C29'—H29E | 0.9600 |
| C72—H72D | 0.9600 | C29'—H29F | 0.9600 |
| C72—H72E | 0.9600 | C30'—H30D | 0.9600 |
| C72—H72F | 0.9600 | C30'—H30E | 0.9600 |
| S5'—C48' | 1.792 (19) | C30'—H30F | 0.9600 |
| S5'—C45 | 1.827 (17) | C31—C32 | 1.380 (3) |

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|-----------|------------|-----------|------------|
| S6'—C56' | 1.740 (14) | C31—C36 | 1.405 (3) |
| S6'—C53 | 1.787 (10) | C32—C33 | 1.388 (4) |
| S7'—C61 | 1.734 (10) | C32—H32 | 0.9300 |
| S7'—C64' | 1.760 (13) | C33—C34 | 1.389 (3) |
| S8'—C69 | 1.756 (10) | C33—C37 | 1.532 (4) |
| S8'—C72' | 1.812 (17) | C34—C35 | 1.387 (3) |
| C48'—H48D | 0.9600 | C34—H34 | 0.9300 |
| C48'—H48E | 0.9600 | C35—C36 | 1.384 (3) |
| C48'—H48F | 0.9600 | C37—C38 | 1.416 (8) |
| C56'—H56D | 0.9600 | C37—C40' | 1.423 (16) |
| C56'—H56E | 0.9600 | C37—C39' | 1.437 (9) |
| C56'—H56F | 0.9600 | C37—C40 | 1.506 (11) |
| C64'—H64D | 0.9600 | C37—C39 | 1.678 (7) |
| C64'—H64E | 0.9600 | C37—C38' | 1.733 (9) |
| C64'—H64F | 0.9600 | C38—H38A | 0.9600 |
| C72'—H72A | 0.9600 | C38—H38B | 0.9600 |
| C72'—H72B | 0.9600 | C38—H38C | 0.9600 |
| C72'—H72C | 0.9600 | C39—H39A | 0.9600 |
| O1—C6 | 1.370 (3) | C39—H39B | 0.9600 |
| O1—C41 | 1.375 (4) | C39—H39C | 0.9600 |
| O2—C16 | 1.371 (3) | C40—H40A | 0.9600 |
| O2—C49 | 1.421 (3) | C40—H40B | 0.9600 |
| O3—C26 | 1.372 (3) | C40—H40C | 0.9600 |
| O3—C57 | 1.433 (3) | C38'—H38D | 0.9600 |
| O4—C36 | 1.376 (3) | C38'—H38E | 0.9600 |
| O4—C65 | 1.440 (4) | C38'—H38F | 0.9600 |
| C1—C2 | 1.379 (3) | C39'—H39D | 0.9600 |
| C1—C6 | 1.400 (3) | C39'—H39E | 0.9600 |
| C2—C3 | 1.396 (4) | C39'—H39F | 0.9600 |
| C2—H2 | 0.9300 | C40'—H40D | 0.9600 |
| C3—C4 | 1.373 (4) | C40'—H40E | 0.9600 |
| C3—C7 | 1.542 (4) | C40'—H40F | 0.9600 |
| C4—C5 | 1.387 (3) | C41—C42 | 1.482 (4) |
| C4—H4 | 0.9300 | C41—H41A | 0.9700 |
| C5—C6 | 1.384 (3) | C41—H41B | 0.9700 |
| C7—C10 | 1.512 (5) | C42—C43 | 1.366 (4) |
| C7—C8 | 1.522 (5) | C42—C47 | 1.373 (4) |
| C7—C9 | 1.527 (4) | C43—C44 | 1.357 (4) |
| C8—H8A | 0.9600 | C43—H43 | 0.9300 |
| C8—H8B | 0.9600 | C44—C45 | 1.345 (4) |
| C8—H8C | 0.9600 | C44—H44 | 0.9300 |
| C9—H9A | 0.9600 | C45—C46 | 1.357 (4) |
| C9—H9B | 0.9600 | C46—C47 | 1.388 (5) |
| C9—H9C | 0.9600 | C46—H46 | 0.9300 |
| C10—H10A | 0.9600 | C47—H47 | 0.9300 |
| C10—H10B | 0.9600 | C49—C50 | 1.489 (4) |
| C10—H10C | 0.9600 | C49—H49A | 0.9700 |
| C11—C12 | 1.383 (4) | C49—H49B | 0.9700 |
| C11—C16 | 1.393 (4) | C50—C55 | 1.371 (4) |

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|---------------|-------------|----------------|-----------|
| C12—C13 | 1.390 (4) | C50—C51 | 1.382 (4) |
| C12—H12 | 0.9300 | C51—C52 | 1.374 (5) |
| C13—C14 | 1.378 (4) | C51—H51 | 0.9300 |
| C13—C17 | 1.533 (4) | C52—C53 | 1.361 (5) |
| C14—C15 | 1.395 (4) | C52—H52 | 0.9300 |
| C14—H14 | 0.9300 | C53—C54 | 1.385 (5) |
| C15—C16 | 1.386 (4) | C54—C55 | 1.383 (4) |
| C17—C20' | 1.457 (14) | C54—H54 | 0.9300 |
| C17—C18' | 1.46 (2) | C55—H55 | 0.9300 |
| C17—C19 | 1.534 (11) | C57—C58 | 1.504 (4) |
| C17—C19' | 1.566 (18) | C57—H57A | 0.9700 |
| C17—C18 | 1.592 (18) | C57—H57B | 0.9700 |
| C17—C20 | 1.624 (13) | C58—C59 | 1.375 (4) |
| C18—H18A | 0.9600 | C58—C63 | 1.386 (4) |
| C18—H18B | 0.9600 | C59—C60 | 1.372 (4) |
| C18—H18C | 0.9600 | C59—H59 | 0.9300 |
| C19—H19A | 0.9600 | C60—C61 | 1.388 (4) |
| C19—H19B | 0.9600 | C60—H60 | 0.9300 |
| C19—H19C | 0.9600 | C61—C62 | 1.380 (4) |
| C20—H20A | 0.9600 | C62—C63 | 1.361 (4) |
| C20—H20B | 0.9600 | C62—H62 | 0.9300 |
| C20—H20C | 0.9600 | C63—H63 | 0.9300 |
| C18'—H18D | 0.9600 | C65—C66 | 1.498 (4) |
| C18'—H18E | 0.9600 | C65—H65A | 0.9700 |
| C18'—H18F | 0.9600 | C65—H65B | 0.9700 |
| C19'—H19D | 0.9600 | C66—C67 | 1.354 (5) |
| C19'—H19E | 0.9600 | C66—C71 | 1.373 (5) |
| C19'—H19F | 0.9600 | C67—C68 | 1.402 (6) |
| C20'—H20D | 0.9600 | C67—H67 | 0.9300 |
| C20'—H20E | 0.9600 | C68—C69 | 1.325 (6) |
| C20'—H20F | 0.9600 | C68—H68 | 0.9300 |
| C21—C26 | 1.383 (4) | C69—C70 | 1.364 (5) |
| C21—C22 | 1.399 (4) | C70—C71 | 1.376 (5) |
| C22—C23 | 1.386 (4) | C70—H70 | 0.9300 |
| C22—H22 | 0.9300 | C71—H71 | 0.9300 |
| | | | |
| C1—S1—C35 | 106.14 (11) | C27—C30—H30B | 109.5 |
| C11—S2—C5 | 108.71 (11) | C27—C30—H30C | 109.5 |
| C15—S3—C21 | 108.63 (12) | C27—C28'—H28D | 109.5 |
| C25—S4—C31 | 108.22 (11) | C27—C28'—H28E | 109.5 |
| C45—S5—C48 | 106.3 (4) | H28D—C28'—H28E | 109.5 |
| C53—S6—C56 | 100.8 (7) | C27—C28'—H28F | 109.5 |
| C64—S7—C61 | 100.0 (6) | H28D—C28'—H28F | 109.5 |
| C69—S8—C72 | 102.6 (6) | H28E—C28'—H28F | 109.5 |
| C48'—S5'—C45 | 82.1 (9) | C27—C29'—H29D | 109.5 |
| C56'—S6'—C53 | 102.5 (8) | C27—C29'—H29E | 109.5 |
| C61—S7'—C64' | 107.7 (8) | H29D—C29'—H29E | 109.5 |
| C69—S8'—C72' | 107.6 (11) | C27—C29'—H29F | 109.5 |
| S5'—C48'—H48D | 109.5 | H29D—C29'—H29F | 109.5 |

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|----------------|-------------|----------------|-------------|
| S5'—C48'—H48E | 109.5 | H29E—C29'—H29F | 109.5 |
| H48D—C48'—H48E | 109.5 | C27—C30'—H30D | 109.5 |
| S5'—C48'—H48F | 109.5 | C27—C30'—H30E | 109.5 |
| H48D—C48'—H48F | 109.5 | H30D—C30'—H30E | 109.5 |
| H48E—C48'—H48F | 109.5 | C27—C30'—H30F | 109.5 |
| S6'—C56'—H56D | 109.5 | H30D—C30'—H30F | 109.5 |
| S6'—C56'—H56E | 109.5 | H30E—C30'—H30F | 109.5 |
| H56D—C56'—H56E | 109.5 | C32—C31—C36 | 120.3 (2) |
| S6'—C56'—H56F | 109.5 | C32—C31—S4 | 117.03 (18) |
| H56D—C56'—H56F | 109.5 | C36—C31—S4 | 122.17 (19) |
| H56E—C56'—H56F | 109.5 | C31—C32—C33 | 122.4 (2) |
| S7'—C64'—H64D | 109.5 | C31—C32—H32 | 118.8 |
| S7'—C64'—H64E | 109.5 | C33—C32—H32 | 118.8 |
| H64D—C64'—H64E | 109.5 | C32—C33—C34 | 116.4 (2) |
| S7'—C64'—H64F | 109.5 | C32—C33—C37 | 121.2 (2) |
| H64D—C64'—H64F | 109.5 | C34—C33—C37 | 122.5 (2) |
| H64E—C64'—H64F | 109.5 | C35—C34—C33 | 122.4 (2) |
| S8'—C72'—H72A | 109.5 | C35—C34—H34 | 118.8 |
| S8'—C72'—H72B | 109.5 | C33—C34—H34 | 118.8 |
| H72A—C72'—H72B | 109.5 | C36—C35—C34 | 120.5 (2) |
| S8'—C72'—H72C | 109.5 | C36—C35—S1 | 124.13 (19) |
| H72A—C72'—H72C | 109.5 | C34—C35—S1 | 115.11 (18) |
| H72B—C72'—H72C | 109.5 | O4—C36—C35 | 123.7 (2) |
| C6—O1—C41 | 124.3 (2) | O4—C36—C31 | 118.2 (2) |
| C16—O2—C49 | 114.5 (2) | C35—C36—C31 | 117.9 (2) |
| C26—O3—C57 | 113.88 (18) | C38—C37—C40' | 128.2 (8) |
| C36—O4—C65 | 116.4 (2) | C38—C37—C39' | 56.3 (6) |
| C2—C1—C6 | 120.1 (2) | C40'—C37—C39' | 117.1 (7) |
| C2—C1—S1 | 117.5 (2) | C38—C37—C40 | 117.8 (7) |
| C6—C1—S1 | 122.04 (19) | C40'—C37—C40 | 25.5 (7) |
| C1—C2—C3 | 122.3 (2) | C39'—C37—C40 | 135.4 (5) |
| C1—C2—H2 | 118.8 | C38—C37—C33 | 115.0 (4) |
| C3—C2—H2 | 118.8 | C40'—C37—C33 | 114.3 (7) |
| C4—C3—C2 | 116.4 (2) | C39'—C37—C33 | 110.9 (4) |
| C4—C3—C7 | 123.2 (2) | C40—C37—C33 | 110.3 (4) |
| C2—C3—C7 | 120.3 (3) | C38—C37—C39 | 106.5 (6) |
| C3—C4—C5 | 122.6 (2) | C40'—C37—C39 | 74.4 (6) |
| C3—C4—H4 | 118.7 | C39'—C37—C39 | 52.7 (5) |
| C5—C4—H4 | 118.7 | C40—C37—C39 | 99.8 (4) |
| C6—C5—C4 | 120.4 (2) | C33—C37—C39 | 105.5 (3) |
| C6—C5—S2 | 123.38 (19) | C38—C37—C38' | 45.7 (5) |
| C4—C5—S2 | 115.79 (18) | C40'—C37—C38' | 105.0 (7) |
| O1—C6—C5 | 122.5 (2) | C39'—C37—C38' | 101.7 (6) |
| O1—C6—C1 | 119.2 (2) | C40—C37—C38' | 82.6 (5) |
| C5—C6—C1 | 118.0 (2) | C33—C37—C38' | 106.2 (3) |
| C10—C7—C8 | 107.3 (3) | C39—C37—C38' | 145.1 (4) |
| C10—C7—C9 | 110.5 (3) | C37—C38—H38A | 109.5 |
| C8—C7—C9 | 108.6 (3) | C37—C38—H38B | 109.5 |
| C10—C7—C3 | 110.8 (2) | C37—C38—H38C | 109.5 |

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| C8—C7—C3 | 111.5 (3) | C37—C39—H39A | 109.5 |
| C9—C7—C3 | 108.1 (2) | C37—C39—H39B | 109.5 |
| C7—C8—H8A | 109.5 | C37—C39—H39C | 109.5 |
| C7—C8—H8B | 109.5 | C37—C40—H40A | 109.5 |
| H8A—C8—H8B | 109.5 | C37—C40—H40B | 109.5 |
| C7—C8—H8C | 109.5 | C37—C40—H40C | 109.5 |
| H8A—C8—H8C | 109.5 | C37—C38'—H38D | 109.5 |
| H8B—C8—H8C | 109.5 | C37—C38'—H38E | 109.5 |
| C7—C9—H9A | 109.5 | H38D—C38'—H38E | 109.5 |
| C7—C9—H9B | 109.5 | C37—C38'—H38F | 109.5 |
| H9A—C9—H9B | 109.5 | H38D—C38'—H38F | 109.5 |
| C7—C9—H9C | 109.5 | H38E—C38'—H38F | 109.5 |
| H9A—C9—H9C | 109.5 | C37—C39'—H39D | 109.5 |
| H9B—C9—H9C | 109.5 | C37—C39'—H39E | 109.5 |
| C7—C10—H10A | 109.5 | H39D—C39'—H39E | 109.5 |
| C7—C10—H10B | 109.5 | C37—C39'—H39F | 109.5 |
| H10A—C10—H10B | 109.5 | H39D—C39'—H39F | 109.5 |
| C7—C10—H10C | 109.5 | H39E—C39'—H39F | 109.5 |
| H10A—C10—H10C | 109.5 | C37—C40'—H40D | 109.5 |
| H10B—C10—H10C | 109.5 | C37—C40'—H40E | 109.5 |
| C12—C11—C16 | 119.9 (2) | H40D—C40'—H40E | 109.5 |
| C12—C11—S2 | 116.2 (2) | C37—C40'—H40F | 109.5 |
| C16—C11—S2 | 123.2 (2) | H40D—C40'—H40F | 109.5 |
| C11—C12—C13 | 122.3 (2) | H40E—C40'—H40F | 109.5 |
| C11—C12—H12 | 118.8 | O1—C41—C42 | 120.6 (3) |
| C13—C12—H12 | 118.8 | O1—C41—H41A | 107.2 |
| C14—C13—C12 | 116.9 (2) | C42—C41—H41A | 107.2 |
| C14—C13—C17 | 120.9 (3) | O1—C41—H41B | 107.2 |
| C12—C13—C17 | 122.2 (3) | C42—C41—H41B | 107.2 |
| C13—C14—C15 | 122.1 (3) | H41A—C41—H41B | 106.8 |
| C13—C14—H14 | 119.0 | C43—C42—C47 | 115.1 (3) |
| C15—C14—H14 | 119.0 | C43—C42—C41 | 123.2 (3) |
| C16—C15—C14 | 120.1 (2) | C47—C42—C41 | 121.6 (3) |
| C16—C15—S3 | 124.2 (2) | C44—C43—C42 | 123.4 (3) |
| C14—C15—S3 | 115.2 (2) | C44—C43—H43 | 118.3 |
| O2—C16—C15 | 120.7 (2) | C42—C43—H43 | 118.3 |
| O2—C16—C11 | 120.6 (2) | C45—C44—C43 | 120.4 (3) |
| C15—C16—C11 | 118.7 (2) | C45—C44—H44 | 119.8 |
| C20'—C17—C18' | 117.9 (10) | C43—C44—H44 | 119.8 |
| C20'—C17—C13 | 114.7 (6) | C44—C45—C46 | 119.1 (3) |
| C18'—C17—C13 | 115.0 (8) | C44—C45—S5 | 115.1 (3) |
| C20'—C17—C19 | 89.3 (6) | C46—C45—S5 | 125.7 (3) |
| C18'—C17—C19 | 108.1 (7) | C44—C45—S5' | 122.0 (6) |
| C13—C17—C19 | 108.0 (5) | C46—C45—S5' | 118.5 (6) |
| C20'—C17—C19' | 114.6 (8) | S5—C45—S5' | 10.0 (10) |
| C18'—C17—C19' | 86.7 (8) | C45—C46—C47 | 119.6 (3) |
| C13—C17—C19' | 103.6 (7) | C45—C46—H46 | 120.2 |
| C19—C17—C19' | 27.2 (6) | C47—C46—H46 | 120.2 |
| C20'—C17—C18 | 110.2 (9) | C42—C47—C46 | 122.2 (3) |

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| C18'—C17—C18 | 18.6 (9) | C42—C47—H47 | 118.9 |
| C13—C17—C18 | 107.7 (7) | C46—C47—H47 | 118.9 |
| C19—C17—C18 | 126.3 (7) | O2—C49—C50 | 109.5 (3) |
| C19'—C17—C18 | 105.3 (9) | O2—C49—H49A | 109.8 |
| C20'—C17—C20 | 20.8 (7) | C50—C49—H49A | 109.8 |
| C18'—C17—C20 | 107.1 (9) | O2—C49—H49B | 109.8 |
| C13—C17—C20 | 108.8 (5) | C50—C49—H49B | 109.8 |
| C19—C17—C20 | 109.9 (6) | H49A—C49—H49B | 108.2 |
| C19'—C17—C20 | 134.2 (8) | C55—C50—C51 | 117.9 (3) |
| C18—C17—C20 | 94.8 (9) | C55—C50—C49 | 123.2 (3) |
| C17—C18—H18A | 109.5 | C51—C50—C49 | 118.9 (3) |
| C17—C18—H18B | 109.5 | C52—C51—C50 | 121.2 (4) |
| C17—C18—H18C | 109.5 | C52—C51—H51 | 119.4 |
| C17—C19—H19A | 109.5 | C50—C51—H51 | 119.4 |
| C17—C19—H19B | 109.5 | C53—C52—C51 | 121.2 (3) |
| C17—C19—H19C | 109.5 | C53—C52—H52 | 119.4 |
| C17—C20—H20A | 109.5 | C51—C52—H52 | 119.4 |
| C17—C20—H20B | 109.5 | C52—C53—C54 | 118.2 (3) |
| C17—C20—H20C | 109.5 | C52—C53—S6 | 114.4 (4) |
| C17—C18'—H18D | 109.5 | C54—C53—S6 | 126.9 (5) |
| C17—C18'—H18E | 109.5 | C52—C53—S6' | 120.3 (5) |
| H18D—C18'—H18E | 109.5 | C54—C53—S6' | 120.9 (5) |
| C17—C18'—H18F | 109.5 | S6—C53—S6' | 15.5 (5) |
| H18D—C18'—H18F | 109.5 | C55—C54—C53 | 120.7 (3) |
| H18E—C18'—H18F | 109.5 | C55—C54—H54 | 119.7 |
| C17—C19'—H19D | 109.5 | C53—C54—H54 | 119.7 |
| C17—C19'—H19E | 109.5 | C50—C55—C54 | 120.9 (3) |
| H19D—C19'—H19E | 109.5 | C50—C55—H55 | 119.5 |
| C17—C19'—H19F | 109.5 | C54—C55—H55 | 119.5 |
| H19D—C19'—H19F | 109.5 | O3—C57—C58 | 109.3 (2) |
| H19E—C19'—H19F | 109.5 | O3—C57—H57A | 109.8 |
| C17—C20'—H20D | 109.5 | C58—C57—H57A | 109.8 |
| C17—C20'—H20E | 109.5 | O3—C57—H57B | 109.8 |
| H20D—C20'—H20E | 109.5 | C58—C57—H57B | 109.8 |
| C17—C20'—H20F | 109.5 | H57A—C57—H57B | 108.3 |
| H20D—C20'—H20F | 109.5 | C59—C58—C63 | 118.2 (2) |
| H20E—C20'—H20F | 109.5 | C59—C58—C57 | 123.4 (2) |
| C26—C21—C22 | 120.6 (2) | C63—C58—C57 | 118.4 (2) |
| C26—C21—S3 | 123.6 (2) | C60—C59—C58 | 120.4 (3) |
| C22—C21—S3 | 115.3 (2) | C60—C59—H59 | 119.8 |
| C23—C22—C21 | 121.2 (3) | C58—C59—H59 | 119.8 |
| C23—C22—H22 | 119.4 | C59—C60—C61 | 121.2 (3) |
| C21—C22—H22 | 119.4 | C59—C60—H60 | 119.4 |
| C24—C23—C22 | 117.2 (2) | C61—C60—H60 | 119.4 |
| C24—C23—C27 | 122.4 (3) | C62—C61—C60 | 118.1 (3) |
| C22—C23—C27 | 120.4 (3) | C62—C61—S7' | 120.1 (4) |
| C23—C24—C25 | 122.7 (3) | C60—C61—S7' | 121.8 (4) |
| C23—C24—H24 | 118.7 | C62—C61—S7 | 128.9 (4) |
| C25—C24—H24 | 118.7 | C60—C61—S7 | 112.9 (4) |

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| C26—C25—C24 | 119.6 (2) | S7'—C61—S7 | 10.2 (7) |
| C26—C25—S4 | 123.81 (19) | C63—C62—C61 | 120.4 (3) |
| C24—C25—S4 | 115.7 (2) | C63—C62—H62 | 119.8 |
| O3—C26—C21 | 120.5 (2) | C61—C62—H62 | 119.8 |
| O3—C26—C25 | 120.8 (2) | C62—C63—C58 | 121.6 (3) |
| C21—C26—C25 | 118.7 (2) | C62—C63—H63 | 119.2 |
| C30'—C27—C28 | 124.7 (8) | C58—C63—H63 | 119.2 |
| C30'—C27—C29 | 108.4 (8) | O4—C65—C66 | 114.4 (2) |
| C28—C27—C29 | 85.6 (7) | O4—C65—H65A | 108.7 |
| C30'—C27—C23 | 111.6 (7) | C66—C65—H65A | 108.7 |
| C28—C27—C23 | 112.3 (5) | O4—C65—H65B | 108.7 |
| C29—C27—C23 | 110.4 (5) | C66—C65—H65B | 108.7 |
| C30'—C27—C29' | 79.6 (7) | H65A—C65—H65B | 107.6 |
| C28—C27—C29' | 112.4 (7) | C67—C66—C71 | 115.9 (3) |
| C29—C27—C29' | 31.4 (5) | C67—C66—C65 | 122.3 (3) |
| C23—C27—C29' | 111.6 (5) | C71—C66—C65 | 121.7 (3) |
| C30'—C27—C30 | 25.2 (6) | C66—C67—C68 | 122.2 (4) |
| C28—C27—C30 | 108.9 (6) | C66—C67—H67 | 118.9 |
| C29—C27—C30 | 130.7 (6) | C68—C67—H67 | 118.9 |
| C23—C27—C30 | 106.8 (4) | C69—C68—C67 | 120.8 (4) |
| C29'—C27—C30 | 104.2 (6) | C69—C68—H68 | 119.6 |
| C30'—C27—C28' | 110.4 (9) | C67—C68—H68 | 119.6 |
| C28—C27—C28' | 21.6 (9) | C68—C69—C70 | 118.0 (4) |
| C29—C27—C28' | 106.3 (8) | C68—C69—S8' | 117.1 (6) |
| C23—C27—C28' | 109.6 (7) | C70—C69—S8' | 124.8 (5) |
| C29'—C27—C28' | 129.6 (8) | C68—C69—S8 | 129.1 (5) |
| C30—C27—C28' | 90.2 (7) | C70—C69—S8 | 112.8 (4) |
| C27—C28—H28A | 109.5 | S8'—C69—S8 | 12.7 (7) |
| C27—C28—H28B | 109.5 | C69—C70—C71 | 121.3 (4) |
| C27—C28—H28C | 109.5 | C69—C70—H70 | 119.4 |
| C27—C29—H29A | 109.5 | C71—C70—H70 | 119.4 |
| C27—C29—H29B | 109.5 | C66—C71—C70 | 121.6 (4) |
| C27—C29—H29C | 109.5 | C66—C71—H71 | 119.2 |
| C27—C30—H30A | 109.5 | C70—C71—H71 | 119.2 |
| | | | |
| C35—S1—C1—C2 | -128.12 (19) | C1—S1—C35—C34 | -133.1 (2) |
| C35—S1—C1—C6 | 58.3 (2) | C65—O4—C36—C35 | 70.1 (3) |
| C6—C1—C2—C3 | -1.1 (4) | C65—O4—C36—C31 | -115.1 (3) |
| S1—C1—C2—C3 | -174.75 (19) | C34—C35—C36—O4 | 178.6 (2) |
| C1—C2—C3—C4 | -1.7 (4) | S1—C35—C36—O4 | -7.8 (4) |
| C1—C2—C3—C7 | 179.2 (2) | C34—C35—C36—C31 | 3.8 (4) |
| C2—C3—C4—C5 | 2.2 (4) | S1—C35—C36—C31 | 177.35 (19) |
| C7—C3—C4—C5 | -178.7 (2) | C32—C31—C36—O4 | -178.8 (2) |
| C3—C4—C5—C6 | 0.0 (4) | S4—C31—C36—O4 | 9.2 (3) |
| C3—C4—C5—S2 | 172.9 (2) | C32—C31—C36—C35 | -3.7 (4) |
| C11—S2—C5—C6 | -56.4 (2) | S4—C31—C36—C35 | -175.69 (19) |
| C11—S2—C5—C4 | 130.9 (2) | C32—C33—C37—C38 | 168.4 (7) |
| C41—O1—C6—C5 | -79.4 (4) | C34—C33—C37—C38 | -11.2 (8) |
| C41—O1—C6—C1 | 106.7 (3) | C32—C33—C37—C40' | -28.2 (8) |

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| C4—C5—C6—O1 | -176.8 (2) | C34—C33—C37—C40' | 152.3 (7) |
| S2—C5—C6—O1 | 10.8 (3) | C32—C33—C37—C39' | 106.8 (6) |
| C4—C5—C6—C1 | -2.7 (3) | C34—C33—C37—C39' | -72.7 (7) |
| S2—C5—C6—C1 | -175.14 (18) | C32—C33—C37—C40 | -55.5 (5) |
| C2—C1—C6—O1 | 177.5 (2) | C34—C33—C37—C40 | 125.0 (5) |
| S1—C1—C6—O1 | -9.1 (3) | C32—C33—C37—C39 | 51.4 (4) |
| C2—C1—C6—C5 | 3.3 (3) | C34—C33—C37—C39 | -128.1 (4) |
| S1—C1—C6—C5 | 176.64 (17) | C32—C33—C37—C38' | -143.4 (4) |
| C4—C3—C7—C10 | -127.8 (3) | C34—C33—C37—C38' | 37.0 (5) |
| C2—C3—C7—C10 | 51.3 (4) | C6—O1—C41—C42 | -21.9 (5) |
| C4—C3—C7—C8 | -8.4 (4) | O1—C41—C42—C43 | -80.9 (5) |
| C2—C3—C7—C8 | 170.7 (3) | O1—C41—C42—C47 | 102.2 (4) |
| C4—C3—C7—C9 | 110.9 (3) | C47—C42—C43—C44 | 3.1 (5) |
| C2—C3—C7—C9 | -70.0 (3) | C41—C42—C43—C44 | -174.0 (3) |
| C5—S2—C11—C12 | 139.5 (2) | C42—C43—C44—C45 | -2.3 (6) |
| C5—S2—C11—C16 | -49.6 (2) | C43—C44—C45—C46 | 0.8 (5) |
| C16—C11—C12—C13 | -0.2 (4) | C43—C44—C45—S5 | 179.0 (5) |
| S2—C11—C12—C13 | 171.0 (2) | C43—C44—C45—S5' | -172.7 (11) |
| C11—C12—C13—C14 | 1.1 (4) | C48—S5—C45—C44 | -177.8 (5) |
| C11—C12—C13—C17 | -177.4 (3) | C48—S5—C45—C46 | 0.4 (8) |
| C12—C13—C14—C15 | -1.5 (4) | C48—S5—C45—S5' | 47 (6) |
| C17—C13—C14—C15 | 177.0 (3) | C48'—S5'—C45—C44 | -153.6 (7) |
| C13—C14—C15—C16 | 0.9 (4) | C48'—S5'—C45—C46 | 32.9 (13) |
| C13—C14—C15—S3 | -171.2 (2) | C48'—S5'—C45—S5 | -105 (7) |
| C21—S3—C15—C16 | 46.1 (3) | C44—C45—C46—C47 | -0.3 (6) |
| C21—S3—C15—C14 | -142.2 (2) | S5—C45—C46—C47 | -178.3 (5) |
| C49—O2—C16—C15 | 89.0 (3) | S5'—C45—C46—C47 | 173.4 (11) |
| C49—O2—C16—C11 | -92.3 (3) | C43—C42—C47—C46 | -2.6 (5) |
| C14—C15—C16—O2 | 178.7 (2) | C41—C42—C47—C46 | 174.6 (3) |
| S3—C15—C16—O2 | -9.9 (4) | C45—C46—C47—C42 | 1.3 (6) |
| C14—C15—C16—C11 | 0.0 (4) | C16—O2—C49—C50 | -177.7 (2) |
| S3—C15—C16—C11 | 171.4 (2) | O2—C49—C50—C55 | 7.8 (4) |
| C12—C11—C16—O2 | -179.1 (2) | O2—C49—C50—C51 | -173.5 (3) |
| S2—C11—C16—O2 | 10.3 (3) | C55—C50—C51—C52 | -0.6 (5) |
| C12—C11—C16—C15 | -0.3 (4) | C49—C50—C51—C52 | -179.4 (3) |
| S2—C11—C16—C15 | -170.97 (19) | C50—C51—C52—C53 | 1.8 (6) |
| C14—C13—C17—C20' | 17.0 (7) | C51—C52—C53—C54 | -2.1 (6) |
| C12—C13—C17—C20' | -164.6 (6) | C51—C52—C53—S6 | -174.7 (4) |
| C14—C13—C17—C18' | 158.5 (7) | C51—C52—C53—S6' | 169.2 (4) |
| C12—C13—C17—C18' | -23.1 (8) | C56—S6—C53—C52 | -173.0 (5) |
| C14—C13—C17—C19 | -80.8 (5) | C56—S6—C53—C54 | 15.2 (8) |
| C12—C13—C17—C19 | 97.6 (5) | C56—S6—C53—S6' | -57 (3) |
| C14—C13—C17—C19' | -108.7 (7) | C56'—S6'—C53—C52 | 150.9 (6) |
| C12—C13—C17—C19' | 69.7 (7) | C56'—S6'—C53—C54 | -38.0 (8) |
| C14—C13—C17—C18 | 140.1 (7) | C56'—S6'—C53—S6 | 79 (3) |
| C12—C13—C17—C18 | -41.5 (7) | C52—C53—C54—C55 | 1.4 (5) |
| C14—C13—C17—C20 | 38.5 (6) | S6—C53—C54—C55 | 172.9 (4) |
| C12—C13—C17—C20 | -143.1 (6) | S6'—C53—C54—C55 | -169.8 (4) |
| C15—S3—C21—C26 | 49.1 (2) | C51—C50—C55—C54 | -0.1 (5) |

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| C15—S3—C21—C22 | -138.9 (2) | C49—C50—C55—C54 | 178.6 (3) |
| C26—C21—C22—C23 | -0.2 (4) | C53—C54—C55—C50 | -0.3 (5) |
| S3—C21—C22—C23 | -172.4 (2) | C26—O3—C57—C58 | -173.4 (2) |
| C21—C22—C23—C24 | -0.7 (4) | O3—C57—C58—C59 | 1.3 (4) |
| C21—C22—C23—C27 | 177.2 (2) | O3—C57—C58—C63 | -177.6 (2) |
| C22—C23—C24—C25 | 1.0 (4) | C63—C58—C59—C60 | 1.1 (5) |
| C27—C23—C24—C25 | -176.8 (2) | C57—C58—C59—C60 | -177.8 (3) |
| C23—C24—C25—C26 | -0.6 (4) | C58—C59—C60—C61 | 0.7 (5) |
| C23—C24—C25—S4 | 169.39 (19) | C59—C60—C61—C62 | -2.4 (5) |
| C31—S4—C25—C26 | -47.7 (2) | C59—C60—C61—S7' | 175.8 (5) |
| C31—S4—C25—C24 | 142.83 (19) | C59—C60—C61—S7 | -178.5 (4) |
| C57—O3—C26—C21 | 89.2 (3) | C64'—S7'—C61—C62 | 38.4 (9) |
| C57—O3—C26—C25 | -92.4 (3) | C64'—S7'—C61—C60 | -139.8 (7) |
| C22—C21—C26—O3 | 179.1 (2) | C64'—S7'—C61—S7 | -171 (4) |
| S3—C21—C26—O3 | -9.3 (3) | C64—S7—C61—C62 | 15.1 (9) |
| C22—C21—C26—C25 | 0.7 (4) | C64—S7—C61—C60 | -169.4 (5) |
| S3—C21—C26—C25 | 172.24 (18) | C64—S7—C61—S7' | -17 (3) |
| C24—C25—C26—O3 | -178.8 (2) | C60—C61—C62—C63 | 2.3 (5) |
| S4—C25—C26—O3 | 12.1 (3) | S7'—C61—C62—C63 | -176.0 (5) |
| C24—C25—C26—C21 | -0.3 (4) | S7—C61—C62—C63 | 177.6 (5) |
| S4—C25—C26—C21 | -169.42 (18) | C61—C62—C63—C58 | -0.4 (5) |
| C24—C23—C27—C30' | 80.8 (7) | C59—C58—C63—C62 | -1.3 (5) |
| C22—C23—C27—C30' | -97.1 (7) | C57—C58—C63—C62 | 177.7 (3) |
| C24—C23—C27—C28 | -133.6 (6) | C36—O4—C65—C66 | 81.3 (3) |
| C22—C23—C27—C28 | 48.6 (6) | O4—C65—C66—C67 | -99.8 (4) |
| C24—C23—C27—C29 | -39.9 (6) | O4—C65—C66—C71 | 81.0 (4) |
| C22—C23—C27—C29 | 142.3 (6) | C71—C66—C67—C68 | 1.7 (7) |
| C24—C23—C27—C29' | -6.3 (6) | C65—C66—C67—C68 | -177.6 (4) |
| C22—C23—C27—C29' | 175.9 (5) | C66—C67—C68—C69 | 2.2 (8) |
| C24—C23—C27—C30 | 107.0 (5) | C67—C68—C69—C70 | -5.1 (7) |
| C22—C23—C27—C30 | -70.8 (5) | C67—C68—C69—S8' | 172.1 (6) |
| C24—C23—C27—C28' | -156.6 (7) | C67—C68—C69—S8 | 177.0 (5) |
| C22—C23—C27—C28' | 25.6 (7) | C72'—S8'—C69—C68 | 15.4 (12) |
| C25—S4—C31—C32 | 128.5 (2) | C72'—S8'—C69—C70 | -167.7 (10) |
| C25—S4—C31—C36 | -59.2 (2) | C72'—S8'—C69—S8 | -147 (3) |
| C36—C31—C32—C33 | 0.4 (4) | C72—S8—C69—C68 | 19.2 (8) |
| S4—C31—C32—C33 | 172.8 (2) | C72—S8—C69—C70 | -158.8 (6) |
| C31—C32—C33—C34 | 2.8 (4) | C72—S8—C69—S8' | 39 (2) |
| C31—C32—C33—C37 | -176.8 (3) | C68—C69—C70—C71 | 4.2 (6) |
| C32—C33—C34—C35 | -2.7 (4) | S8'—C69—C70—C71 | -172.7 (5) |
| C37—C33—C34—C35 | 176.9 (3) | S8—C69—C70—C71 | -177.6 (4) |
| C33—C34—C35—C36 | -0.6 (4) | C67—C66—C71—C70 | -2.6 (6) |
| C33—C34—C35—S1 | -174.7 (2) | C65—C66—C71—C70 | 176.7 (3) |
| C1—S1—C35—C36 | 53.0 (2) | C69—C70—C71—C66 | -0.3 (6) |