

1-(4-Chlorophenyl)-2-phenyl-2-(3-phenyl-1-isoquinolylsulfanyl)ethanone

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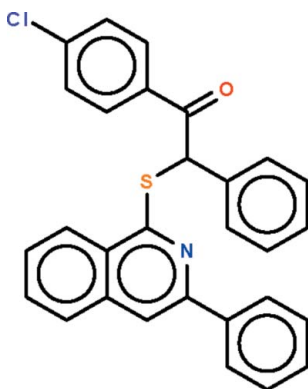
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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.079; wR factor = 0.170; data-to-parameter ratio = 14.0.

The title compound, $\text{C}_{29}\text{H}_{20}\text{ClNOS}$, is a 1-substituted-3-phenylisoquinoline that crystallizes with four independent molecules in the asymmetric unit. The four molecules have similar C—S—C angles. The most noteworthy differences between the molecules relate to the inclination of the 3-phenyl substituent with respect to the isoquinoline fused-ring [dihedral angles of 21.2 (1), 25.6 (2), 34.3 (1) and 36.5 (2)°].

Related literature

For the crystal structure of 1-(4-chloro-3-fluorophenyl)-2-[(3-phenylisoquinolin-1-yl)sulfanyl]ethanone, see: Manivel *et al.* (2009).



Experimental

Crystal data

| | |
|--|-----------------------------------|
| $\text{C}_{29}\text{H}_{20}\text{ClNOS}$ | $\gamma = 90.043$ (1)° |
| $M_r = 465.97$ | $V = 4743.9$ (5) Å ³ |
| Triclinic, $P\bar{1}$ | $Z = 8$ |
| $a = 10.2808$ (6) Å | Mo $K\alpha$ radiation |
| $b = 11.1145$ (7) Å | $\mu = 0.27$ mm ⁻¹ |
| $c = 42.169$ (3) Å | $T = 290$ K |
| $\alpha = 97.562$ (1)° | $0.30 \times 0.24 \times 0.17$ mm |
| $\beta = 96.647$ (2)° | |

Data collection

| | |
|---|---|
| Bruker SMART area-detector diffractometer | 45825 measured reflections |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | 16659 independent reflections |
| $T_{\min} = 0.923$, $T_{\max} = 0.955$ | 10228 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.048$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.079$ | 1189 parameters |
| $wR(F^2) = 0.170$ | H-atom parameters constrained |
| $S = 1.18$ | $\Delta\rho_{\text{max}} = 0.20$ e Å ⁻³ |
| 16659 reflections | $\Delta\rho_{\text{min}} = -0.20$ e Å ⁻³ |

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2556).

References

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 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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supplementary materials

Acta Cryst. (2009). E65, o2732 [doi:10.1107/S1600536809041282]

1-(4-Chlorophenyl)-2-phenyl-2-(3-phenyl-1-isoquinolylsulfanyl)ethanone

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Experimental

1-Mercapto-3-phenylisoquinoline (10.0 mmol) and 2-bromo-1-(4-chlorophenyl)-2-phenylethanone (10.5 mmol) were heated in ethanol (50 ml) under a nitrogen atmosphere for 2 h. The solid product was collected and dissolved in chloroform. The chloroform solution was washed with water and dried; the dry solution was concentrated. The solid material was purified by recrystallization from ether.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.98 Å) and were included in the refinement in the riding model approximation with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$.

Figures

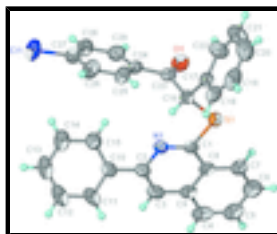


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of one of the four independent molecules of $\text{C}_{29}\text{H}_{20}\text{NOS}$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

1-(4-Chlorophenyl)-2-phenyl-2-(3-phenyl-1-isoquinolylsulfanyl)ethanone

Crystal data

$\text{C}_{29}\text{H}_{20}\text{ClNOS}$

$M_r = 465.97$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 10.2808$ (6) Å

$b = 11.1145$ (7) Å

$c = 42.169$ (3) Å

$\alpha = 97.562$ (1)°

$\beta = 96.647$ (2)°

$\gamma = 90.043$ (1)°

$V = 4743.9$ (5) Å³

$Z = 8$

$F_{000} = 1936$

$D_x = 1.305$ Mg m⁻³

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

Cell parameters from 1324 reflections

$\theta = 1.6$ – 24.3 °

$\mu = 0.27$ mm⁻¹

$T = 290$ K

Block, colorless

$0.30 \times 0.24 \times 0.17$ mm

supplementary materials

Data collection

| | |
|---|---|
| Bruker SMART area-detector diffractometer | 16659 independent reflections |
| Radiation source: fine-focus sealed tube | 10228 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.048$ |
| $T = 290$ K | $\theta_{\text{max}} = 25.0^\circ$ |
| φ and ω scans | $\theta_{\text{min}} = 1.5^\circ$ |
| Absorption correction: Multi-scan (SADABS; Sheldrick, 1996) | $h = -12 \rightarrow 12$ |
| $T_{\text{min}} = 0.923$, $T_{\text{max}} = 0.955$ | $k = -13 \rightarrow 13$ |
| 45825 measured reflections | $l = -50 \rightarrow 50$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.079$ | H-atom parameters constrained |
| $wR(F^2) = 0.170$ | $w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 2.6389P]$ |
| $S = 1.18$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 16659 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 1189 parameters | $\Delta\rho_{\text{max}} = 0.20 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$ |
| | Extinction correction: none |

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| S1 | 0.42109 (11) | 0.61616 (11) | 0.07142 (3) | 0.0553 (3) |
| S2 | 0.14531 (11) | 0.11317 (11) | 0.06884 (3) | 0.0579 (3) |
| S3 | 0.07836 (11) | 0.54707 (11) | 0.42913 (3) | 0.0567 (3) |
| S4 | 0.35545 (11) | 0.04298 (11) | 0.43006 (3) | 0.0585 (3) |
| Cl1 | 0.10000 (18) | 1.01418 (16) | 0.22600 (4) | 0.1147 (6) |
| Cl2 | 0.61254 (15) | 0.50839 (14) | 0.22440 (3) | 0.0899 (5) |
| Cl3 | 0.39882 (16) | 0.78415 (17) | 0.27399 (4) | 0.1059 (6) |
| Cl4 | -0.10384 (17) | 0.28896 (15) | 0.27441 (4) | 0.1043 (5) |
| O1 | 0.2278 (3) | 0.5609 (3) | 0.11499 (8) | 0.0651 (9) |
| O2 | 0.3808 (3) | 0.0567 (3) | 0.11194 (8) | 0.0649 (9) |
| O3 | 0.2759 (3) | 0.4471 (3) | 0.38692 (7) | 0.0641 (9) |
| O4 | 0.1214 (3) | -0.0536 (3) | 0.38623 (8) | 0.0676 (9) |
| N1 | 0.5469 (3) | 0.7207 (3) | 0.12701 (8) | 0.0449 (8) |
| N2 | 0.0699 (3) | 0.2136 (3) | 0.12441 (9) | 0.0497 (9) |
| N3 | -0.0485 (3) | 0.5935 (3) | 0.37340 (8) | 0.0443 (8) |
| N4 | 0.4325 (3) | 0.0908 (3) | 0.37470 (8) | 0.0488 (9) |
| C1 | 0.5563 (4) | 0.6405 (4) | 0.10171 (10) | 0.0442 (10) |

| | | | | |
|-----|------------|------------|--------------|-------------|
| C2 | 0.6565 (4) | 0.7432 (4) | 0.14938 (11) | 0.0513 (11) |
| C3 | 0.7697 (4) | 0.6814 (4) | 0.14609 (12) | 0.0599 (13) |
| H3 | 0.8414 | 0.6982 | 0.1617 | 0.072* |
| C4 | 0.8947 (5) | 0.5242 (5) | 0.11514 (15) | 0.0709 (15) |
| H4 | 0.9686 | 0.5384 | 0.1301 | 0.085* |
| C5 | 0.8961 (5) | 0.4388 (5) | 0.08922 (15) | 0.0751 (15) |
| H5 | 0.9715 | 0.3940 | 0.0868 | 0.090* |
| C6 | 0.7863 (5) | 0.4157 (5) | 0.06576 (15) | 0.0820 (16) |
| H6 | 0.7897 | 0.3571 | 0.0480 | 0.098* |
| C7 | 0.6758 (5) | 0.4798 (4) | 0.06949 (12) | 0.0651 (13) |
| H7 | 0.6030 | 0.4643 | 0.0542 | 0.078* |
| C8 | 0.6694 (4) | 0.5695 (4) | 0.09612 (11) | 0.0503 (11) |
| C9 | 0.7796 (4) | 0.5918 (4) | 0.11926 (12) | 0.0535 (12) |
| C10 | 0.6416 (5) | 0.8365 (4) | 0.17693 (11) | 0.0534 (12) |
| C11 | 0.7456 (5) | 0.9117 (5) | 0.19087 (12) | 0.0718 (15) |
| H11 | 0.8258 | 0.9046 | 0.1827 | 0.086* |
| C12 | 0.7303 (7) | 0.9976 (5) | 0.21713 (14) | 0.0850 (18) |
| H12 | 0.8012 | 1.0469 | 0.2266 | 0.102* |
| C13 | 0.6139 (7) | 1.0107 (5) | 0.22922 (12) | 0.0787 (17) |
| H13 | 0.6056 | 1.0683 | 0.2470 | 0.094* |
| C14 | 0.5096 (6) | 0.9402 (5) | 0.21551 (12) | 0.0765 (16) |
| H14 | 0.4295 | 0.9497 | 0.2237 | 0.092* |
| C15 | 0.5225 (5) | 0.8539 (4) | 0.18924 (11) | 0.0645 (13) |
| H15 | 0.4501 | 0.8067 | 0.1797 | 0.077* |
| C16 | 0.3010 (4) | 0.7185 (4) | 0.08743 (10) | 0.0469 (11) |
| H16 | 0.3427 | 0.7977 | 0.0954 | 0.056* |
| C17 | 0.1996 (4) | 0.7312 (4) | 0.05883 (10) | 0.0496 (11) |
| C18 | 0.2187 (5) | 0.8173 (4) | 0.03890 (11) | 0.0610 (13) |
| H18 | 0.2907 | 0.8699 | 0.0437 | 0.073* |
| C19 | 0.1304 (6) | 0.8252 (5) | 0.01176 (12) | 0.0798 (17) |
| H19 | 0.1432 | 0.8839 | -0.0014 | 0.096* |
| C20 | 0.0249 (7) | 0.7478 (7) | 0.00426 (14) | 0.0926 (19) |
| H20 | -0.0326 | 0.7525 | -0.0143 | 0.111* |
| C21 | 0.0041 (6) | 0.6640 (6) | 0.02393 (15) | 0.0936 (19) |
| H21 | -0.0691 | 0.6129 | 0.0193 | 0.112* |
| C22 | 0.0919 (5) | 0.6549 (5) | 0.05077 (13) | 0.0753 (15) |
| H22 | 0.0781 | 0.5957 | 0.0637 | 0.090* |
| C23 | 0.2408 (4) | 0.6697 (4) | 0.11495 (10) | 0.0482 (11) |
| C24 | 0.1986 (4) | 0.7581 (4) | 0.14110 (10) | 0.0457 (10) |
| C25 | 0.1895 (4) | 0.8808 (4) | 0.13938 (11) | 0.0604 (13) |
| H25 | 0.2056 | 0.9108 | 0.1206 | 0.073* |
| C26 | 0.1565 (5) | 0.9601 (5) | 0.16544 (13) | 0.0741 (15) |
| H26 | 0.1500 | 1.0428 | 0.1643 | 0.089* |
| C27 | 0.1340 (5) | 0.9144 (5) | 0.19270 (13) | 0.0713 (15) |
| C28 | 0.1417 (5) | 0.7926 (5) | 0.19530 (13) | 0.0746 (15) |
| H28 | 0.1265 | 0.7635 | 0.2143 | 0.090* |
| C29 | 0.1725 (4) | 0.7147 (5) | 0.16909 (12) | 0.0633 (13) |
| H29 | 0.1759 | 0.6317 | 0.1702 | 0.076* |
| C30 | 0.0383 (4) | 0.1341 (4) | 0.09883 (10) | 0.0474 (11) |

supplementary materials

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|-----|-------------|-------------|--------------|-------------|
| C31 | -0.0183 (4) | 0.2355 (4) | 0.14699 (11) | 0.0530 (12) |
| C32 | -0.1345 (5) | 0.1720 (4) | 0.14294 (13) | 0.0637 (13) |
| H32 | -0.1921 | 0.1874 | 0.1584 | 0.076* |
| C33 | -0.2871 (5) | 0.0162 (5) | 0.11128 (14) | 0.0670 (14) |
| H33 | -0.3471 | 0.0290 | 0.1262 | 0.080* |
| C34 | -0.3135 (5) | -0.0676 (5) | 0.08507 (15) | 0.0759 (16) |
| H34 | -0.3916 | -0.1121 | 0.0823 | 0.091* |
| C35 | -0.2260 (5) | -0.0891 (5) | 0.06191 (14) | 0.0786 (16) |
| H35 | -0.2461 | -0.1472 | 0.0440 | 0.094* |
| C36 | -0.1107 (5) | -0.0242 (4) | 0.06574 (13) | 0.0694 (14) |
| H36 | -0.0522 | -0.0382 | 0.0504 | 0.083* |
| C37 | -0.0807 (4) | 0.0637 (4) | 0.09289 (11) | 0.0503 (11) |
| C38 | -0.1695 (4) | 0.0842 (4) | 0.11611 (12) | 0.0556 (12) |
| C39 | 0.0227 (5) | 0.3273 (4) | 0.17488 (11) | 0.0524 (11) |
| C40 | -0.0677 (5) | 0.3925 (5) | 0.19212 (13) | 0.0769 (15) |
| H40 | -0.1568 | 0.3788 | 0.1859 | 0.092* |
| C41 | -0.0271 (6) | 0.4763 (5) | 0.21811 (14) | 0.0840 (17) |
| H41 | -0.0894 | 0.5174 | 0.2295 | 0.101* |
| C42 | 0.1039 (6) | 0.5015 (5) | 0.22784 (12) | 0.0741 (15) |
| H42 | 0.1307 | 0.5587 | 0.2456 | 0.089* |
| C43 | 0.1937 (5) | 0.4391 (5) | 0.21048 (12) | 0.0710 (14) |
| H43 | 0.2827 | 0.4541 | 0.2165 | 0.085* |
| C44 | 0.1530 (5) | 0.3547 (4) | 0.18427 (11) | 0.0637 (13) |
| H44 | 0.2155 | 0.3151 | 0.1726 | 0.076* |
| C45 | 0.2801 (4) | 0.2157 (4) | 0.08546 (10) | 0.0477 (11) |
| H45 | 0.2453 | 0.2937 | 0.0941 | 0.057* |
| C46 | 0.3547 (4) | 0.2334 (4) | 0.05736 (10) | 0.0482 (11) |
| C47 | 0.3183 (5) | 0.3232 (4) | 0.03839 (11) | 0.0622 (13) |
| H47 | 0.2504 | 0.3748 | 0.0435 | 0.075* |
| C48 | 0.3820 (6) | 0.3371 (6) | 0.01172 (13) | 0.0824 (17) |
| H48 | 0.3573 | 0.3982 | -0.0007 | 0.099* |
| C49 | 0.4815 (7) | 0.2608 (7) | 0.00379 (13) | 0.091 (2) |
| H49 | 0.5244 | 0.2700 | -0.0140 | 0.109* |
| C50 | 0.5168 (6) | 0.1716 (6) | 0.02208 (15) | 0.0924 (19) |
| H50 | 0.5837 | 0.1193 | 0.0166 | 0.111* |
| C51 | 0.4549 (5) | 0.1579 (5) | 0.04858 (13) | 0.0778 (16) |
| H51 | 0.4810 | 0.0967 | 0.0609 | 0.093* |
| C52 | 0.3672 (4) | 0.1656 (4) | 0.11212 (10) | 0.0466 (11) |
| C53 | 0.4354 (4) | 0.2524 (4) | 0.13870 (10) | 0.0444 (10) |
| C54 | 0.4428 (4) | 0.3758 (4) | 0.13719 (11) | 0.0572 (12) |
| H54 | 0.4097 | 0.4065 | 0.1185 | 0.069* |
| C55 | 0.4995 (5) | 0.4535 (4) | 0.16347 (12) | 0.0643 (13) |
| H55 | 0.5043 | 0.5364 | 0.1623 | 0.077* |
| C56 | 0.5484 (4) | 0.4096 (5) | 0.19114 (11) | 0.0602 (13) |
| C57 | 0.5453 (5) | 0.2867 (5) | 0.19298 (11) | 0.0633 (13) |
| H57 | 0.5806 | 0.2564 | 0.2116 | 0.076* |
| C58 | 0.4886 (4) | 0.2090 (4) | 0.16647 (11) | 0.0552 (12) |
| H58 | 0.4864 | 0.1259 | 0.1675 | 0.066* |
| C59 | -0.0568 (4) | 0.5391 (4) | 0.39884 (11) | 0.0469 (11) |

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|-----|-------------|------------|--------------|-------------|
| C60 | -0.1576 (4) | 0.5924 (4) | 0.35095 (11) | 0.0512 (11) |
| C61 | -0.2698 (4) | 0.5344 (4) | 0.35485 (12) | 0.0602 (13) |
| H61 | -0.3419 | 0.5355 | 0.3394 | 0.072* |
| C62 | -0.3943 (4) | 0.4108 (4) | 0.38677 (13) | 0.0650 (14) |
| H62 | -0.4691 | 0.4103 | 0.3721 | 0.078* |
| C63 | -0.3958 (5) | 0.3520 (5) | 0.41298 (15) | 0.0745 (16) |
| H63 | -0.4718 | 0.3117 | 0.4160 | 0.089* |
| C64 | -0.2857 (5) | 0.3513 (5) | 0.43526 (14) | 0.0769 (15) |
| H64 | -0.2878 | 0.3090 | 0.4528 | 0.092* |
| C65 | -0.1745 (5) | 0.4121 (4) | 0.43169 (13) | 0.0689 (14) |
| H65 | -0.1017 | 0.4125 | 0.4470 | 0.083* |
| C66 | -0.1693 (4) | 0.4742 (4) | 0.40486 (11) | 0.0514 (11) |
| C67 | -0.2806 (4) | 0.4724 (4) | 0.38164 (12) | 0.0534 (12) |
| C68 | -0.1420 (4) | 0.6565 (4) | 0.32276 (10) | 0.0501 (11) |
| C69 | -0.2493 (5) | 0.6979 (5) | 0.30449 (13) | 0.0786 (16) |
| H69 | -0.3329 | 0.6863 | 0.3101 | 0.094* |
| C70 | -0.2342 (6) | 0.7561 (5) | 0.27811 (14) | 0.0853 (17) |
| H70 | -0.3077 | 0.7814 | 0.2659 | 0.102* |
| C71 | -0.1128 (6) | 0.7768 (4) | 0.26987 (12) | 0.0688 (14) |
| H71 | -0.1026 | 0.8159 | 0.2521 | 0.083* |
| C72 | -0.0060 (5) | 0.7390 (4) | 0.28833 (12) | 0.0678 (14) |
| H72 | 0.0775 | 0.7538 | 0.2831 | 0.081* |
| C73 | -0.0196 (5) | 0.6797 (4) | 0.31429 (11) | 0.0584 (12) |
| H73 | 0.0546 | 0.6547 | 0.3264 | 0.070* |
| C74 | 0.2000 (4) | 0.6320 (4) | 0.41328 (10) | 0.0469 (11) |
| H74 | 0.1588 | 0.7026 | 0.4049 | 0.056* |
| C75 | 0.3000 (4) | 0.6750 (4) | 0.44182 (10) | 0.0482 (11) |
| C76 | 0.4083 (5) | 0.6089 (5) | 0.45012 (13) | 0.0773 (16) |
| H76 | 0.4253 | 0.5377 | 0.4371 | 0.093* |
| C77 | 0.4928 (6) | 0.6470 (6) | 0.47773 (16) | 0.0961 (19) |
| H77 | 0.5639 | 0.5992 | 0.4833 | 0.115* |
| C78 | 0.4744 (7) | 0.7507 (7) | 0.49652 (14) | 0.096 (2) |
| H78 | 0.5338 | 0.7766 | 0.5145 | 0.115* |
| C79 | 0.3670 (7) | 0.8181 (6) | 0.48887 (13) | 0.0870 (18) |
| H79 | 0.3519 | 0.8891 | 0.5022 | 0.104* |
| C80 | 0.2798 (5) | 0.7818 (4) | 0.46142 (11) | 0.0625 (13) |
| H80 | 0.2080 | 0.8294 | 0.4563 | 0.075* |
| C81 | 0.2611 (4) | 0.5553 (4) | 0.38657 (10) | 0.0472 (11) |
| C82 | 0.3034 (4) | 0.6155 (4) | 0.35966 (10) | 0.0447 (10) |
| C83 | 0.3152 (4) | 0.7404 (4) | 0.36117 (11) | 0.0596 (12) |
| H83 | 0.3011 | 0.7899 | 0.3800 | 0.071* |
| C84 | 0.3475 (5) | 0.7917 (5) | 0.33525 (12) | 0.0681 (14) |
| H84 | 0.3568 | 0.8755 | 0.3366 | 0.082* |
| C85 | 0.3660 (4) | 0.7189 (5) | 0.30744 (12) | 0.0635 (13) |
| C86 | 0.3579 (5) | 0.5957 (5) | 0.30527 (12) | 0.0692 (14) |
| H86 | 0.3729 | 0.5471 | 0.2864 | 0.083* |
| C87 | 0.3269 (4) | 0.5436 (4) | 0.33184 (11) | 0.0578 (12) |
| H87 | 0.3220 | 0.4596 | 0.3307 | 0.069* |
| C88 | 0.4639 (4) | 0.0348 (4) | 0.40022 (10) | 0.0458 (10) |

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|------|-------------|-------------|--------------|-------------|
| C89 | 0.5224 (4) | 0.0906 (4) | 0.35278 (11) | 0.0526 (11) |
| C90 | 0.6387 (5) | 0.0307 (4) | 0.35657 (12) | 0.0630 (13) |
| H90 | 0.6969 | 0.0315 | 0.3413 | 0.076* |
| C91 | 0.7890 (5) | -0.0957 (5) | 0.38808 (14) | 0.0703 (14) |
| H91 | 0.8493 | -0.0974 | 0.3732 | 0.084* |
| C92 | 0.8152 (5) | -0.1544 (5) | 0.41401 (16) | 0.0795 (16) |
| H92 | 0.8933 | -0.1960 | 0.4168 | 0.095* |
| C93 | 0.7265 (5) | -0.1536 (5) | 0.43686 (15) | 0.0801 (16) |
| H93 | 0.7455 | -0.1949 | 0.4546 | 0.096* |
| C94 | 0.6115 (5) | -0.0917 (4) | 0.43297 (12) | 0.0674 (14) |
| H94 | 0.5529 | -0.0905 | 0.4482 | 0.081* |
| C95 | 0.5820 (4) | -0.0305 (4) | 0.40621 (11) | 0.0514 (11) |
| C96 | 0.6712 (4) | -0.0315 (4) | 0.38316 (12) | 0.0556 (12) |
| C97 | 0.4834 (5) | 0.1576 (4) | 0.32549 (11) | 0.0552 (12) |
| C98 | 0.5761 (5) | 0.2219 (5) | 0.31243 (12) | 0.0709 (14) |
| H98 | 0.6635 | 0.2228 | 0.3211 | 0.085* |
| C99 | 0.5390 (7) | 0.2846 (5) | 0.28655 (14) | 0.0857 (18) |
| H99 | 0.6015 | 0.3279 | 0.2782 | 0.103* |
| C100 | 0.4091 (7) | 0.2830 (5) | 0.27303 (13) | 0.0848 (18) |
| H100 | 0.3841 | 0.3231 | 0.2553 | 0.102* |
| C101 | 0.3186 (6) | 0.2213 (5) | 0.28635 (14) | 0.0843 (17) |
| H101 | 0.2311 | 0.2207 | 0.2777 | 0.101* |
| C102 | 0.3546 (5) | 0.1608 (5) | 0.31200 (12) | 0.0690 (14) |
| H102 | 0.2906 | 0.1205 | 0.3207 | 0.083* |
| C103 | 0.2225 (4) | 0.1309 (4) | 0.41367 (10) | 0.0470 (11) |
| H103 | 0.2586 | 0.2010 | 0.4056 | 0.056* |
| C104 | 0.1470 (4) | 0.1752 (4) | 0.44165 (10) | 0.0510 (11) |
| C105 | 0.1837 (5) | 0.2833 (4) | 0.46091 (11) | 0.0619 (13) |
| H105 | 0.2514 | 0.3305 | 0.4559 | 0.074* |
| C106 | 0.1194 (6) | 0.3217 (6) | 0.48775 (13) | 0.0834 (17) |
| H106 | 0.1444 | 0.3945 | 0.5006 | 0.100* |
| C107 | 0.0206 (7) | 0.2535 (7) | 0.49527 (14) | 0.097 (2) |
| H107 | -0.0224 | 0.2801 | 0.5131 | 0.116* |
| C108 | -0.0157 (6) | 0.1463 (6) | 0.47688 (16) | 0.098 (2) |
| H108 | -0.0823 | 0.0990 | 0.4823 | 0.118* |
| C109 | 0.0469 (5) | 0.1076 (5) | 0.45008 (13) | 0.0753 (15) |
| H109 | 0.0210 | 0.0346 | 0.4375 | 0.090* |
| C110 | 0.1354 (4) | 0.0551 (4) | 0.38612 (11) | 0.0501 (11) |
| C111 | 0.0696 (4) | 0.1168 (4) | 0.35991 (10) | 0.0467 (11) |
| C112 | 0.0135 (5) | 0.0459 (4) | 0.33201 (11) | 0.0608 (13) |
| H112 | 0.0133 | -0.0382 | 0.3309 | 0.073* |
| C113 | -0.0416 (5) | 0.0984 (5) | 0.30600 (12) | 0.0707 (14) |
| H113 | -0.0778 | 0.0504 | 0.2873 | 0.085* |
| C114 | -0.0425 (5) | 0.2222 (5) | 0.30788 (12) | 0.0665 (14) |
| C115 | 0.0082 (5) | 0.2946 (4) | 0.33513 (13) | 0.0690 (14) |
| H115 | 0.0052 | 0.3786 | 0.3361 | 0.083* |
| C116 | 0.0638 (4) | 0.2421 (4) | 0.36114 (11) | 0.0614 (13) |
| H116 | 0.0979 | 0.2913 | 0.3798 | 0.074* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| S1 | 0.0443 (7) | 0.0687 (8) | 0.0495 (7) | 0.0062 (6) | 0.0026 (5) | -0.0020 (6) |
| S2 | 0.0463 (7) | 0.0730 (8) | 0.0533 (7) | -0.0078 (6) | 0.0113 (6) | -0.0007 (6) |
| S3 | 0.0434 (7) | 0.0755 (9) | 0.0520 (7) | -0.0070 (6) | 0.0014 (5) | 0.0147 (6) |
| S4 | 0.0492 (7) | 0.0738 (9) | 0.0550 (7) | 0.0076 (6) | 0.0096 (6) | 0.0142 (6) |
| Cl1 | 0.1194 (14) | 0.1273 (14) | 0.0909 (12) | -0.0069 (11) | 0.0413 (10) | -0.0355 (10) |
| Cl2 | 0.0963 (11) | 0.0992 (11) | 0.0664 (9) | -0.0146 (9) | -0.0021 (8) | -0.0074 (8) |
| Cl3 | 0.1045 (12) | 0.1482 (15) | 0.0782 (11) | 0.0078 (11) | 0.0266 (9) | 0.0498 (10) |
| Cl4 | 0.1242 (14) | 0.1077 (12) | 0.0787 (11) | 0.0035 (10) | -0.0172 (9) | 0.0288 (9) |
| O1 | 0.073 (2) | 0.050 (2) | 0.077 (2) | 0.0054 (17) | 0.0175 (18) | 0.0164 (17) |
| O2 | 0.069 (2) | 0.049 (2) | 0.080 (2) | 0.0000 (16) | 0.0094 (18) | 0.0180 (17) |
| O3 | 0.074 (2) | 0.045 (2) | 0.073 (2) | -0.0001 (17) | 0.0129 (18) | 0.0022 (16) |
| O4 | 0.072 (2) | 0.048 (2) | 0.080 (2) | -0.0001 (17) | 0.0017 (18) | 0.0042 (17) |
| N1 | 0.041 (2) | 0.048 (2) | 0.045 (2) | -0.0026 (16) | 0.0011 (17) | 0.0085 (17) |
| N2 | 0.045 (2) | 0.054 (2) | 0.053 (2) | 0.0075 (18) | 0.0102 (18) | 0.0140 (19) |
| N3 | 0.038 (2) | 0.046 (2) | 0.047 (2) | 0.0000 (16) | 0.0005 (17) | 0.0034 (17) |
| N4 | 0.046 (2) | 0.052 (2) | 0.048 (2) | -0.0023 (17) | 0.0098 (18) | 0.0003 (18) |
| C1 | 0.036 (2) | 0.049 (3) | 0.049 (3) | -0.002 (2) | 0.004 (2) | 0.014 (2) |
| C2 | 0.051 (3) | 0.050 (3) | 0.053 (3) | -0.006 (2) | 0.002 (2) | 0.012 (2) |
| C3 | 0.044 (3) | 0.068 (3) | 0.066 (3) | -0.002 (2) | -0.006 (2) | 0.017 (3) |
| C4 | 0.045 (3) | 0.066 (4) | 0.107 (5) | 0.009 (3) | 0.010 (3) | 0.030 (3) |
| C5 | 0.060 (4) | 0.067 (4) | 0.104 (5) | 0.019 (3) | 0.023 (3) | 0.021 (3) |
| C6 | 0.068 (4) | 0.073 (4) | 0.104 (5) | 0.015 (3) | 0.019 (4) | 0.002 (3) |
| C7 | 0.048 (3) | 0.076 (4) | 0.070 (3) | 0.009 (3) | 0.008 (3) | 0.003 (3) |
| C8 | 0.042 (3) | 0.050 (3) | 0.061 (3) | 0.000 (2) | 0.012 (2) | 0.011 (2) |
| C9 | 0.045 (3) | 0.052 (3) | 0.067 (3) | 0.001 (2) | 0.009 (2) | 0.018 (2) |
| C10 | 0.056 (3) | 0.053 (3) | 0.050 (3) | 0.000 (2) | -0.006 (2) | 0.014 (2) |
| C11 | 0.067 (3) | 0.073 (4) | 0.066 (3) | -0.005 (3) | -0.019 (3) | 0.000 (3) |
| C12 | 0.100 (5) | 0.070 (4) | 0.071 (4) | 0.005 (3) | -0.030 (4) | -0.005 (3) |
| C13 | 0.112 (5) | 0.066 (4) | 0.051 (3) | 0.025 (4) | -0.012 (4) | -0.001 (3) |
| C14 | 0.099 (5) | 0.078 (4) | 0.052 (3) | 0.016 (3) | 0.006 (3) | 0.009 (3) |
| C15 | 0.071 (4) | 0.069 (3) | 0.053 (3) | -0.004 (3) | 0.004 (3) | 0.011 (3) |
| C16 | 0.046 (3) | 0.048 (3) | 0.047 (3) | 0.000 (2) | 0.006 (2) | 0.007 (2) |
| C17 | 0.045 (3) | 0.060 (3) | 0.044 (3) | 0.009 (2) | 0.002 (2) | 0.008 (2) |
| C18 | 0.061 (3) | 0.069 (3) | 0.056 (3) | 0.013 (3) | 0.012 (3) | 0.012 (3) |
| C19 | 0.100 (5) | 0.093 (4) | 0.052 (3) | 0.034 (4) | 0.016 (3) | 0.026 (3) |
| C20 | 0.091 (5) | 0.117 (6) | 0.062 (4) | 0.026 (4) | -0.016 (3) | 0.004 (4) |
| C21 | 0.077 (4) | 0.104 (5) | 0.089 (5) | -0.001 (4) | -0.028 (4) | 0.008 (4) |
| C22 | 0.063 (4) | 0.083 (4) | 0.078 (4) | -0.006 (3) | -0.012 (3) | 0.020 (3) |
| C23 | 0.037 (2) | 0.054 (3) | 0.056 (3) | 0.002 (2) | 0.002 (2) | 0.014 (2) |
| C24 | 0.041 (3) | 0.057 (3) | 0.042 (3) | 0.004 (2) | 0.007 (2) | 0.017 (2) |
| C25 | 0.071 (3) | 0.063 (3) | 0.052 (3) | 0.013 (3) | 0.017 (3) | 0.016 (2) |
| C26 | 0.083 (4) | 0.062 (3) | 0.081 (4) | 0.021 (3) | 0.026 (3) | 0.008 (3) |
| C27 | 0.059 (3) | 0.081 (4) | 0.070 (4) | -0.003 (3) | 0.013 (3) | -0.009 (3) |
| C28 | 0.081 (4) | 0.088 (4) | 0.057 (3) | -0.010 (3) | 0.021 (3) | 0.007 (3) |

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|-----|-----------|-----------|-----------|------------|------------|------------|
| C29 | 0.063 (3) | 0.068 (3) | 0.062 (3) | -0.005 (3) | 0.010 (3) | 0.016 (3) |
| C30 | 0.044 (3) | 0.049 (3) | 0.050 (3) | 0.005 (2) | 0.005 (2) | 0.012 (2) |
| C31 | 0.049 (3) | 0.060 (3) | 0.056 (3) | 0.015 (2) | 0.016 (2) | 0.019 (2) |
| C32 | 0.050 (3) | 0.070 (3) | 0.078 (4) | 0.007 (3) | 0.023 (3) | 0.021 (3) |
| C33 | 0.050 (3) | 0.068 (3) | 0.088 (4) | -0.004 (3) | 0.015 (3) | 0.023 (3) |
| C34 | 0.051 (3) | 0.069 (4) | 0.109 (5) | -0.008 (3) | 0.005 (3) | 0.021 (3) |
| C35 | 0.069 (4) | 0.073 (4) | 0.089 (4) | -0.016 (3) | 0.005 (3) | -0.003 (3) |
| C36 | 0.049 (3) | 0.074 (4) | 0.084 (4) | -0.010 (3) | 0.009 (3) | 0.002 (3) |
| C37 | 0.042 (3) | 0.052 (3) | 0.060 (3) | 0.001 (2) | 0.004 (2) | 0.018 (2) |
| C38 | 0.041 (3) | 0.057 (3) | 0.073 (3) | 0.002 (2) | 0.011 (2) | 0.021 (3) |
| C39 | 0.055 (3) | 0.056 (3) | 0.051 (3) | 0.011 (2) | 0.017 (2) | 0.013 (2) |
| C40 | 0.064 (3) | 0.095 (4) | 0.072 (4) | 0.004 (3) | 0.026 (3) | -0.003 (3) |
| C41 | 0.083 (4) | 0.094 (4) | 0.075 (4) | 0.014 (3) | 0.030 (3) | -0.007 (3) |
| C42 | 0.092 (4) | 0.075 (4) | 0.055 (3) | -0.002 (3) | 0.017 (3) | 0.002 (3) |
| C43 | 0.066 (3) | 0.087 (4) | 0.060 (3) | 0.009 (3) | 0.004 (3) | 0.008 (3) |
| C44 | 0.061 (3) | 0.078 (4) | 0.052 (3) | 0.016 (3) | 0.011 (3) | 0.005 (3) |
| C45 | 0.043 (3) | 0.051 (3) | 0.051 (3) | 0.001 (2) | 0.010 (2) | 0.009 (2) |
| C46 | 0.044 (3) | 0.055 (3) | 0.044 (3) | -0.008 (2) | 0.006 (2) | 0.003 (2) |
| C47 | 0.062 (3) | 0.066 (3) | 0.060 (3) | -0.008 (3) | 0.001 (3) | 0.016 (3) |
| C48 | 0.093 (5) | 0.102 (5) | 0.054 (3) | -0.036 (4) | -0.005 (3) | 0.027 (3) |
| C49 | 0.100 (5) | 0.124 (6) | 0.050 (4) | -0.037 (4) | 0.026 (3) | 0.000 (4) |
| C50 | 0.092 (5) | 0.108 (5) | 0.087 (5) | 0.005 (4) | 0.050 (4) | 0.013 (4) |
| C51 | 0.076 (4) | 0.083 (4) | 0.083 (4) | 0.012 (3) | 0.034 (3) | 0.020 (3) |
| C52 | 0.042 (3) | 0.050 (3) | 0.051 (3) | 0.000 (2) | 0.013 (2) | 0.015 (2) |
| C53 | 0.040 (2) | 0.052 (3) | 0.043 (3) | 0.004 (2) | 0.008 (2) | 0.012 (2) |
| C54 | 0.063 (3) | 0.056 (3) | 0.055 (3) | -0.002 (2) | -0.001 (2) | 0.021 (2) |
| C55 | 0.073 (3) | 0.059 (3) | 0.061 (3) | -0.012 (3) | -0.001 (3) | 0.019 (3) |
| C56 | 0.050 (3) | 0.076 (4) | 0.056 (3) | -0.003 (3) | 0.012 (2) | 0.009 (3) |
| C57 | 0.073 (3) | 0.074 (4) | 0.046 (3) | 0.016 (3) | 0.008 (3) | 0.019 (3) |
| C58 | 0.059 (3) | 0.055 (3) | 0.054 (3) | 0.010 (2) | 0.009 (2) | 0.015 (2) |
| C59 | 0.040 (3) | 0.043 (3) | 0.055 (3) | 0.005 (2) | 0.003 (2) | 0.000 (2) |
| C60 | 0.041 (3) | 0.048 (3) | 0.060 (3) | 0.000 (2) | -0.001 (2) | -0.003 (2) |
| C61 | 0.042 (3) | 0.064 (3) | 0.069 (3) | 0.000 (2) | -0.007 (2) | 0.002 (3) |
| C62 | 0.041 (3) | 0.065 (3) | 0.084 (4) | -0.009 (2) | 0.006 (3) | -0.007 (3) |
| C63 | 0.050 (3) | 0.065 (4) | 0.112 (5) | -0.008 (3) | 0.023 (3) | 0.012 (3) |
| C64 | 0.065 (4) | 0.083 (4) | 0.089 (4) | -0.010 (3) | 0.020 (3) | 0.025 (3) |
| C65 | 0.053 (3) | 0.078 (4) | 0.078 (4) | -0.010 (3) | 0.007 (3) | 0.019 (3) |
| C66 | 0.043 (3) | 0.046 (3) | 0.063 (3) | -0.001 (2) | 0.008 (2) | 0.000 (2) |
| C67 | 0.038 (3) | 0.048 (3) | 0.071 (3) | 0.000 (2) | 0.006 (2) | -0.003 (2) |
| C68 | 0.051 (3) | 0.046 (3) | 0.049 (3) | 0.003 (2) | -0.008 (2) | 0.002 (2) |
| C69 | 0.058 (3) | 0.091 (4) | 0.086 (4) | -0.003 (3) | -0.013 (3) | 0.029 (3) |
| C70 | 0.067 (4) | 0.099 (5) | 0.089 (4) | 0.002 (3) | -0.023 (3) | 0.037 (4) |
| C71 | 0.086 (4) | 0.058 (3) | 0.059 (3) | -0.001 (3) | -0.005 (3) | 0.007 (2) |
| C72 | 0.066 (3) | 0.075 (4) | 0.062 (3) | 0.010 (3) | 0.007 (3) | 0.007 (3) |
| C73 | 0.049 (3) | 0.067 (3) | 0.057 (3) | 0.009 (2) | -0.004 (2) | 0.009 (2) |
| C74 | 0.043 (3) | 0.049 (3) | 0.048 (3) | 0.000 (2) | 0.004 (2) | 0.007 (2) |
| C75 | 0.047 (3) | 0.057 (3) | 0.042 (3) | -0.011 (2) | 0.009 (2) | 0.008 (2) |
| C76 | 0.064 (4) | 0.082 (4) | 0.078 (4) | 0.001 (3) | -0.019 (3) | 0.004 (3) |
| C77 | 0.080 (4) | 0.111 (5) | 0.090 (5) | -0.003 (4) | -0.027 (4) | 0.015 (4) |

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| C78 | 0.090 (5) | 0.125 (6) | 0.065 (4) | -0.038 (4) | -0.022 (4) | 0.011 (4) |
| C79 | 0.111 (5) | 0.092 (4) | 0.052 (4) | -0.044 (4) | 0.013 (3) | -0.013 (3) |
| C80 | 0.067 (3) | 0.067 (3) | 0.052 (3) | -0.009 (3) | 0.011 (3) | 0.001 (3) |
| C81 | 0.036 (2) | 0.050 (3) | 0.052 (3) | -0.005 (2) | -0.003 (2) | -0.002 (2) |
| C82 | 0.036 (2) | 0.047 (3) | 0.049 (3) | -0.001 (2) | 0.006 (2) | -0.002 (2) |
| C83 | 0.061 (3) | 0.058 (3) | 0.058 (3) | -0.003 (2) | 0.009 (2) | 0.002 (2) |
| C84 | 0.078 (4) | 0.061 (3) | 0.067 (4) | -0.016 (3) | 0.012 (3) | 0.013 (3) |
| C85 | 0.051 (3) | 0.088 (4) | 0.053 (3) | -0.002 (3) | 0.009 (2) | 0.012 (3) |
| C86 | 0.070 (4) | 0.092 (4) | 0.044 (3) | 0.014 (3) | 0.009 (3) | 0.001 (3) |
| C87 | 0.059 (3) | 0.054 (3) | 0.057 (3) | 0.010 (2) | 0.002 (2) | -0.003 (2) |
| C88 | 0.041 (3) | 0.049 (3) | 0.046 (3) | -0.006 (2) | 0.007 (2) | 0.001 (2) |
| C89 | 0.051 (3) | 0.051 (3) | 0.056 (3) | -0.006 (2) | 0.015 (2) | -0.001 (2) |
| C90 | 0.060 (3) | 0.064 (3) | 0.067 (3) | 0.000 (3) | 0.023 (3) | 0.001 (3) |
| C91 | 0.043 (3) | 0.070 (4) | 0.096 (4) | 0.005 (3) | 0.012 (3) | 0.001 (3) |
| C92 | 0.058 (4) | 0.063 (4) | 0.118 (5) | 0.019 (3) | 0.008 (4) | 0.013 (3) |
| C93 | 0.064 (4) | 0.077 (4) | 0.102 (5) | 0.017 (3) | 0.002 (3) | 0.026 (3) |
| C94 | 0.059 (3) | 0.071 (3) | 0.073 (4) | 0.011 (3) | 0.007 (3) | 0.013 (3) |
| C95 | 0.042 (3) | 0.048 (3) | 0.062 (3) | -0.002 (2) | 0.003 (2) | 0.002 (2) |
| C96 | 0.046 (3) | 0.048 (3) | 0.070 (3) | -0.004 (2) | 0.011 (2) | -0.002 (2) |
| C97 | 0.065 (3) | 0.050 (3) | 0.051 (3) | 0.004 (2) | 0.017 (3) | -0.003 (2) |
| C98 | 0.074 (4) | 0.080 (4) | 0.065 (3) | 0.004 (3) | 0.026 (3) | 0.014 (3) |
| C99 | 0.119 (6) | 0.081 (4) | 0.067 (4) | 0.008 (4) | 0.044 (4) | 0.016 (3) |
| C100 | 0.117 (5) | 0.084 (4) | 0.056 (4) | 0.028 (4) | 0.019 (4) | 0.011 (3) |
| C101 | 0.092 (5) | 0.090 (4) | 0.068 (4) | 0.013 (4) | 0.004 (3) | 0.003 (3) |
| C102 | 0.071 (4) | 0.076 (4) | 0.060 (3) | 0.000 (3) | 0.006 (3) | 0.013 (3) |
| C103 | 0.043 (3) | 0.049 (3) | 0.049 (3) | -0.002 (2) | 0.005 (2) | 0.007 (2) |
| C104 | 0.049 (3) | 0.055 (3) | 0.048 (3) | 0.009 (2) | 0.002 (2) | 0.005 (2) |
| C105 | 0.065 (3) | 0.065 (3) | 0.052 (3) | 0.010 (3) | -0.001 (3) | 0.002 (2) |
| C106 | 0.100 (5) | 0.088 (4) | 0.055 (4) | 0.026 (4) | -0.005 (3) | -0.008 (3) |
| C107 | 0.106 (5) | 0.125 (6) | 0.065 (4) | 0.045 (5) | 0.031 (4) | 0.016 (4) |
| C108 | 0.106 (5) | 0.105 (5) | 0.094 (5) | 0.011 (4) | 0.054 (4) | 0.016 (4) |
| C109 | 0.080 (4) | 0.075 (4) | 0.075 (4) | -0.003 (3) | 0.027 (3) | 0.005 (3) |
| C110 | 0.042 (3) | 0.049 (3) | 0.058 (3) | 0.002 (2) | 0.012 (2) | -0.004 (2) |
| C111 | 0.043 (3) | 0.047 (3) | 0.047 (3) | 0.000 (2) | 0.005 (2) | -0.004 (2) |
| C112 | 0.071 (3) | 0.053 (3) | 0.055 (3) | -0.013 (2) | 0.008 (3) | -0.004 (2) |
| C113 | 0.077 (4) | 0.071 (4) | 0.059 (3) | -0.012 (3) | 0.002 (3) | -0.006 (3) |
| C114 | 0.058 (3) | 0.070 (4) | 0.070 (4) | 0.000 (3) | 0.000 (3) | 0.008 (3) |
| C115 | 0.074 (4) | 0.049 (3) | 0.079 (4) | 0.012 (3) | -0.006 (3) | 0.003 (3) |
| C116 | 0.066 (3) | 0.053 (3) | 0.058 (3) | 0.002 (2) | -0.008 (3) | -0.007 (2) |

Geometric parameters (Å, °)

| | | | |
|--------|-----------|---------|-----------|
| S1—C1 | 1.770 (4) | C51—H51 | 0.9300 |
| S1—C16 | 1.807 (4) | C52—C53 | 1.487 (6) |
| S2—C30 | 1.763 (4) | C53—C58 | 1.380 (6) |
| S2—C45 | 1.809 (4) | C53—C54 | 1.384 (5) |
| S3—C59 | 1.769 (4) | C54—C55 | 1.382 (6) |
| S3—C74 | 1.805 (4) | C54—H54 | 0.9300 |
| S4—C88 | 1.769 (4) | C55—C56 | 1.367 (6) |

supplementary materials

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|----------|-----------|---------|-----------|
| S4—C103 | 1.806 (4) | C55—H55 | 0.9300 |
| C11—C27 | 1.740 (5) | C56—C57 | 1.379 (6) |
| C12—C56 | 1.728 (5) | C57—C58 | 1.390 (6) |
| C13—C85 | 1.735 (5) | C57—H57 | 0.9300 |
| C14—C114 | 1.735 (5) | C58—H58 | 0.9300 |
| O1—C23 | 1.217 (5) | C59—C66 | 1.428 (6) |
| O2—C52 | 1.217 (5) | C60—C61 | 1.359 (6) |
| O3—C81 | 1.214 (5) | C60—C68 | 1.488 (6) |
| O4—C110 | 1.218 (5) | C61—C67 | 1.413 (6) |
| N1—C1 | 1.310 (5) | C61—H61 | 0.9300 |
| N1—C2 | 1.383 (5) | C62—C63 | 1.357 (7) |
| N2—C30 | 1.311 (5) | C62—C67 | 1.407 (6) |
| N2—C31 | 1.389 (5) | C62—H62 | 0.9300 |
| N3—C59 | 1.309 (5) | C63—C64 | 1.386 (7) |
| N3—C60 | 1.380 (5) | C63—H63 | 0.9300 |
| N4—C88 | 1.322 (5) | C64—C65 | 1.360 (6) |
| N4—C89 | 1.380 (5) | C64—H64 | 0.9300 |
| C1—C8 | 1.430 (5) | C65—C66 | 1.407 (6) |
| C2—C3 | 1.364 (6) | C65—H65 | 0.9300 |
| C2—C10 | 1.475 (6) | C66—C67 | 1.416 (6) |
| C3—C9 | 1.419 (6) | C68—C73 | 1.380 (6) |
| C3—H3 | 0.9300 | C68—C69 | 1.385 (6) |
| C4—C5 | 1.351 (7) | C69—C70 | 1.382 (7) |
| C4—C9 | 1.418 (6) | C69—H69 | 0.9300 |
| C4—H4 | 0.9300 | C70—C71 | 1.361 (7) |
| C5—C6 | 1.412 (7) | C70—H70 | 0.9300 |
| C5—H5 | 0.9300 | C71—C72 | 1.371 (6) |
| C6—C7 | 1.355 (6) | C71—H71 | 0.9300 |
| C6—H6 | 0.9300 | C72—C73 | 1.370 (6) |
| C7—C8 | 1.408 (6) | C72—H72 | 0.9300 |
| C7—H7 | 0.9300 | C73—H73 | 0.9300 |
| C8—C9 | 1.406 (6) | C74—C81 | 1.517 (6) |
| C10—C11 | 1.382 (6) | C74—C75 | 1.515 (6) |
| C10—C15 | 1.388 (6) | C74—H74 | 0.9800 |
| C11—C12 | 1.387 (7) | C75—C76 | 1.372 (6) |
| C11—H11 | 0.9300 | C75—C80 | 1.384 (6) |
| C12—C13 | 1.355 (7) | C76—C77 | 1.387 (7) |
| C12—H12 | 0.9300 | C76—H76 | 0.9300 |
| C13—C14 | 1.355 (7) | C77—C78 | 1.337 (8) |
| C13—H13 | 0.9300 | C77—H77 | 0.9300 |
| C14—C15 | 1.386 (7) | C78—C79 | 1.366 (8) |
| C14—H14 | 0.9300 | C78—H78 | 0.9300 |
| C15—H15 | 0.9300 | C79—C80 | 1.394 (7) |
| C16—C17 | 1.522 (5) | C79—H79 | 0.9300 |
| C16—C23 | 1.534 (6) | C80—H80 | 0.9300 |
| C16—H16 | 0.9800 | C81—C82 | 1.496 (6) |
| C17—C22 | 1.377 (6) | C82—C87 | 1.375 (6) |
| C17—C18 | 1.382 (6) | C82—C83 | 1.386 (6) |
| C18—C19 | 1.389 (7) | C83—C84 | 1.371 (6) |

| | | | |
|---------|-----------|-----------|-----------|
| C18—H18 | 0.9300 | C83—H83 | 0.9300 |
| C19—C20 | 1.365 (8) | C84—C85 | 1.367 (7) |
| C19—H19 | 0.9300 | C84—H84 | 0.9300 |
| C20—C21 | 1.358 (8) | C85—C86 | 1.362 (6) |
| C20—H20 | 0.9300 | C86—C87 | 1.394 (6) |
| C21—C22 | 1.378 (7) | C86—H86 | 0.9300 |
| C21—H21 | 0.9300 | C87—H87 | 0.9300 |
| C22—H22 | 0.9300 | C88—C95 | 1.429 (6) |
| C23—C24 | 1.482 (6) | C89—C90 | 1.373 (6) |
| C24—C25 | 1.378 (6) | C89—C97 | 1.470 (6) |
| C24—C29 | 1.386 (6) | C90—C96 | 1.402 (6) |
| C25—C26 | 1.390 (6) | C90—H90 | 0.9300 |
| C25—H25 | 0.9300 | C91—C92 | 1.346 (7) |
| C26—C27 | 1.359 (7) | C91—C96 | 1.415 (6) |
| C26—H26 | 0.9300 | C91—H91 | 0.9300 |
| C27—C28 | 1.374 (7) | C92—C93 | 1.400 (7) |
| C28—C29 | 1.379 (6) | C92—H92 | 0.9300 |
| C28—H28 | 0.9300 | C93—C94 | 1.373 (6) |
| C29—H29 | 0.9300 | C93—H93 | 0.9300 |
| C30—C37 | 1.430 (6) | C94—C95 | 1.397 (6) |
| C31—C32 | 1.369 (6) | C94—H94 | 0.9300 |
| C31—C39 | 1.473 (6) | C95—C96 | 1.410 (6) |
| C32—C38 | 1.405 (6) | C97—C102 | 1.383 (6) |
| C32—H32 | 0.9300 | C97—C98 | 1.395 (6) |
| C33—C34 | 1.350 (7) | C98—C99 | 1.388 (7) |
| C33—C38 | 1.406 (6) | C98—H98 | 0.9300 |
| C33—H33 | 0.9300 | C99—C100 | 1.389 (8) |
| C34—C35 | 1.401 (7) | C99—H99 | 0.9300 |
| C34—H34 | 0.9300 | C100—C101 | 1.368 (8) |
| C35—C36 | 1.369 (6) | C100—H100 | 0.9300 |
| C35—H35 | 0.9300 | C101—C102 | 1.363 (7) |
| C36—C37 | 1.409 (6) | C101—H101 | 0.9300 |
| C36—H36 | 0.9300 | C102—H102 | 0.9300 |
| C37—C38 | 1.412 (6) | C103—C104 | 1.516 (6) |
| C39—C44 | 1.374 (6) | C103—C110 | 1.537 (6) |
| C39—C40 | 1.391 (6) | C103—H103 | 0.9800 |
| C40—C41 | 1.367 (7) | C104—C109 | 1.379 (6) |
| C40—H40 | 0.9300 | C104—C105 | 1.385 (6) |
| C41—C42 | 1.379 (7) | C105—C106 | 1.395 (7) |
| C41—H41 | 0.9300 | C105—H105 | 0.9300 |
| C42—C43 | 1.375 (6) | C106—C107 | 1.358 (8) |
| C42—H42 | 0.9300 | C106—H106 | 0.9300 |
| C43—C44 | 1.377 (6) | C107—C108 | 1.360 (8) |
| C43—H43 | 0.9300 | C107—H107 | 0.9300 |
| C44—H44 | 0.9300 | C108—C109 | 1.385 (7) |
| C45—C46 | 1.518 (5) | C108—H108 | 0.9300 |
| C45—C52 | 1.519 (6) | C109—H109 | 0.9300 |
| C45—H45 | 0.9800 | C110—C111 | 1.475 (6) |
| C46—C51 | 1.382 (6) | C111—C116 | 1.388 (6) |

supplementary materials

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|-------------|-----------|-------------|-----------|
| C46—C47 | 1.385 (6) | C111—C112 | 1.392 (6) |
| C47—C48 | 1.391 (7) | C112—C113 | 1.375 (6) |
| C47—H47 | 0.9300 | C112—H112 | 0.9300 |
| C48—C49 | 1.372 (8) | C113—C114 | 1.368 (6) |
| C48—H48 | 0.9300 | C113—H113 | 0.9300 |
| C49—C50 | 1.359 (8) | C114—C115 | 1.362 (6) |
| C49—H49 | 0.9300 | C115—C116 | 1.376 (6) |
| C50—C51 | 1.373 (7) | C115—H115 | 0.9300 |
| C50—H50 | 0.9300 | C116—H116 | 0.9300 |
| C1—S1—C16 | 102.4 (2) | C58—C57—H57 | 120.6 |
| C30—S2—C45 | 102.6 (2) | C53—C58—C57 | 121.4 (4) |
| C59—S3—C74 | 103.3 (2) | C53—C58—H58 | 119.3 |
| C88—S4—C103 | 102.6 (2) | C57—C58—H58 | 119.3 |
| C1—N1—C2 | 117.8 (4) | N3—C59—C66 | 125.1 (4) |
| C30—N2—C31 | 118.9 (4) | N3—C59—S3 | 119.2 (3) |
| C59—N3—C60 | 118.3 (4) | C66—C59—S3 | 115.7 (3) |
| C88—N4—C89 | 117.8 (4) | C61—C60—N3 | 120.8 (4) |
| N1—C1—C8 | 125.0 (4) | C61—C60—C68 | 123.6 (4) |
| N1—C1—S1 | 119.0 (3) | N3—C60—C68 | 115.6 (4) |
| C8—C1—S1 | 116.0 (3) | C60—C61—C67 | 122.1 (4) |
| C3—C2—N1 | 121.7 (4) | C60—C61—H61 | 118.9 |
| C3—C2—C10 | 122.8 (4) | C67—C61—H61 | 118.9 |
| N1—C2—C10 | 115.6 (4) | C63—C62—C67 | 120.6 (5) |
| C2—C3—C9 | 120.9 (4) | C63—C62—H62 | 119.7 |
| C2—C3—H3 | 119.5 | C67—C62—H62 | 119.7 |
| C9—C3—H3 | 119.5 | C62—C63—C64 | 120.8 (5) |
| C5—C4—C9 | 119.4 (5) | C62—C63—H63 | 119.6 |
| C5—C4—H4 | 120.3 | C64—C63—H63 | 119.6 |
| C9—C4—H4 | 120.3 | C65—C64—C63 | 120.6 (5) |
| C4—C5—C6 | 121.8 (5) | C65—C64—H64 | 119.7 |
| C4—C5—H5 | 119.1 | C63—C64—H64 | 119.7 |
| C6—C5—H5 | 119.1 | C64—C65—C66 | 120.1 (5) |
| C7—C6—C5 | 119.2 (5) | C64—C65—H65 | 119.9 |
| C7—C6—H6 | 120.4 | C66—C65—H65 | 119.9 |
| C5—C6—H6 | 120.4 | C65—C66—C67 | 119.3 (4) |
| C6—C7—C8 | 121.1 (5) | C65—C66—C59 | 124.3 (4) |
| C6—C7—H7 | 119.4 | C67—C66—C59 | 116.4 (4) |
| C8—C7—H7 | 119.4 | C62—C67—C61 | 124.4 (5) |
| C7—C8—C9 | 119.1 (4) | C62—C67—C66 | 118.4 (5) |
| C7—C8—C1 | 124.3 (4) | C61—C67—C66 | 117.2 (4) |
| C9—C8—C1 | 116.6 (4) | C73—C68—C69 | 117.4 (5) |
| C8—C9—C3 | 117.8 (4) | C73—C68—C60 | 121.1 (4) |
| C8—C9—C4 | 119.4 (5) | C69—C68—C60 | 121.4 (4) |
| C3—C9—C4 | 122.8 (5) | C70—C69—C68 | 121.1 (5) |
| C11—C10—C15 | 117.8 (5) | C70—C69—H69 | 119.5 |
| C11—C10—C2 | 120.8 (5) | C68—C69—H69 | 119.5 |
| C15—C10—C2 | 121.4 (4) | C71—C70—C69 | 120.7 (5) |
| C10—C11—C12 | 120.0 (5) | C71—C70—H70 | 119.7 |
| C10—C11—H11 | 120.0 | C69—C70—H70 | 119.7 |

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|-------------|-----------|-------------|-----------|
| C12—C11—H11 | 120.0 | C70—C71—C72 | 118.6 (5) |
| C13—C12—C11 | 121.1 (6) | C70—C71—H71 | 120.7 |
| C13—C12—H12 | 119.5 | C72—C71—H71 | 120.7 |
| C11—C12—H12 | 119.5 | C73—C72—C71 | 121.4 (5) |
| C14—C13—C12 | 120.1 (5) | C73—C72—H72 | 119.3 |
| C14—C13—H13 | 120.0 | C71—C72—H72 | 119.3 |
| C12—C13—H13 | 120.0 | C72—C73—C68 | 120.8 (4) |
| C13—C14—C15 | 119.8 (6) | C72—C73—H73 | 119.6 |
| C13—C14—H14 | 120.1 | C68—C73—H73 | 119.6 |
| C15—C14—H14 | 120.1 | C81—C74—C75 | 112.1 (3) |
| C14—C15—C10 | 121.1 (5) | C81—C74—S3 | 111.7 (3) |
| C14—C15—H15 | 119.4 | C75—C74—S3 | 105.5 (3) |
| C10—C15—H15 | 119.4 | C81—C74—H74 | 109.2 |
| C17—C16—C23 | 112.3 (3) | C75—C74—H74 | 109.2 |
| C17—C16—S1 | 105.0 (3) | S3—C74—H74 | 109.2 |
| C23—C16—S1 | 111.6 (3) | C76—C75—C80 | 117.9 (4) |
| C17—C16—H16 | 109.3 | C76—C75—C74 | 122.4 (4) |
| C23—C16—H16 | 109.3 | C80—C75—C74 | 119.7 (4) |
| S1—C16—H16 | 109.3 | C75—C76—C77 | 120.7 (5) |
| C22—C17—C18 | 118.0 (4) | C75—C76—H76 | 119.7 |
| C22—C17—C16 | 122.3 (4) | C77—C76—H76 | 119.7 |
| C18—C17—C16 | 119.6 (4) | C78—C77—C76 | 121.6 (6) |
| C17—C18—C19 | 120.0 (5) | C78—C77—H77 | 119.2 |
| C17—C18—H18 | 120.0 | C76—C77—H77 | 119.2 |
| C19—C18—H18 | 120.0 | C77—C78—C79 | 118.9 (6) |
| C20—C19—C18 | 120.7 (5) | C77—C78—H78 | 120.6 |
| C20—C19—H19 | 119.7 | C79—C78—H78 | 120.6 |
| C18—C19—H19 | 119.7 | C78—C79—C80 | 120.9 (6) |
| C21—C20—C19 | 119.7 (6) | C78—C79—H79 | 119.5 |
| C21—C20—H20 | 120.1 | C80—C79—H79 | 119.5 |
| C19—C20—H20 | 120.1 | C75—C80—C79 | 120.0 (5) |
| C20—C21—C22 | 119.9 (6) | C75—C80—H80 | 120.0 |
| C20—C21—H21 | 120.1 | C79—C80—H80 | 120.0 |
| C22—C21—H21 | 120.1 | O3—C81—C82 | 120.3 (4) |
| C21—C22—C17 | 121.6 (5) | O3—C81—C74 | 120.9 (4) |
| C21—C22—H22 | 119.2 | C82—C81—C74 | 118.8 (4) |
| C17—C22—H22 | 119.2 | C87—C82—C83 | 118.8 (4) |
| O1—C23—C24 | 121.2 (4) | C87—C82—C81 | 118.4 (4) |
| O1—C23—C16 | 120.3 (4) | C83—C82—C81 | 122.8 (4) |
| C24—C23—C16 | 118.5 (4) | C84—C83—C82 | 120.7 (4) |
| C25—C24—C29 | 118.9 (4) | C84—C83—H83 | 119.6 |
| C25—C24—C23 | 123.2 (4) | C82—C83—H83 | 119.6 |
| C29—C24—C23 | 117.8 (4) | C83—C84—C85 | 119.5 (5) |
| C24—C25—C26 | 120.6 (4) | C83—C84—H84 | 120.2 |
| C24—C25—H25 | 119.7 | C85—C84—H84 | 120.2 |
| C26—C25—H25 | 119.7 | C86—C85—C84 | 121.4 (5) |
| C27—C26—C25 | 118.8 (5) | C86—C85—Cl3 | 119.1 (4) |
| C27—C26—H26 | 120.6 | C84—C85—Cl3 | 119.5 (4) |
| C25—C26—H26 | 120.6 | C85—C86—C87 | 118.9 (4) |

supplementary materials

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| C26—C27—C28 | 122.3 (5) | C85—C86—H86 | 120.6 |
| C26—C27—C11 | 118.9 (5) | C87—C86—H86 | 120.6 |
| C28—C27—C11 | 118.7 (5) | C82—C87—C86 | 120.6 (5) |
| C27—C28—C29 | 118.3 (5) | C82—C87—H87 | 119.7 |
| C27—C28—H28 | 120.9 | C86—C87—H87 | 119.7 |
| C29—C28—H28 | 120.9 | N4—C88—C95 | 124.8 (4) |
| C28—C29—C24 | 121.0 (5) | N4—C88—S4 | 118.6 (3) |
| C28—C29—H29 | 119.5 | C95—C88—S4 | 116.5 (3) |
| C24—C29—H29 | 119.5 | C90—C89—N4 | 121.5 (4) |
| N2—C30—C37 | 124.3 (4) | C90—C89—C97 | 123.3 (4) |
| N2—C30—S2 | 119.0 (3) | N4—C89—C97 | 115.1 (4) |
| C37—C30—S2 | 116.7 (3) | C89—C90—C96 | 121.0 (4) |
| C32—C31—N2 | 120.2 (4) | C89—C90—H90 | 119.5 |
| C32—C31—C39 | 123.8 (4) | C96—C90—H90 | 119.5 |
| N2—C31—C39 | 116.0 (4) | C92—C91—C96 | 121.0 (5) |
| C31—C32—C38 | 122.0 (4) | C92—C91—H91 | 119.5 |
| C31—C32—H32 | 119.0 | C96—C91—H91 | 119.5 |
| C38—C32—H32 | 119.0 | C91—C92—C93 | 120.9 (5) |
| C34—C33—C38 | 120.4 (5) | C91—C92—H92 | 119.5 |
| C34—C33—H33 | 119.8 | C93—C92—H92 | 119.5 |
| C38—C33—H33 | 119.8 | C94—C93—C92 | 119.8 (5) |
| C33—C34—C35 | 121.5 (5) | C94—C93—H93 | 120.1 |
| C33—C34—H34 | 119.2 | C92—C93—H93 | 120.1 |
| C35—C34—H34 | 119.2 | C93—C94—C95 | 120.4 (5) |
| C36—C35—C34 | 119.7 (5) | C93—C94—H94 | 119.8 |
| C36—C35—H35 | 120.1 | C95—C94—H94 | 119.8 |
| C34—C35—H35 | 120.1 | C94—C95—C96 | 119.9 (4) |
| C35—C36—C37 | 119.9 (5) | C94—C95—C88 | 123.8 (4) |
| C35—C36—H36 | 120.0 | C96—C95—C88 | 116.3 (4) |
| C37—C36—H36 | 120.0 | C90—C96—C95 | 118.5 (4) |
| C36—C37—C38 | 119.8 (4) | C90—C96—C91 | 123.3 (5) |
| C36—C37—C30 | 123.3 (4) | C95—C96—C91 | 118.2 (5) |
| C38—C37—C30 | 116.9 (4) | C102—C97—C98 | 117.4 (5) |
| C33—C38—C32 | 123.7 (5) | C102—C97—C89 | 121.8 (4) |
| C33—C38—C37 | 118.6 (5) | C98—C97—C89 | 120.8 (5) |
| C32—C38—C37 | 117.7 (4) | C99—C98—C97 | 120.6 (5) |
| C44—C39—C40 | 117.2 (5) | C99—C98—H98 | 119.7 |
| C44—C39—C31 | 120.9 (4) | C97—C98—H98 | 119.7 |
| C40—C39—C31 | 121.9 (4) | C98—C99—C100 | 120.4 (6) |
| C41—C40—C39 | 120.8 (5) | C98—C99—H99 | 119.8 |
| C41—C40—H40 | 119.6 | C100—C99—H99 | 119.8 |
| C39—C40—H40 | 119.6 | C101—C100—C99 | 118.5 (6) |
| C40—C41—C42 | 121.7 (5) | C101—C100—H100 | 120.7 |
| C40—C41—H41 | 119.1 | C99—C100—H100 | 120.7 |
| C42—C41—H41 | 119.1 | C102—C101—C100 | 121.2 (6) |
| C43—C42—C41 | 117.7 (5) | C102—C101—H101 | 119.4 |
| C43—C42—H42 | 121.1 | C100—C101—H101 | 119.4 |
| C41—C42—H42 | 121.1 | C101—C102—C97 | 121.8 (5) |
| C42—C43—C44 | 120.7 (5) | C101—C102—H102 | 119.1 |

| | | | |
|--------------|------------|----------------|------------|
| C42—C43—H43 | 119.7 | C97—C102—H102 | 119.1 |
| C44—C43—H43 | 119.7 | C104—C103—C110 | 111.8 (3) |
| C39—C44—C43 | 121.8 (5) | C104—C103—S4 | 105.8 (3) |
| C39—C44—H44 | 119.1 | C110—C103—S4 | 111.6 (3) |
| C43—C44—H44 | 119.1 | C104—C103—H103 | 109.2 |
| C46—C45—C52 | 111.6 (3) | C110—C103—H103 | 109.2 |
| C46—C45—S2 | 105.7 (3) | S4—C103—H103 | 109.2 |
| C52—C45—S2 | 111.9 (3) | C109—C104—C105 | 118.0 (5) |
| C46—C45—H45 | 109.2 | C109—C104—C103 | 122.2 (4) |
| C52—C45—H45 | 109.2 | C105—C104—C103 | 119.7 (4) |
| S2—C45—H45 | 109.2 | C104—C105—C106 | 120.2 (5) |
| C51—C46—C47 | 117.6 (4) | C104—C105—H105 | 119.9 |
| C51—C46—C45 | 122.2 (4) | C106—C105—H105 | 119.9 |
| C47—C46—C45 | 120.1 (4) | C107—C106—C105 | 120.4 (6) |
| C46—C47—C48 | 120.7 (5) | C107—C106—H106 | 119.8 |
| C46—C47—H47 | 119.6 | C105—C106—H106 | 119.8 |
| C48—C47—H47 | 119.6 | C108—C107—C106 | 120.3 (6) |
| C49—C48—C47 | 120.0 (5) | C108—C107—H107 | 119.9 |
| C49—C48—H48 | 120.0 | C106—C107—H107 | 119.9 |
| C47—C48—H48 | 120.0 | C107—C108—C109 | 119.8 (6) |
| C50—C49—C48 | 119.6 (5) | C107—C108—H108 | 120.1 |
| C50—C49—H49 | 120.2 | C109—C108—H108 | 120.1 |
| C48—C49—H49 | 120.2 | C104—C109—C108 | 121.4 (5) |
| C49—C50—C51 | 120.7 (6) | C104—C109—H109 | 119.3 |
| C49—C50—H50 | 119.7 | C108—C109—H109 | 119.3 |
| C51—C50—H50 | 119.7 | O4—C110—C111 | 121.3 (4) |
| C50—C51—C46 | 121.3 (5) | O4—C110—C103 | 120.1 (4) |
| C50—C51—H51 | 119.3 | C111—C110—C103 | 118.7 (4) |
| C46—C51—H51 | 119.3 | C116—C111—C112 | 118.0 (4) |
| O2—C52—C53 | 120.4 (4) | C116—C111—C110 | 123.6 (4) |
| O2—C52—C45 | 121.0 (4) | C112—C111—C110 | 118.4 (4) |
| C53—C52—C45 | 118.6 (4) | C113—C112—C111 | 120.9 (5) |
| C58—C53—C54 | 118.7 (4) | C113—C112—H112 | 119.5 |
| C58—C53—C52 | 118.7 (4) | C111—C112—H112 | 119.5 |
| C54—C53—C52 | 122.5 (4) | C114—C113—C112 | 119.2 (5) |
| C55—C54—C53 | 120.1 (4) | C114—C113—H113 | 120.4 |
| C55—C54—H54 | 119.9 | C112—C113—H113 | 120.4 |
| C53—C54—H54 | 119.9 | C115—C114—C113 | 121.5 (5) |
| C56—C55—C54 | 120.5 (5) | C115—C114—C14 | 119.0 (4) |
| C56—C55—H55 | 119.7 | C113—C114—C14 | 119.5 (4) |
| C54—C55—H55 | 119.7 | C114—C115—C116 | 119.3 (5) |
| C55—C56—C57 | 120.5 (5) | C114—C115—H115 | 120.3 |
| C55—C56—C12 | 120.1 (4) | C116—C115—H115 | 120.3 |
| C57—C56—C12 | 119.4 (4) | C115—C116—C111 | 121.0 (4) |
| C56—C57—C58 | 118.7 (4) | C115—C116—H116 | 119.5 |
| C56—C57—H57 | 120.6 | C111—C116—H116 | 119.5 |
| C2—N1—C1—C8 | 3.4 (6) | C60—N3—C59—C66 | 2.4 (6) |
| C2—N1—C1—S1 | -176.2 (3) | C60—N3—C59—S3 | -176.2 (3) |
| C16—S1—C1—N1 | -1.2 (4) | C74—S3—C59—N3 | -2.1 (4) |

supplementary materials

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| C16—S1—C1—C8 | 179.2 (3) | C74—S3—C59—C66 | 179.2 (3) |
| C1—N1—C2—C3 | -2.4 (6) | C59—N3—C60—C61 | -1.2 (6) |
| C1—N1—C2—C10 | 178.4 (4) | C59—N3—C60—C68 | 179.5 (4) |
| N1—C2—C3—C9 | 0.6 (7) | N3—C60—C61—C67 | -0.3 (7) |
| C10—C2—C3—C9 | 179.7 (4) | C68—C60—C61—C67 | 178.8 (4) |
| C9—C4—C5—C6 | 0.7 (8) | C67—C62—C63—C64 | 0.0 (8) |
| C4—C5—C6—C7 | -0.8 (8) | C62—C63—C64—C65 | 1.5 (8) |
| C5—C6—C7—C8 | 0.6 (8) | C63—C64—C65—C66 | -1.4 (8) |
| C6—C7—C8—C9 | -0.5 (7) | C64—C65—C66—C67 | -0.2 (7) |
| C6—C7—C8—C1 | -179.8 (4) | C64—C65—C66—C59 | -179.2 (5) |
| N1—C1—C8—C7 | 177.0 (4) | N3—C59—C66—C65 | 177.2 (4) |
| S1—C1—C8—C7 | -3.4 (6) | S3—C59—C66—C65 | -4.1 (6) |
| N1—C1—C8—C9 | -2.4 (6) | N3—C59—C66—C67 | -1.8 (6) |
| S1—C1—C8—C9 | 177.2 (3) | S3—C59—C66—C67 | 176.8 (3) |
| C7—C8—C9—C3 | -179.0 (4) | C63—C62—C67—C61 | 179.1 (5) |
| C1—C8—C9—C3 | 0.4 (6) | C63—C62—C67—C66 | -1.6 (7) |
| C7—C8—C9—C4 | 0.4 (6) | C60—C61—C67—C62 | -179.9 (4) |
| C1—C8—C9—C4 | 179.8 (4) | C60—C61—C67—C66 | 0.9 (7) |
| C2—C3—C9—C8 | 0.4 (6) | C65—C66—C67—C62 | 1.7 (6) |
| C2—C3—C9—C4 | -179.0 (4) | C59—C66—C67—C62 | -179.2 (4) |
| C5—C4—C9—C8 | -0.6 (7) | C65—C66—C67—C61 | -179.0 (4) |
| C5—C4—C9—C3 | 178.9 (5) | C59—C66—C67—C61 | 0.1 (6) |
| C3—C2—C10—C11 | 34.8 (7) | C61—C60—C68—C73 | -158.9 (4) |
| N1—C2—C10—C11 | -146.1 (4) | N3—C60—C68—C73 | 20.3 (6) |
| C3—C2—C10—C15 | -146.7 (5) | C61—C60—C68—C69 | 22.7 (7) |
| N1—C2—C10—C15 | 32.4 (6) | N3—C60—C68—C69 | -158.1 (4) |
| C15—C10—C11—C12 | 2.6 (7) | C73—C68—C69—C70 | 2.3 (8) |
| C2—C10—C11—C12 | -178.9 (4) | C60—C68—C69—C70 | -179.2 (5) |
| C10—C11—C12—C13 | -1.0 (8) | C68—C69—C70—C71 | -1.6 (9) |
| C11—C12—C13—C14 | -0.6 (8) | C69—C70—C71—C72 | -0.1 (8) |
| C12—C13—C14—C15 | 0.5 (8) | C70—C71—C72—C73 | 1.0 (8) |
| C13—C14—C15—C10 | 1.1 (8) | C71—C72—C73—C68 | -0.2 (7) |
| C11—C10—C15—C14 | -2.6 (7) | C69—C68—C73—C72 | -1.4 (7) |
| C2—C10—C15—C14 | 178.8 (4) | C60—C68—C73—C72 | -179.9 (4) |
| C1—S1—C16—C17 | 163.3 (3) | C59—S3—C74—C81 | -75.1 (3) |
| C1—S1—C16—C23 | -74.8 (3) | C59—S3—C74—C75 | 162.9 (3) |
| C23—C16—C17—C22 | -31.6 (6) | C81—C74—C75—C76 | -30.6 (6) |
| S1—C16—C17—C22 | 89.8 (5) | S3—C74—C75—C76 | 91.1 (5) |
| C23—C16—C17—C18 | 152.3 (4) | C81—C74—C75—C80 | 152.6 (4) |
| S1—C16—C17—C18 | -86.3 (4) | S3—C74—C75—C80 | -85.7 (4) |
| C22—C17—C18—C19 | 0.3 (7) | C80—C75—C76—C77 | 1.5 (8) |
| C16—C17—C18—C19 | 176.5 (4) | C74—C75—C76—C77 | -175.4 (5) |
| C17—C18—C19—C20 | -0.7 (8) | C75—C76—C77—C78 | -2.3 (10) |
| C18—C19—C20—C21 | 1.6 (9) | C76—C77—C78—C79 | 2.5 (10) |
| C19—C20—C21—C22 | -2.1 (10) | C77—C78—C79—C80 | -2.0 (9) |
| C20—C21—C22—C17 | 1.8 (9) | C76—C75—C80—C79 | -1.0 (7) |
| C18—C17—C22—C21 | -0.8 (8) | C74—C75—C80—C79 | 175.9 (4) |
| C16—C17—C22—C21 | -177.0 (5) | C78—C79—C80—C75 | 1.3 (8) |
| C17—C16—C23—O1 | 85.8 (5) | C75—C74—C81—O3 | 85.2 (5) |

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| S1—C16—C23—O1 | -31.8 (5) | S3—C74—C81—O3 | -32.9 (5) |
| C17—C16—C23—C24 | -93.8 (4) | C75—C74—C81—C82 | -94.6 (4) |
| S1—C16—C23—C24 | 148.6 (3) | S3—C74—C81—C82 | 147.3 (3) |
| O1—C23—C24—C25 | -168.1 (4) | O3—C81—C82—C87 | 16.5 (6) |
| C16—C23—C24—C25 | 11.5 (6) | C74—C81—C82—C87 | -163.6 (4) |
| O1—C23—C24—C29 | 14.7 (6) | O3—C81—C82—C83 | -165.9 (4) |
| C16—C23—C24—C29 | -165.7 (4) | C74—C81—C82—C83 | 14.0 (6) |
| C29—C24—C25—C26 | 0.9 (7) | C87—C82—C83—C84 | 1.1 (6) |
| C23—C24—C25—C26 | -176.3 (4) | C81—C82—C83—C84 | -176.5 (4) |
| C24—C25—C26—C27 | 0.3 (8) | C82—C83—C84—C85 | 1.1 (7) |
| C25—C26—C27—C28 | -0.5 (8) | C83—C84—C85—C86 | -2.5 (8) |
| C25—C26—C27—C11 | 177.1 (4) | C83—C84—C85—C13 | 176.8 (4) |
| C26—C27—C28—C29 | -0.5 (8) | C84—C85—C86—C87 | 1.6 (7) |
| C11—C27—C28—C29 | -178.1 (4) | C13—C85—C86—C87 | -177.7 (4) |
| C27—C28—C29—C24 | 1.7 (7) | C83—C82—C87—C86 | -2.0 (6) |
| C25—C24—C29—C28 | -1.9 (7) | C81—C82—C87—C86 | 175.7 (4) |
| C23—C24—C29—C28 | 175.4 (4) | C85—C86—C87—C82 | 0.7 (7) |
| C31—N2—C30—C37 | -2.3 (6) | C89—N4—C88—C95 | -2.7 (6) |
| C31—N2—C30—S2 | 175.9 (3) | C89—N4—C88—S4 | 175.6 (3) |
| C45—S2—C30—N2 | 1.8 (4) | C103—S4—C88—N4 | 1.5 (4) |
| C45—S2—C30—C37 | -179.8 (3) | C103—S4—C88—C95 | 179.9 (3) |
| C30—N2—C31—C32 | 2.0 (6) | C88—N4—C89—C90 | 2.3 (6) |
| C30—N2—C31—C39 | -179.1 (4) | C88—N4—C89—C97 | -178.2 (4) |
| N2—C31—C32—C38 | -0.5 (7) | N4—C89—C90—C96 | -0.7 (7) |
| C39—C31—C32—C38 | -179.4 (4) | C97—C89—C90—C96 | 179.8 (4) |
| C38—C33—C34—C35 | -0.3 (8) | C96—C91—C92—C93 | 0.0 (8) |
| C33—C34—C35—C36 | 0.1 (8) | C91—C92—C93—C94 | -0.4 (8) |
| C34—C35—C36—C37 | -0.1 (8) | C92—C93—C94—C95 | 0.6 (8) |
| C35—C36—C37—C38 | 0.3 (7) | C93—C94—C95—C96 | -0.4 (7) |
| C35—C36—C37—C30 | 179.2 (4) | C93—C94—C95—C88 | 179.2 (4) |
| N2—C30—C37—C36 | -177.8 (4) | N4—C88—C95—C94 | -178.3 (4) |
| S2—C30—C37—C36 | 3.9 (6) | S4—C88—C95—C94 | 3.4 (6) |
| N2—C30—C37—C38 | 1.2 (6) | N4—C88—C95—C96 | 1.4 (6) |
| S2—C30—C37—C38 | -177.1 (3) | S4—C88—C95—C96 | -176.9 (3) |
| C34—C33—C38—C32 | -179.3 (5) | C89—C90—C96—C95 | -0.6 (7) |
| C34—C33—C38—C37 | 0.6 (7) | C89—C90—C96—C91 | 179.3 (4) |
| C31—C32—C38—C33 | 179.2 (4) | C94—C95—C96—C90 | 180.0 (4) |
| C31—C32—C38—C37 | -0.6 (7) | C88—C95—C96—C90 | 0.3 (6) |
| C36—C37—C38—C33 | -0.5 (7) | C94—C95—C96—C91 | 0.1 (6) |
| C30—C37—C38—C33 | -179.5 (4) | C88—C95—C96—C91 | -179.6 (4) |
| C36—C37—C38—C32 | 179.3 (4) | C92—C91—C96—C90 | -179.8 (5) |
| C30—C37—C38—C32 | 0.4 (6) | C92—C91—C96—C95 | 0.1 (7) |
| C32—C31—C39—C44 | 155.4 (5) | C90—C89—C97—C102 | 144.5 (5) |
| N2—C31—C39—C44 | -23.5 (6) | N4—C89—C97—C102 | -35.0 (6) |
| C32—C31—C39—C40 | -26.7 (7) | C90—C89—C97—C98 | -36.2 (7) |
| N2—C31—C39—C40 | 154.4 (4) | N4—C89—C97—C98 | 144.3 (4) |
| C44—C39—C40—C41 | -2.7 (8) | C102—C97—C98—C99 | -1.0 (7) |
| C31—C39—C40—C41 | 179.3 (5) | C89—C97—C98—C99 | 179.7 (4) |
| C39—C40—C41—C42 | 1.4 (9) | C97—C98—C99—C100 | -0.7 (8) |

supplementary materials

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| C40—C41—C42—C43 | 0.0 (9) | C98—C99—C100—C101 | 1.8 (8) |
| C41—C42—C43—C44 | 0.1 (8) | C99—C100—C101—C102 | -1.1 (8) |
| C40—C39—C44—C43 | 2.7 (7) | C100—C101—C102—C97 | -0.8 (8) |
| C31—C39—C44—C43 | -179.2 (4) | C98—C97—C102—C101 | 1.8 (7) |
| C42—C43—C44—C39 | -1.5 (8) | C89—C97—C102—C101 | -178.9 (5) |
| C30—S2—C45—C46 | -162.6 (3) | C88—S4—C103—C104 | -162.9 (3) |
| C30—S2—C45—C52 | 75.8 (3) | C88—S4—C103—C110 | 75.3 (3) |
| C52—C45—C46—C51 | 32.9 (6) | C110—C103—C104—C109 | 33.8 (6) |
| S2—C45—C46—C51 | -88.9 (5) | S4—C103—C104—C109 | -87.9 (5) |
| C52—C45—C46—C47 | -150.8 (4) | C110—C103—C104—C105 | -150.4 (4) |
| S2—C45—C46—C47 | 87.4 (4) | S4—C103—C104—C105 | 88.0 (4) |
| C51—C46—C47—C48 | -0.8 (7) | C109—C104—C105—C106 | -0.5 (7) |
| C45—C46—C47—C48 | -177.2 (4) | C103—C104—C105—C106 | -176.6 (4) |
| C46—C47—C48—C49 | 0.6 (8) | C104—C105—C106—C107 | 0.1 (8) |
| C47—C48—C49—C50 | 0.1 (9) | C105—C106—C107—C108 | 0.7 (9) |
| C48—C49—C50—C51 | -0.6 (9) | C106—C107—C108—C109 | -1.1 (10) |
| C49—C50—C51—C46 | 0.4 (9) | C105—C104—C109—C108 | 0.2 (8) |
| C47—C46—C51—C50 | 0.3 (8) | C103—C104—C109—C108 | 176.1 (5) |
| C45—C46—C51—C50 | 176.6 (5) | C107—C108—C109—C104 | 0.7 (9) |
| C46—C45—C52—O2 | -87.7 (5) | C104—C103—C110—O4 | -87.2 (5) |
| S2—C45—C52—O2 | 30.5 (5) | S4—C103—C110—O4 | 31.0 (5) |
| C46—C45—C52—C53 | 92.7 (4) | C104—C103—C110—C111 | 92.7 (4) |
| S2—C45—C52—C53 | -149.2 (3) | S4—C103—C110—C111 | -149.1 (3) |
| O2—C52—C53—C58 | -14.9 (6) | O4—C110—C111—C116 | 168.7 (4) |
| C45—C52—C53—C58 | 164.8 (4) | C103—C110—C111—C116 | -11.1 (6) |
| O2—C52—C53—C54 | 167.9 (4) | O4—C110—C111—C112 | -13.2 (6) |
| C45—C52—C53—C54 | -12.4 (6) | C103—C110—C111—C112 | 166.9 (4) |
| C58—C53—C54—C55 | -1.7 (7) | C116—C111—C112—C113 | 2.4 (7) |
| C52—C53—C54—C55 | 175.5 (4) | C110—C111—C112—C113 | -175.8 (4) |
| C53—C54—C55—C56 | -0.1 (7) | C111—C112—C113—C114 | -0.9 (8) |
| C54—C55—C56—C57 | 1.8 (7) | C112—C113—C114—C115 | -1.0 (8) |
| C54—C55—C56—C12 | -177.2 (4) | C112—C113—C114—C14 | 176.5 (4) |
| C55—C56—C57—C58 | -1.6 (7) | C113—C114—C115—C116 | 1.2 (8) |
| C12—C56—C57—C58 | 177.4 (4) | C14—C114—C115—C116 | -176.3 (4) |
| C54—C53—C58—C57 | 1.9 (7) | C114—C115—C116—C111 | 0.4 (8) |
| C52—C53—C58—C57 | -175.4 (4) | C112—C111—C116—C115 | -2.2 (7) |
| C56—C57—C58—C53 | -0.3 (7) | C110—C111—C116—C115 | 175.9 (4) |

Fig. 1

