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# [Hydridotris(pyrazol-1-yl)borato-$\kappa^3N,N',N''$][5,10,15,20-tetrakis(4-methylphenyl)porphyrinato-$\kappa^4N,N',N'',N'''$]samarium(III) toluene 1.75-solvate

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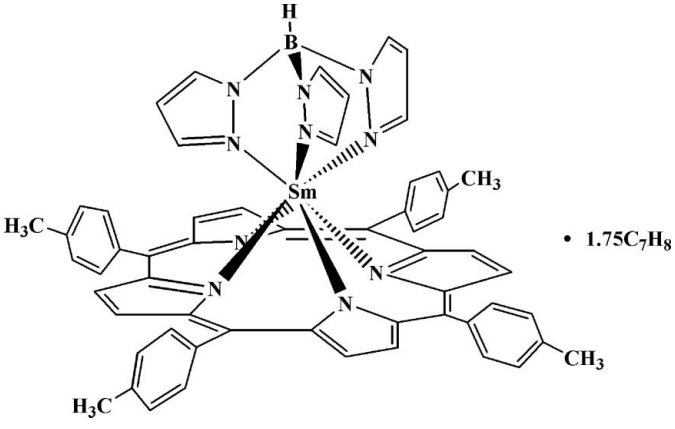
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; disorder in solvent or counterion; $R$ factor = 0.033; $wR$ factor = 0.089; data-to-parameter ratio = 15.8.

In the title complex, $[Sm(C_9H_{10}BN_6)(C_{48}H_{36}N_4)]\cdot 1.75C_7H_8$, there are two independent complex molecules in the asymmetric unit, in each of which the $Sm^{III}$ ion is coordinated by seven N atoms, four from a (4-methylphenyl)porphyrinate ligand and three from a hydridotris(pyrazol-1-yl)borate ligand, to form a capped trigonal-prismatic geometry. The $Sm^{III}$ ion is 'sandwiched' between two ligands and is located 1.2647 (13) and 1.2549 (14)Å from the porphyrin ring in the two complex molecules. The asymmetric unit also contains 3.5 molecules of toluene, the half-occupancy molecule being located close to a crystallographic inversion center. The porphyrin groups have 'dome'-like geometries.

## Related literature

For related literature, see: He, Guo *et al.* (2004); He, Wong *et al.* (2004*a*,*b*); Foley *et al.* (2003).




## Experimental

### Crystal data

$[Sm(C_9H_{10}BN_6)(C_{48}H_{36}N_4)]\cdot 1.75C_7H_8$
$M_r$ = 1193.43
Triclinic, $P\overline{1}$
$a$ = 16.6210 (2) Å
$b$ = 16.5696 (2) Å
$c$ = 25.4414 (3) Å
$\alpha$ = 79.318 (1)°
$\beta$ = 79.064 (1)°
$\gamma$ = 61.248 (1)°
$V$ = 5995.10 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.03 mm$^{-1}$
$T$ = 293 (2) K
0.30 × 0.30 × 0.30 mm

### Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min}$ = 0.748, $T_{max}$ = 0.748
73453 measured reflections
21056 independent reflections
17078 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.089
$S$ = 1.02
21056 reflections
1335 parameters
154 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.88 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2527).

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# supplementary materials

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# [Hydridotris(pyrazol-1-yl)borato-$\kappa^3N,N',N''$][5,10,15,20-tetrakis(4-methylphenyl)porphyrinato-$\kappa^4N,N',N'',N'''$]samarium(III) toluene 1.75-solvate

**H. He, G. He and S. W. Ng**

## Comment

Several monoporphyrinate lanthanide complexes with hydridotrispyrazolylborate anions have been reported recently (He, Guo *et al.*, 2004; He *et al.* 2004*a*,b; Foley *et al.* 2003). These complexes exhibit strong luminescence in the near-infrared region and have potential in fluoroimmunoassay and photonic devices (He, Guo *et al.* 2004). However, light rare earth complexes are uncommon. Reported herein is the single-crystal structure of a Sm(III) complex.

In the title compound, there are two independent molecules in the asymmetric unit. In each, the $Sm^{III}$ ion is "sandwiched" between a porphyrin ring and a tripodal ligand. The conformation of each complex molecule is different only in the relative orientaions of the phenyl groups. In each molecule, four N atoms from a 5,10,15,20-tetrakis(4-methyl)porphyrinate ligand ($TTP^{2-}$) and three N atoms from hydridotris (pyrazol-1-yl)borate anion ($TpH^{-}$) ligand coordinate to the central $Sm^{III}$ ion to form a capped trigonal prismatic geometry. The distances between atom Sm1 and the least-squared planes N1/N2/N3/N4 and N5/N7/N9 are 1.2647 (13) and 1.8713 (17) Å, respectively. The distances between atom Sm2 and the least-squared planes N11/N12/N13/N14 and N15/N17/N19 are 1.2549 (14) and 1.8778 (18) Å, respectively. The distances Sm1···B1 and Sm2···B2 are 3.690 (4) and 3.677 (4) Å, respectively. In each independent molecules the orientation of the three arms of the tripodal ligand are different with respect to the phenyl rings. For the molecule containing Sm1 the three arms are located between the phenyl groups, whereas in the molecule containing Sm2 one arm of tripodal ligand is very close to one of the phenyl groups.

## Experimental

*n*-BuLi (3.0 ml, 1.6 mol/l in hexane, 4.8 mmol) was added slowly over a period of 30 min to a solution of $(Me_3Si)_2NH$ (0.78 g, 4.8 mmol) in THF (15 ml) cooled in an ice bath. The reaction mixture was stirred, warmed up slowly to room temperature and stirred for another 12 h until a clear pale yellow solution was obtained. Then the resultant solution was transferred slowly to a suspension of $SmCl_3$ (0.41 g, 1.6 mmol) in THF (10 ml). The reaction mixture was stirred for 24 h at room temperature until all of the $SmCl_3$ was consumed. The resulting solution was centrifuged and filtered. The filtrate was transferred to a solution of 5,10,15,20-tetrakis(4-methyl phenyl)porphyrin (0.20 g, 0.32 mmol) in bis(2-methoxyethyl)ether (8 ml) under a nitrogen atmosphere. The resulting solution was refluxed 24 h and the progress of the reaction was monitored by UV-Vis absorption spectroscopy. After the reaction, the mixture was cooled to room temperature, potassium hydridotris(pyrazole-1-yl)borate (0.1 g, 0.40 mmol) was added and the resulting solution was magnetically stirred at room temperature for 12 h. Then all solvent was removed under vacuum and chloroform (5 ml) was added. After filtration, methanol was diffused into the filtrate and a purple solid crystallized. Yield: 89%. The single-crystal suitable for data analysis were obtained from slow evaporation of toluene solution of sample at room temperature for two weeks.

### Refinement

All hydrogen atoms were geometrically constrained and refined in riding mode as follows: methyl d(C—H) = 0.96 Å, $U_{iso}$(H) = 1.5$U_{eq}$(C); aromatic d(C—H) = 0.93 Å, $U_{iso}$(H) = 1.2$U_{eq}$(C).

### Figures

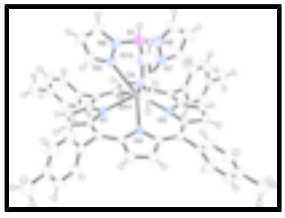

Fig. 1. Side view of the molecule containing atom Sm1, with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are drawn as small circles of arbitrary radii.

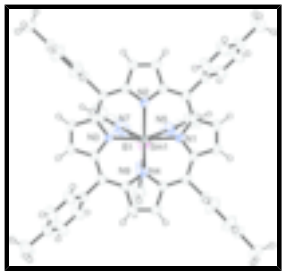

Fig. 2. Top view of the molecule containing atom Sm1, with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are drawn as small circles of arbitrary radii.

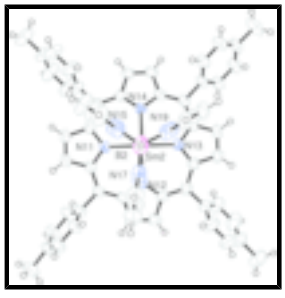

Fig. 3. Top view of the molecule containing atom Sm2 with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are drawn as small circles of arbitrary radii.

### [Hydridotris(pyrazol-1-yl)borato-κ$^3$*N*,*N*',*N*'']\[5,10,15,20-tetrakis(4- methylphenyl)porphyrinato-κ$^4$*N*,*N*',*N*'',*N*''']samarium(III) toluene 1.75-solvate

*Crystal data*

| | |
|---|---|
| $[Sm(C_9H_{10}BN_6)(C_{48}H_{36}N_4)]\cdot 1.75C_7H_8$ | $Z = 4$ |
| $M_r = 1193.43$ | $F_{000} = 2450$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.322$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| $a = 16.6210$ (2) Å | Cell parameters from 42602 reflections |
| $b = 16.5696$ (2) Å | θ = 1.5–28.6º |
| $c = 25.4414$ (3) Å | μ = 1.03 mm$^{-1}$ |
| α = 79.318 (1)º | $T = 293$ (2) K |
| β = 79.064 (1)º | Block, purple |

| | |
|---|---|
| γ = 61.248 (1)° | 0.30 × 0.30 × 0.30 mm |
| $V$ = 5995.10 (12) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART 1K CCD diffractometer | 21056 independent reflections |
| Radiation source: fine-focus sealed tube | 17078 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.030 |
| $T$ = 293(2) K | $\theta_{max}$ = 25.0° |
| φ and ω scans | $\theta_{min}$ = 1.5° |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2002) | $h$ = −19→19 |
| $T_{min}$ = 0.748, $T_{max}$ = 0.748 | $k$ = −19→19 |
| 73453 measured reflections | $l$ = −30→30 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.033 | H-atom parameters constrained |
| $wR(F^2)$ = 0.089 | $w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 6.7364P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.02 | $(\Delta/\sigma)_{max}$ = 0.069 |
| 21056 reflections | $\Delta\rho_{max}$ = 0.88 e Å$^{-3}$ |
| 1335 parameters | $\Delta\rho_{min}$ = −0.46 e Å$^{-3}$ |
| 154 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Special details*

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

**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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Sm1 | 0.482762 (11) | 0.261500 (10) | 0.657833 (6) | 0.03049 (5) | |
| Sm2 | 0.836393 (12) | 0.385772 (11) | 0.877913 (7) | 0.03729 (6) | |

| | | | | |
|---|---|---|---|---|
| N1 | 0.57515 (18) | 0.33192 (16) | 0.60674 (10) | 0.0332 (6) |
| N2 | 0.61809 (18) | 0.13848 (16) | 0.61386 (11) | 0.0343 (6) |
| N3 | 0.42424 (18) | 0.19426 (16) | 0.60740 (11) | 0.0340 (6) |
| N4 | 0.37984 (18) | 0.38779 (16) | 0.60053 (11) | 0.0340 (6) |
| N5 | 0.5620 (2) | 0.2652 (2) | 0.73429 (12) | 0.0493 (7) |
| N6 | 0.5280 (2) | 0.2599 (2) | 0.78690 (11) | 0.0465 (7) |
| N7 | 0.4574 (2) | 0.1496 (2) | 0.73743 (12) | 0.0525 (8) |
| N8 | 0.4453 (2) | 0.1652 (2) | 0.78978 (12) | 0.0504 (8) |
| N9 | 0.3531 (2) | 0.3617 (2) | 0.72682 (12) | 0.0495 (7) |
| N10 | 0.3560 (2) | 0.3373 (2) | 0.78131 (12) | 0.0475 (7) |
| N11 | 0.72354 (19) | 0.3572 (2) | 0.94114 (12) | 0.0436 (7) |
| N12 | 0.7011 (2) | 0.53405 (19) | 0.88392 (12) | 0.0437 (7) |
| N13 | 0.88912 (19) | 0.48524 (19) | 0.90085 (11) | 0.0409 (6) |
| N14 | 0.91109 (19) | 0.30930 (19) | 0.95994 (11) | 0.0411 (7) |
| N15 | 0.8714 (3) | 0.2294 (2) | 0.84721 (13) | 0.0581 (9) |
| N16 | 0.9031 (3) | 0.2101 (2) | 0.79554 (13) | 0.0592 (9) |
| N17 | 0.7806 (2) | 0.4239 (2) | 0.78406 (13) | 0.0578 (8) |
| N18 | 0.8272 (3) | 0.3681 (2) | 0.74437 (13) | 0.0600 (9) |
| N19 | 0.9848 (2) | 0.3372 (2) | 0.80925 (12) | 0.0515 (8) |
| N20 | 0.9935 (2) | 0.2984 (2) | 0.76415 (12) | 0.0544 (8) |
| B1 | 0.4381 (3) | 0.2529 (3) | 0.80599 (17) | 0.0478 (10) |
| H1 | 0.4263 | 0.2510 | 0.8453 | 0.057* |
| B2 | 0.9177 (4) | 0.2795 (4) | 0.75097 (19) | 0.0613 (13) |
| H2B1 | 0.9391 | 0.2516 | 0.7170 | 0.074* |
| C1 | 0.5421 (2) | 0.4265 (2) | 0.59702 (12) | 0.0338 (7) |
| C2 | 0.6185 (2) | 0.4470 (2) | 0.58272 (14) | 0.0424 (8) |
| H2 | 0.6148 | 0.5057 | 0.5756 | 0.051* |
| C3 | 0.6963 (3) | 0.3663 (2) | 0.58138 (15) | 0.0433 (8) |
| H3 | 0.7562 | 0.3588 | 0.5723 | 0.052* |
| C4 | 0.6697 (2) | 0.2937 (2) | 0.59658 (13) | 0.0352 (7) |
| C5 | 0.7315 (2) | 0.1991 (2) | 0.59826 (13) | 0.0366 (7) |
| C6 | 0.7067 (2) | 0.1276 (2) | 0.60636 (13) | 0.0361 (7) |
| C7 | 0.7713 (2) | 0.0313 (2) | 0.60227 (16) | 0.0473 (9) |
| H7 | 0.8354 | 0.0051 | 0.5986 | 0.057* |
| C8 | 0.7214 (2) | −0.0131 (2) | 0.60476 (16) | 0.0474 (9) |
| H8 | 0.7448 | −0.0761 | 0.6029 | 0.057* |
| C9 | 0.6254 (2) | 0.0533 (2) | 0.61076 (13) | 0.0369 (7) |
| C10 | 0.5523 (2) | 0.0355 (2) | 0.60797 (13) | 0.0354 (7) |
| C11 | 0.4588 (2) | 0.1013 (2) | 0.60601 (13) | 0.0359 (7) |
| C12 | 0.3857 (2) | 0.0817 (2) | 0.60086 (14) | 0.0432 (8) |
| H12D | 0.3911 | 0.0235 | 0.5999 | 0.052* |
| C13 | 0.3081 (2) | 0.1622 (2) | 0.59768 (15) | 0.0444 (8) |
| H13 | 0.2498 | 0.1702 | 0.5946 | 0.053* |
| C14 | 0.3321 (2) | 0.2337 (2) | 0.59998 (13) | 0.0359 (7) |
| C15 | 0.2721 (2) | 0.3287 (2) | 0.59151 (13) | 0.0358 (7) |
| C16 | 0.2965 (2) | 0.3996 (2) | 0.58994 (13) | 0.0355 (7) |
| C17 | 0.2375 (2) | 0.4961 (2) | 0.57527 (15) | 0.0452 (8) |
| H17 | 0.1776 | 0.5221 | 0.5664 | 0.054* |
| C18 | 0.2857 (2) | 0.5415 (2) | 0.57690 (15) | 0.0454 (9) |

| | | | | |
|---|---|---|---|---|
| H18 | 0.2648 | 0.6050 | 0.5697 | 0.054* |
| C19 | 0.3758 (2) | 0.4737 (2) | 0.59192 (13) | 0.0358 (7) |
| C20 | 0.4494 (2) | 0.4923 (2) | 0.59349 (13) | 0.0349 (7) |
| C21 | 0.83363 (11) | 0.17318 (17) | 0.58430 (9) | 0.0386 (7) |
| C22 | 0.88201 (15) | 0.18067 (18) | 0.62054 (8) | 0.0565 (10) |
| H22 | 0.8525 | 0.2000 | 0.6541 | 0.068* |
| C23 | 0.97456 (15) | 0.1592 (2) | 0.60660 (10) | 0.0654 (12) |
| H23 | 1.0069 | 0.1642 | 0.6308 | 0.079* |
| C24 | 1.01873 (12) | 0.13027 (19) | 0.55641 (11) | 0.0554 (10) |
| C25 | 0.97036 (16) | 0.1228 (2) | 0.52016 (8) | 0.0642 (11) |
| H25 | 0.9999 | 0.1034 | 0.4866 | 0.077* |
| C26 | 0.87781 (15) | 0.14423 (19) | 0.53411 (8) | 0.0578 (10) |
| H26 | 0.8454 | 0.1392 | 0.5099 | 0.069* |
| C27 | 1.1214 (3) | 0.1058 (4) | 0.5413 (2) | 0.0821 (15) |
| H27A | 1.1548 | 0.0701 | 0.5714 | 0.123* |
| H27B | 1.1273 | 0.1617 | 0.5320 | 0.123* |
| H27C | 1.1460 | 0.0703 | 0.5111 | 0.123* |
| C28 | 0.57628 (17) | −0.06230 (11) | 0.60141 (9) | 0.0380 (7) |
| C29 | 0.58805 (19) | −0.08589 (13) | 0.54983 (7) | 0.0554 (10) |
| H29 | 0.5829 | −0.0421 | 0.5202 | 0.067* |
| C30 | 0.60747 (19) | −0.17488 (15) | 0.54261 (8) | 0.0590 (11) |
| H30 | 0.6153 | −0.1907 | 0.5081 | 0.071* |
| C31 | 0.61512 (18) | −0.24027 (11) | 0.58696 (10) | 0.0485 (9) |
| C32 | 0.60335 (19) | −0.21668 (13) | 0.63854 (8) | 0.0606 (11) |
| H32 | 0.6085 | −0.2604 | 0.6682 | 0.073* |
| C33 | 0.58393 (19) | −0.12769 (14) | 0.64576 (7) | 0.0548 (10) |
| H33 | 0.5761 | −0.1119 | 0.6803 | 0.066* |
| C34 | 0.6364 (3) | −0.3371 (2) | 0.5793 (2) | 0.0718 (13) |
| H34A | 0.5914 | −0.3529 | 0.6015 | 0.108* |
| H34B | 0.6968 | −0.3801 | 0.5892 | 0.108* |
| H34C | 0.6347 | −0.3399 | 0.5422 | 0.108* |
| C35 | 0.17531 (12) | 0.35731 (16) | 0.57932 (9) | 0.0371 (7) |
| C36 | 0.16265 (14) | 0.33895 (18) | 0.53122 (9) | 0.0587 (10) |
| H36 | 0.2132 | 0.3113 | 0.5059 | 0.070* |
| C37 | 0.07448 (17) | 0.3619 (2) | 0.52100 (9) | 0.0657 (12) |
| H37 | 0.0660 | 0.3496 | 0.4888 | 0.079* |
| C38 | −0.00104 (13) | 0.40317 (19) | 0.55889 (11) | 0.0574 (10) |
| C39 | 0.01161 (13) | 0.42154 (19) | 0.60699 (10) | 0.0670 (12) |
| H39 | −0.0389 | 0.4492 | 0.6323 | 0.080* |
| C40 | 0.09979 (15) | 0.39861 (18) | 0.61721 (8) | 0.0552 (10) |
| H40 | 0.1083 | 0.4109 | 0.6494 | 0.066* |
| C41 | −0.0978 (3) | 0.4262 (4) | 0.5474 (2) | 0.0895 (17) |
| H41A | −0.1412 | 0.4469 | 0.5788 | 0.134* |
| H41B | −0.0965 | 0.3719 | 0.5382 | 0.134* |
| H41C | −0.1162 | 0.4743 | 0.5179 | 0.134* |
| C42 | 0.42917 (18) | 0.59212 (11) | 0.58439 (8) | 0.0366 (7) |
| C43 | 0.4098 (2) | 0.64024 (15) | 0.62826 (7) | 0.0590 (11) |
| H43 | 0.4113 | 0.6101 | 0.6630 | 0.071* |
| C44 | 0.3883 (2) | 0.73339 (15) | 0.62018 (9) | 0.0721 (13) |

| | | | | |
|---|---|---|---|---|
| H44 | 0.3754 | 0.7656 | 0.6495 | 0.086* |
| C45 | 0.3861 (2) | 0.77844 (11) | 0.56822 (11) | 0.0551 (10) |
| C46 | 0.4055 (2) | 0.73032 (15) | 0.52435 (8) | 0.0660 (12) |
| H46 | 0.4040 | 0.7605 | 0.4896 | 0.079* |
| C47 | 0.4270 (2) | 0.63716 (14) | 0.53243 (7) | 0.0634 (12) |
| H47 | 0.4400 | 0.6050 | 0.5031 | 0.076* |
| C48 | 0.3611 (4) | 0.8805 (3) | 0.5584 (3) | 0.0918 (18) |
| H48A | 0.3245 | 0.9092 | 0.5290 | 0.138* |
| H48B | 0.4165 | 0.8872 | 0.5499 | 0.138* |
| H48C | 0.3264 | 0.9097 | 0.5903 | 0.138* |
| C49 | 0.6371 (3) | 0.2746 (3) | 0.73369 (17) | 0.0662 (12) |
| H49 | 0.6745 | 0.2804 | 0.7026 | 0.079* |
| C50 | 0.6529 (3) | 0.2747 (4) | 0.78521 (19) | 0.0753 (14) |
| H50 | 0.7010 | 0.2799 | 0.7953 | 0.090* |
| C51 | 0.5826 (3) | 0.2656 (3) | 0.81738 (17) | 0.0625 (11) |
| H51 | 0.5733 | 0.2635 | 0.8547 | 0.075* |
| C52 | 0.4525 (4) | 0.0720 (3) | 0.73958 (18) | 0.0801 (15) |
| H52 | 0.4579 | 0.0446 | 0.7095 | 0.096* |
| C53 | 0.4384 (5) | 0.0365 (4) | 0.7919 (2) | 0.104 (2) |
| H53 | 0.4331 | −0.0175 | 0.8037 | 0.124* |
| C54 | 0.4340 (4) | 0.0974 (3) | 0.82229 (18) | 0.0786 (15) |
| H54 | 0.4246 | 0.0929 | 0.8597 | 0.094* |
| C55 | 0.2720 (3) | 0.4349 (3) | 0.72112 (17) | 0.0562 (10) |
| H55 | 0.2515 | 0.4662 | 0.6882 | 0.067* |
| C56 | 0.2217 (3) | 0.4589 (3) | 0.77061 (18) | 0.0631 (11) |
| H56 | 0.1629 | 0.5075 | 0.7774 | 0.076* |
| C57 | 0.2776 (3) | 0.3952 (3) | 0.80749 (17) | 0.0580 (10) |
| H57 | 0.2630 | 0.3928 | 0.8447 | 0.070* |
| C58 | 0.7418 (2) | 0.2770 (2) | 0.97547 (14) | 0.0447 (8) |
| C59 | 0.6632 (3) | 0.2596 (3) | 0.98277 (17) | 0.0558 (10) |
| H59 | 0.6582 | 0.2095 | 1.0037 | 0.067* |
| C60 | 0.5982 (3) | 0.3290 (3) | 0.95392 (17) | 0.0573 (10) |
| H60 | 0.5408 | 0.3348 | 0.9506 | 0.069* |
| C61 | 0.6343 (2) | 0.3919 (3) | 0.92943 (15) | 0.0457 (8) |
| C62 | 0.5815 (2) | 0.4807 (3) | 0.90399 (15) | 0.0461 (8) |
| C63 | 0.6114 (2) | 0.5482 (2) | 0.88756 (15) | 0.0471 (9) |
| C64 | 0.5520 (3) | 0.6445 (3) | 0.87306 (18) | 0.0595 (11) |
| H64 | 0.4884 | 0.6720 | 0.8725 | 0.071* |
| C65 | 0.6050 (3) | 0.6872 (3) | 0.86049 (18) | 0.0614 (11) |
| H65 | 0.5847 | 0.7500 | 0.8494 | 0.074* |
| C66 | 0.6991 (3) | 0.6189 (2) | 0.86710 (15) | 0.0477 (9) |
| C67 | 0.7752 (3) | 0.6366 (2) | 0.85929 (15) | 0.0490 (9) |
| C68 | 0.8648 (3) | 0.5729 (2) | 0.87425 (14) | 0.0447 (8) |
| C69 | 0.9417 (3) | 0.5923 (3) | 0.86766 (16) | 0.0535 (10) |
| H69 | 0.9437 | 0.6460 | 0.8501 | 0.064* |
| C70 | 1.0104 (3) | 0.5186 (3) | 0.89149 (16) | 0.0522 (9) |
| H70 | 1.0688 | 0.5117 | 0.8932 | 0.063* |
| C71 | 0.9772 (2) | 0.4528 (2) | 0.91367 (14) | 0.0435 (8) |
| C72 | 1.0247 (2) | 0.3694 (2) | 0.94671 (14) | 0.0417 (8) |

| | | | | |
|---|---|---|---|---|
| C73 | 0.9894 (2) | 0.3082 (2) | 0.97117 (14) | 0.0425 (8) |
| C74 | 1.0267 (3) | 0.2377 (3) | 1.01523 (15) | 0.0532 (10) |
| H74 | 1.0798 | 0.2224 | 1.0302 | 0.064* |
| C75 | 0.9705 (3) | 0.1984 (3) | 1.03051 (15) | 0.0523 (9) |
| H75 | 0.9776 | 0.1510 | 1.0582 | 0.063* |
| C76 | 0.8975 (2) | 0.2427 (2) | 0.99650 (14) | 0.0429 (8) |
| C77 | 0.8220 (2) | 0.2243 (2) | 1.00157 (14) | 0.0450 (8) |
| C78 | 0.48192 (12) | 0.50799 (18) | 0.89787 (10) | 0.0480 (9) |
| C79 | 0.45767 (15) | 0.51111 (19) | 0.84789 (8) | 0.0578 (10) |
| H79 | 0.5028 | 0.4939 | 0.8184 | 0.069* |
| C80 | 0.36602 (17) | 0.5400 (2) | 0.84192 (9) | 0.0640 (11) |
| H80 | 0.3498 | 0.5421 | 0.8085 | 0.077* |
| C81 | 0.29863 (12) | 0.56571 (19) | 0.88593 (11) | 0.0570 (10) |
| C82 | 0.32287 (14) | 0.5626 (2) | 0.93591 (9) | 0.0677 (12) |
| H82 | 0.2778 | 0.5798 | 0.9654 | 0.081* |
| C83 | 0.41452 (16) | 0.5337 (2) | 0.94188 (8) | 0.0673 (12) |
| H83 | 0.4307 | 0.5316 | 0.9753 | 0.081* |
| C84 | 0.1964 (3) | 0.6028 (4) | 0.8796 (2) | 0.0860 (16) |
| H84A | 0.1663 | 0.5832 | 0.9116 | 0.129* |
| H84B | 0.1916 | 0.5792 | 0.8493 | 0.129* |
| H84C | 0.1673 | 0.6692 | 0.8740 | 0.129* |
| C85 | 0.7594 (2) | 0.73294 (14) | 0.83665 (11) | 0.0548 (10) |
| C86 | 0.7408 (3) | 0.76536 (19) | 0.78365 (11) | 0.0844 (15) |
| H86 | 0.7391 | 0.7271 | 0.7618 | 0.101* |
| C87 | 0.7246 (3) | 0.8550 (2) | 0.76327 (11) | 0.0950 (18) |
| H87 | 0.7122 | 0.8767 | 0.7278 | 0.114* |
| C88 | 0.7271 (2) | 0.91228 (15) | 0.79588 (15) | 0.0833 (15) |
| C89 | 0.7457 (3) | 0.87986 (18) | 0.84888 (14) | 0.0903 (17) |
| H89 | 0.7474 | 0.9182 | 0.8707 | 0.108* |
| C90 | 0.7618 (2) | 0.7902 (2) | 0.86926 (10) | 0.0760 (13) |
| H90 | 0.7743 | 0.7685 | 0.9047 | 0.091* |
| C91 | 0.7080 (5) | 1.0114 (3) | 0.7720 (3) | 0.125 (3) |
| H91A | 0.6778 | 1.0280 | 0.7402 | 0.187* |
| H91B | 0.7653 | 1.0144 | 0.7629 | 0.187* |
| H91C | 0.6690 | 1.0537 | 0.7980 | 0.187* |
| C92 | 1.12048 (12) | 0.34652 (17) | 0.95883 (10) | 0.0458 (8) |
| C93 | 1.13340 (14) | 0.40831 (14) | 0.98216 (11) | 0.0550 (10) |
| H93 | 1.0832 | 0.4639 | 0.9913 | 0.066* |
| C94 | 1.22140 (17) | 0.38707 (18) | 0.99181 (11) | 0.0609 (11) |
| H94 | 1.2300 | 0.4284 | 1.0074 | 0.073* |
| C95 | 1.29646 (12) | 0.3040 (2) | 0.97812 (12) | 0.0636 (11) |
| C96 | 1.28354 (13) | 0.24225 (16) | 0.95479 (12) | 0.0655 (11) |
| H96 | 1.3338 | 0.1867 | 0.9456 | 0.079* |
| C97 | 1.19555 (16) | 0.26349 (15) | 0.94514 (11) | 0.0569 (10) |
| H97 | 1.1869 | 0.2221 | 0.9295 | 0.068* |
| C98 | 1.3932 (3) | 0.2829 (5) | 0.9880 (3) | 0.105 (2) |
| H98A | 1.3945 | 0.2812 | 1.0258 | 0.158* |
| H98B | 1.4081 | 0.3303 | 0.9683 | 0.158* |
| H98C | 1.4377 | 0.2240 | 0.9761 | 0.158* |

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|---|---|---|---|---|
| C99 | 0.82433 (19) | 0.14297 (14) | 1.04081 (9) | 0.0479 (9) |
| C100 | 0.8828 (2) | 0.05375 (17) | 1.02709 (10) | 0.0803 (15) |
| H100 | 0.9194 | 0.0448 | 0.9940 | 0.096* |
| C101 | 0.8864 (2) | −0.02211 (13) | 1.06279 (12) | 0.0907 (17) |
| H101 | 0.9255 | −0.0818 | 1.0536 | 0.109* |
| C102 | 0.8317 (2) | −0.00875 (16) | 1.11219 (11) | 0.0704 (12) |
| C103 | 0.7733 (2) | 0.08048 (19) | 1.12591 (9) | 0.0846 (16) |
| H103 | 0.7367 | 0.0894 | 1.1590 | 0.101* |
| C104 | 0.7696 (2) | 0.15634 (14) | 1.09022 (10) | 0.0752 (14) |
| H104 | 0.7305 | 0.2160 | 1.0994 | 0.090* |
| C105 | 0.8367 (5) | −0.0927 (4) | 1.1519 (2) | 0.107 (2) |
| H10A | 0.7771 | −0.0777 | 1.1718 | 0.160* |
| H10B | 0.8809 | −0.1084 | 1.1763 | 0.160* |
| H10C | 0.8554 | −0.1443 | 1.1323 | 0.160* |
| C106 | 0.8696 (4) | 0.1533 (3) | 0.8743 (2) | 0.0813 (15) |
| H106 | 0.8511 | 0.1467 | 0.9110 | 0.098* |
| C107 | 0.8985 (5) | 0.0862 (4) | 0.8408 (2) | 0.0979 (19) |
| H107 | 0.9030 | 0.0273 | 0.8499 | 0.118* |
| C108 | 0.9192 (4) | 0.1245 (3) | 0.7915 (2) | 0.0807 (15) |
| H108 | 0.9410 | 0.0956 | 0.7601 | 0.097* |
| C109 | 0.7038 (3) | 0.4920 (3) | 0.76419 (17) | 0.0660 (12) |
| H109 | 0.6592 | 0.5409 | 0.7829 | 0.079* |
| C110 | 0.6990 (4) | 0.4808 (4) | 0.7129 (2) | 0.0838 (15) |
| H110 | 0.6525 | 0.5182 | 0.6911 | 0.101* |
| C111 | 0.7784 (4) | 0.4021 (4) | 0.70145 (17) | 0.0775 (14) |
| H111 | 0.7962 | 0.3760 | 0.6692 | 0.093* |
| C112 | 1.0653 (3) | 0.3376 (3) | 0.80769 (16) | 0.0552 (10) |
| H112 | 1.0793 | 0.3604 | 0.8336 | 0.066* |
| C113 | 1.1254 (3) | 0.3001 (3) | 0.76312 (17) | 0.0617 (11) |
| H113 | 1.1852 | 0.2927 | 0.7532 | 0.074* |
| C114 | 1.0772 (3) | 0.2766 (3) | 0.73732 (17) | 0.0630 (11) |
| H114 | 1.0991 | 0.2492 | 0.7054 | 0.076* |
| C115 | 0.9965 (8) | 0.7857 (9) | 0.7792 (3) | 0.305 (8) |
| H11A | 1.0375 | 0.7236 | 0.7926 | 0.458* |
| H11B | 0.9378 | 0.7896 | 0.7764 | 0.458* |
| H11C | 0.9880 | 0.8278 | 0.8034 | 0.458* |
| C116 | 1.0362 (5) | 0.8099 (5) | 0.7259 (2) | 0.164 (3) |
| C117 | 1.1209 (4) | 0.7460 (3) | 0.7028 (3) | 0.152 (3) |
| H117 | 1.1525 | 0.6877 | 0.7212 | 0.183* |
| C118 | 1.1584 (4) | 0.7693 (5) | 0.6523 (3) | 0.197 (5) |
| H18A | 1.2151 | 0.7265 | 0.6369 | 0.237* |
| C119 | 1.1112 (6) | 0.8565 (6) | 0.6249 (2) | 0.169 (4) |
| H119 | 1.1363 | 0.8720 | 0.5911 | 0.203* |
| C120 | 1.0265 (5) | 0.9204 (4) | 0.6480 (3) | 0.183 (4) |
| H120 | 0.9949 | 0.9787 | 0.6297 | 0.220* |
| C121 | 0.9890 (4) | 0.8971 (4) | 0.6985 (3) | 0.154 (3) |
| H121 | 0.9323 | 0.9399 | 0.7140 | 0.184* |
| C122 | 1.0363 (5) | 0.2584 (4) | 0.4021 (2) | 0.141 (3) |
| H12A | 0.9780 | 0.2634 | 0.3976 | 0.211* |

| | | | | | |
|---|---|---|---|---|---|
| H12B | 1.0330 | 0.2744 | 0.4372 | 0.211* | |
| H12C | 1.0838 | 0.1960 | 0.3987 | 0.211* | |
| C123 | 1.0580 (5) | 0.3216 (3) | 0.3608 (2) | 0.1055 (19) | |
| C124 | 1.1425 (4) | 0.3241 (4) | 0.3612 (3) | 0.0979 (18) | |
| H12F | 1.1819 | 0.2863 | 0.3869 | 0.117* | |
| C125 | 1.1641 (5) | 0.3806 (5) | 0.3246 (3) | 0.125 (2) | |
| H125 | 1.2191 | 0.3823 | 0.3250 | 0.151* | |
| C126 | 1.1028 (6) | 0.4416 (4) | 0.2828 (3) | 0.120 (2) | |
| H126 | 1.1179 | 0.4815 | 0.2570 | 0.144* | |
| C127 | 1.0276 (6) | 0.4361 (5) | 0.2842 (3) | 0.119 (2) | |
| H127 | 0.9881 | 0.4728 | 0.2583 | 0.143* | |
| C128 | 1.0022 (4) | 0.3769 (3) | 0.3231 (2) | 0.0951 (17) | |
| H128 | 0.9467 | 0.3762 | 0.3227 | 0.114* | |
| C129 | 0.1921 (5) | 1.0193 (4) | 0.6989 (2) | 0.150 (3) | |
| H12H | 0.1336 | 1.0202 | 0.7003 | 0.225* | |
| H12I | 0.2151 | 1.0298 | 0.6621 | 0.225* | |
| H12J | 0.1846 | 1.0672 | 0.7185 | 0.225* | |
| C130 | 0.2587 (3) | 0.9280 (2) | 0.72326 (13) | 0.0985 (18) | |
| C131 | 0.2295 (3) | 0.8614 (3) | 0.74347 (17) | 0.111 (2) | |
| H131 | 0.1690 | 0.8743 | 0.7416 | 0.133* | |
| C132 | 0.2907 (4) | 0.7753 (3) | 0.76648 (17) | 0.123 (2) | |
| H132 | 0.2711 | 0.7306 | 0.7800 | 0.148* | |
| C133 | 0.3810 (4) | 0.7559 (3) | 0.76928 (16) | 0.124 (2) | |
| H133 | 0.4220 | 0.6983 | 0.7847 | 0.149* | |
| C134 | 0.4103 (2) | 0.8225 (4) | 0.74906 (18) | 0.122 (2) | |
| H124 | 0.4707 | 0.8096 | 0.7509 | 0.147* | |
| C135 | 0.3491 (3) | 0.9086 (3) | 0.72606 (15) | 0.0981 (17) | |
| H135 | 0.3687 | 0.9533 | 0.7125 | 0.118* | |
| C136 | 0.430 (2) | −0.0286 (14) | 0.9639 (11) | 0.370 (17) | 0.50 |
| H13A | 0.3782 | −0.0247 | 0.9899 | 0.555* | 0.50 |
| H13B | 0.4664 | −0.0911 | 0.9552 | 0.555* | 0.50 |
| H13C | 0.4074 | 0.0117 | 0.9319 | 0.555* | 0.50 |
| C137 | 0.4882 (19) | 0.0007 (9) | 0.9872 (9) | 0.370 (17) | 0.50 |
| C138 | 0.457 (2) | 0.0311 (12) | 1.0381 (9) | 0.370 (17) | 0.50 |
| H138 | 0.4023 | 0.0330 | 1.0565 | 0.444* | 0.50 |
| C139 | 0.508 (3) | 0.0587 (11) | 1.0614 (8) | 0.370 (17) | 0.50 |
| H139 | 0.4868 | 0.0791 | 1.0954 | 0.444* | 0.50 |
| C140 | 0.590 (2) | 0.0559 (10) | 1.0339 (10) | 0.370 (17) | 0.50 |
| H140 | 0.6234 | 0.0744 | 1.0496 | 0.444* | 0.50 |
| C141 | 0.621 (2) | 0.0255 (11) | 0.9831 (10) | 0.370 (17) | 0.50 |
| H141 | 0.6755 | 0.0236 | 0.9647 | 0.444* | 0.50 |
| C142 | 0.570 (2) | −0.0022 (9) | 0.9598 (7) | 0.370 (17) | 0.50 |
| H142 | 0.5909 | −0.0225 | 0.9257 | 0.444* | 0.50 |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sm1 | 0.03464 (9) | 0.02702 (8) | 0.03449 (9) | −0.01687 (7) | −0.00639 (7) | −0.00408 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Sm2 | 0.04230 (11) | 0.04041 (10) | 0.03538 (10) | −0.02316 (8) | −0.00873 (8) | −0.00238 (7) |
| N1 | 0.0364 (15) | 0.0282 (13) | 0.0394 (15) | −0.0167 (11) | −0.0076 (12) | −0.0052 (11) |
| N2 | 0.0375 (15) | 0.0273 (13) | 0.0421 (15) | −0.0172 (12) | −0.0073 (12) | −0.0039 (11) |
| N3 | 0.0361 (15) | 0.0257 (12) | 0.0440 (15) | −0.0154 (11) | −0.0082 (12) | −0.0056 (11) |
| N4 | 0.0376 (15) | 0.0280 (13) | 0.0425 (15) | −0.0183 (12) | −0.0070 (12) | −0.0066 (11) |
| N5 | 0.0531 (19) | 0.066 (2) | 0.0404 (17) | −0.0346 (16) | −0.0094 (14) | −0.0081 (14) |
| N6 | 0.0550 (19) | 0.0529 (17) | 0.0384 (17) | −0.0274 (15) | −0.0106 (14) | −0.0081 (13) |
| N7 | 0.078 (2) | 0.0490 (18) | 0.0410 (17) | −0.0397 (17) | −0.0012 (16) | −0.0051 (13) |
| N8 | 0.067 (2) | 0.0486 (17) | 0.0398 (17) | −0.0318 (16) | −0.0041 (15) | −0.0002 (13) |
| N9 | 0.0477 (18) | 0.0492 (17) | 0.0443 (18) | −0.0145 (15) | −0.0048 (14) | −0.0120 (14) |
| N10 | 0.0522 (19) | 0.0498 (17) | 0.0417 (17) | −0.0243 (15) | 0.0000 (14) | −0.0116 (13) |
| N11 | 0.0398 (16) | 0.0472 (16) | 0.0473 (17) | −0.0231 (14) | −0.0102 (13) | 0.0008 (13) |
| N12 | 0.0464 (17) | 0.0446 (16) | 0.0476 (17) | −0.0259 (14) | −0.0132 (14) | −0.0002 (13) |
| N13 | 0.0406 (16) | 0.0445 (16) | 0.0415 (16) | −0.0213 (13) | −0.0103 (13) | −0.0030 (12) |
| N14 | 0.0401 (16) | 0.0460 (16) | 0.0392 (16) | −0.0213 (13) | −0.0071 (13) | −0.0023 (12) |
| N15 | 0.083 (2) | 0.0540 (19) | 0.0503 (19) | −0.0418 (18) | −0.0057 (17) | −0.0091 (15) |
| N16 | 0.079 (2) | 0.061 (2) | 0.054 (2) | −0.0434 (19) | −0.0017 (17) | −0.0176 (16) |
| N17 | 0.068 (2) | 0.070 (2) | 0.0427 (18) | −0.0360 (19) | −0.0159 (16) | −0.0021 (16) |
| N18 | 0.080 (2) | 0.075 (2) | 0.0427 (19) | −0.049 (2) | −0.0120 (17) | −0.0047 (16) |
| N19 | 0.058 (2) | 0.0579 (19) | 0.0475 (18) | −0.0334 (16) | −0.0004 (15) | −0.0134 (15) |
| N20 | 0.070 (2) | 0.0601 (19) | 0.0417 (17) | −0.0373 (18) | 0.0041 (16) | −0.0147 (15) |
| B1 | 0.060 (3) | 0.054 (2) | 0.032 (2) | −0.029 (2) | −0.0063 (19) | −0.0050 (18) |
| B2 | 0.091 (4) | 0.070 (3) | 0.042 (2) | −0.050 (3) | −0.002 (2) | −0.018 (2) |
| C1 | 0.0435 (19) | 0.0308 (16) | 0.0360 (17) | −0.0233 (15) | −0.0050 (14) | −0.0058 (13) |
| C2 | 0.050 (2) | 0.0330 (17) | 0.056 (2) | −0.0273 (16) | −0.0086 (17) | −0.0049 (15) |
| C3 | 0.046 (2) | 0.0426 (19) | 0.055 (2) | −0.0307 (17) | −0.0066 (17) | −0.0076 (16) |
| C4 | 0.0391 (18) | 0.0349 (16) | 0.0388 (18) | −0.0207 (15) | −0.0074 (14) | −0.0073 (13) |
| C5 | 0.0372 (18) | 0.0351 (17) | 0.0416 (18) | −0.0181 (14) | −0.0070 (14) | −0.0073 (14) |
| C6 | 0.0373 (18) | 0.0327 (16) | 0.0415 (18) | −0.0176 (14) | −0.0062 (14) | −0.0053 (13) |
| C7 | 0.0352 (19) | 0.0334 (17) | 0.070 (3) | −0.0130 (15) | −0.0048 (17) | −0.0084 (16) |
| C8 | 0.042 (2) | 0.0278 (16) | 0.071 (3) | −0.0148 (15) | −0.0045 (18) | −0.0095 (16) |
| C9 | 0.0402 (18) | 0.0286 (15) | 0.0439 (19) | −0.0176 (14) | −0.0034 (15) | −0.0049 (13) |
| C10 | 0.0438 (19) | 0.0255 (15) | 0.0402 (18) | −0.0185 (14) | −0.0037 (15) | −0.0052 (13) |
| C11 | 0.0448 (19) | 0.0308 (16) | 0.0396 (18) | −0.0220 (15) | −0.0063 (15) | −0.0062 (13) |
| C12 | 0.052 (2) | 0.0346 (17) | 0.057 (2) | −0.0292 (17) | −0.0089 (17) | −0.0092 (15) |
| C13 | 0.043 (2) | 0.0385 (18) | 0.064 (2) | −0.0248 (16) | −0.0142 (17) | −0.0069 (16) |
| C14 | 0.0376 (18) | 0.0371 (17) | 0.0408 (18) | −0.0217 (15) | −0.0065 (14) | −0.0071 (14) |
| C15 | 0.0368 (18) | 0.0366 (17) | 0.0395 (18) | −0.0191 (14) | −0.0093 (14) | −0.0053 (14) |
| C16 | 0.0389 (18) | 0.0328 (16) | 0.0389 (18) | −0.0169 (14) | −0.0123 (14) | −0.0046 (13) |
| C17 | 0.043 (2) | 0.0358 (17) | 0.058 (2) | −0.0148 (16) | −0.0223 (17) | −0.0006 (15) |
| C18 | 0.050 (2) | 0.0264 (16) | 0.061 (2) | −0.0154 (15) | −0.0209 (18) | 0.0001 (15) |
| C19 | 0.0423 (18) | 0.0266 (15) | 0.0420 (18) | −0.0168 (14) | −0.0099 (15) | −0.0042 (13) |
| C20 | 0.0454 (19) | 0.0272 (15) | 0.0371 (17) | −0.0195 (14) | −0.0063 (14) | −0.0053 (13) |
| C21 | 0.0353 (18) | 0.0339 (16) | 0.050 (2) | −0.0176 (14) | −0.0054 (15) | −0.0062 (14) |
| C22 | 0.042 (2) | 0.069 (3) | 0.062 (3) | −0.0202 (19) | −0.0074 (18) | −0.027 (2) |
| C23 | 0.042 (2) | 0.080 (3) | 0.079 (3) | −0.022 (2) | −0.016 (2) | −0.028 (2) |
| C24 | 0.039 (2) | 0.048 (2) | 0.078 (3) | −0.0196 (17) | −0.008 (2) | −0.0050 (19) |
| C25 | 0.053 (2) | 0.088 (3) | 0.059 (3) | −0.039 (2) | 0.008 (2) | −0.020 (2) |
| C26 | 0.052 (2) | 0.081 (3) | 0.054 (2) | −0.039 (2) | −0.0016 (19) | −0.018 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C27 | 0.042 (2) | 0.093 (4) | 0.107 (4) | −0.029 (2) | −0.003 (2) | −0.012 (3) |
| C28 | 0.0402 (18) | 0.0260 (15) | 0.051 (2) | −0.0171 (14) | −0.0043 (15) | −0.0075 (14) |
| C29 | 0.081 (3) | 0.0353 (18) | 0.052 (2) | −0.0303 (19) | −0.001 (2) | −0.0077 (16) |
| C30 | 0.077 (3) | 0.041 (2) | 0.063 (3) | −0.028 (2) | 0.000 (2) | −0.0207 (18) |
| C31 | 0.040 (2) | 0.0282 (17) | 0.080 (3) | −0.0174 (15) | −0.0029 (18) | −0.0130 (17) |
| C32 | 0.077 (3) | 0.0316 (18) | 0.069 (3) | −0.0249 (19) | −0.008 (2) | 0.0037 (17) |
| C33 | 0.076 (3) | 0.0367 (19) | 0.052 (2) | −0.0246 (19) | −0.011 (2) | −0.0046 (16) |
| C34 | 0.065 (3) | 0.033 (2) | 0.121 (4) | −0.0239 (19) | −0.002 (3) | −0.022 (2) |
| C35 | 0.0380 (18) | 0.0340 (16) | 0.0452 (19) | −0.0204 (14) | −0.0125 (15) | 0.0007 (14) |
| C36 | 0.047 (2) | 0.077 (3) | 0.061 (3) | −0.029 (2) | −0.0092 (19) | −0.023 (2) |
| C37 | 0.061 (3) | 0.086 (3) | 0.068 (3) | −0.042 (2) | −0.022 (2) | −0.013 (2) |
| C38 | 0.045 (2) | 0.055 (2) | 0.078 (3) | −0.0279 (19) | −0.024 (2) | 0.011 (2) |
| C39 | 0.041 (2) | 0.086 (3) | 0.068 (3) | −0.024 (2) | −0.004 (2) | −0.010 (2) |
| C40 | 0.046 (2) | 0.069 (3) | 0.050 (2) | −0.022 (2) | −0.0098 (18) | −0.0119 (19) |
| C41 | 0.054 (3) | 0.102 (4) | 0.122 (5) | −0.042 (3) | −0.034 (3) | 0.010 (3) |
| C42 | 0.0402 (18) | 0.0269 (15) | 0.048 (2) | −0.0173 (14) | −0.0090 (15) | −0.0065 (14) |
| C43 | 0.087 (3) | 0.044 (2) | 0.050 (2) | −0.035 (2) | 0.004 (2) | −0.0128 (17) |
| C44 | 0.100 (4) | 0.045 (2) | 0.075 (3) | −0.037 (2) | 0.012 (3) | −0.028 (2) |
| C45 | 0.049 (2) | 0.0269 (17) | 0.092 (3) | −0.0182 (16) | −0.008 (2) | −0.0085 (19) |
| C46 | 0.102 (4) | 0.043 (2) | 0.062 (3) | −0.039 (2) | −0.032 (2) | 0.0134 (19) |
| C47 | 0.114 (4) | 0.040 (2) | 0.049 (2) | −0.041 (2) | −0.023 (2) | −0.0004 (17) |
| C48 | 0.084 (4) | 0.030 (2) | 0.160 (5) | −0.025 (2) | −0.014 (3) | −0.013 (3) |
| C49 | 0.064 (3) | 0.103 (3) | 0.054 (3) | −0.055 (3) | −0.007 (2) | −0.014 (2) |
| C50 | 0.072 (3) | 0.118 (4) | 0.065 (3) | −0.059 (3) | −0.019 (2) | −0.018 (3) |
| C51 | 0.074 (3) | 0.077 (3) | 0.049 (2) | −0.038 (2) | −0.022 (2) | −0.011 (2) |
| C52 | 0.143 (5) | 0.070 (3) | 0.056 (3) | −0.077 (3) | 0.007 (3) | −0.009 (2) |
| C53 | 0.196 (7) | 0.085 (4) | 0.063 (3) | −0.103 (4) | 0.012 (4) | −0.004 (3) |
| C54 | 0.128 (4) | 0.072 (3) | 0.049 (3) | −0.065 (3) | 0.001 (3) | 0.005 (2) |
| C55 | 0.048 (2) | 0.055 (2) | 0.056 (2) | −0.0122 (19) | −0.0090 (19) | −0.0158 (19) |
| C56 | 0.049 (2) | 0.061 (3) | 0.068 (3) | −0.013 (2) | 0.000 (2) | −0.025 (2) |
| C57 | 0.056 (2) | 0.068 (3) | 0.051 (2) | −0.030 (2) | 0.009 (2) | −0.024 (2) |
| C58 | 0.046 (2) | 0.047 (2) | 0.043 (2) | −0.0255 (17) | −0.0033 (16) | 0.0001 (15) |
| C59 | 0.055 (2) | 0.058 (2) | 0.062 (3) | −0.037 (2) | −0.008 (2) | 0.0064 (19) |
| C60 | 0.046 (2) | 0.067 (3) | 0.070 (3) | −0.036 (2) | −0.012 (2) | 0.001 (2) |
| C61 | 0.040 (2) | 0.054 (2) | 0.048 (2) | −0.0254 (17) | −0.0079 (16) | −0.0036 (16) |
| C62 | 0.040 (2) | 0.056 (2) | 0.047 (2) | −0.0241 (17) | −0.0104 (16) | −0.0045 (17) |
| C63 | 0.044 (2) | 0.050 (2) | 0.051 (2) | −0.0209 (17) | −0.0161 (17) | −0.0037 (16) |
| C64 | 0.044 (2) | 0.052 (2) | 0.081 (3) | −0.0163 (19) | −0.023 (2) | −0.003 (2) |
| C65 | 0.055 (2) | 0.042 (2) | 0.086 (3) | −0.0179 (19) | −0.025 (2) | 0.001 (2) |
| C66 | 0.052 (2) | 0.0418 (19) | 0.054 (2) | −0.0222 (17) | −0.0183 (18) | −0.0007 (16) |
| C67 | 0.057 (2) | 0.044 (2) | 0.051 (2) | −0.0254 (18) | −0.0134 (18) | −0.0024 (16) |
| C68 | 0.052 (2) | 0.0458 (19) | 0.043 (2) | −0.0274 (17) | −0.0081 (17) | −0.0044 (15) |
| C69 | 0.059 (2) | 0.053 (2) | 0.061 (2) | −0.037 (2) | −0.006 (2) | −0.0025 (18) |
| C70 | 0.050 (2) | 0.062 (2) | 0.059 (2) | −0.036 (2) | −0.0069 (19) | −0.0093 (19) |
| C71 | 0.043 (2) | 0.052 (2) | 0.043 (2) | −0.0253 (17) | −0.0030 (16) | −0.0144 (16) |
| C72 | 0.0377 (19) | 0.051 (2) | 0.0407 (19) | −0.0211 (16) | −0.0061 (15) | −0.0104 (16) |
| C73 | 0.0366 (19) | 0.052 (2) | 0.0389 (19) | −0.0191 (16) | −0.0049 (15) | −0.0088 (15) |
| C74 | 0.044 (2) | 0.063 (2) | 0.049 (2) | −0.0209 (19) | −0.0160 (18) | 0.0016 (18) |
| C75 | 0.049 (2) | 0.055 (2) | 0.047 (2) | −0.0210 (19) | −0.0134 (18) | 0.0073 (17) |

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|---|---|---|---|---|---|---|
| C76 | 0.042 (2) | 0.0443 (19) | 0.0372 (19) | −0.0177 (16) | −0.0041 (15) | −0.0001 (15) |
| C77 | 0.046 (2) | 0.0457 (19) | 0.041 (2) | −0.0220 (17) | −0.0022 (16) | 0.0000 (15) |
| C78 | 0.043 (2) | 0.050 (2) | 0.055 (2) | −0.0224 (17) | −0.0164 (18) | −0.0030 (17) |
| C79 | 0.050 (2) | 0.074 (3) | 0.056 (2) | −0.032 (2) | −0.0090 (19) | −0.010 (2) |
| C80 | 0.058 (3) | 0.082 (3) | 0.064 (3) | −0.037 (2) | −0.022 (2) | −0.007 (2) |
| C81 | 0.043 (2) | 0.048 (2) | 0.087 (3) | −0.0203 (18) | −0.020 (2) | −0.014 (2) |
| C82 | 0.046 (2) | 0.084 (3) | 0.077 (3) | −0.026 (2) | −0.006 (2) | −0.031 (2) |
| C83 | 0.050 (2) | 0.096 (3) | 0.060 (3) | −0.029 (2) | −0.009 (2) | −0.026 (2) |
| C84 | 0.049 (3) | 0.093 (4) | 0.122 (4) | −0.026 (3) | −0.024 (3) | −0.031 (3) |
| C85 | 0.055 (2) | 0.045 (2) | 0.068 (3) | −0.0255 (18) | −0.013 (2) | −0.0022 (18) |
| C86 | 0.119 (4) | 0.063 (3) | 0.080 (3) | −0.045 (3) | −0.044 (3) | 0.014 (2) |
| C87 | 0.122 (5) | 0.070 (3) | 0.097 (4) | −0.049 (3) | −0.049 (4) | 0.030 (3) |
| C88 | 0.071 (3) | 0.046 (2) | 0.123 (5) | −0.023 (2) | −0.015 (3) | 0.007 (3) |
| C89 | 0.111 (4) | 0.060 (3) | 0.108 (4) | −0.048 (3) | 0.005 (4) | −0.022 (3) |
| C90 | 0.102 (4) | 0.060 (3) | 0.074 (3) | −0.045 (3) | −0.003 (3) | −0.009 (2) |
| C91 | 0.118 (5) | 0.048 (3) | 0.192 (7) | −0.034 (3) | −0.027 (5) | 0.021 (4) |
| C92 | 0.041 (2) | 0.062 (2) | 0.0390 (19) | −0.0260 (18) | −0.0048 (16) | −0.0083 (16) |
| C93 | 0.044 (2) | 0.069 (3) | 0.058 (2) | −0.0272 (19) | −0.0049 (18) | −0.019 (2) |
| C94 | 0.054 (2) | 0.084 (3) | 0.060 (3) | −0.039 (2) | −0.008 (2) | −0.018 (2) |
| C95 | 0.041 (2) | 0.097 (3) | 0.058 (3) | −0.038 (2) | −0.0065 (19) | −0.004 (2) |
| C96 | 0.041 (2) | 0.076 (3) | 0.072 (3) | −0.020 (2) | −0.003 (2) | −0.013 (2) |
| C97 | 0.046 (2) | 0.062 (2) | 0.064 (3) | −0.023 (2) | −0.0038 (19) | −0.017 (2) |
| C98 | 0.051 (3) | 0.149 (6) | 0.128 (5) | −0.049 (3) | −0.017 (3) | −0.025 (4) |
| C99 | 0.049 (2) | 0.048 (2) | 0.045 (2) | −0.0240 (18) | −0.0050 (17) | 0.0023 (16) |
| C100 | 0.085 (3) | 0.053 (3) | 0.065 (3) | −0.013 (2) | 0.018 (3) | −0.002 (2) |
| C101 | 0.109 (4) | 0.042 (2) | 0.083 (4) | −0.016 (3) | 0.011 (3) | 0.000 (2) |
| C102 | 0.092 (3) | 0.058 (3) | 0.059 (3) | −0.037 (3) | −0.014 (2) | 0.011 (2) |
| C103 | 0.129 (5) | 0.065 (3) | 0.049 (3) | −0.048 (3) | 0.016 (3) | −0.001 (2) |
| C104 | 0.102 (4) | 0.056 (3) | 0.055 (3) | −0.034 (3) | 0.012 (3) | −0.006 (2) |
| C105 | 0.155 (6) | 0.068 (3) | 0.089 (4) | −0.055 (4) | −0.016 (4) | 0.024 (3) |
| C106 | 0.133 (5) | 0.061 (3) | 0.063 (3) | −0.059 (3) | −0.002 (3) | −0.006 (2) |
| C107 | 0.161 (6) | 0.063 (3) | 0.088 (4) | −0.070 (4) | 0.001 (4) | −0.013 (3) |
| C108 | 0.116 (4) | 0.067 (3) | 0.078 (3) | −0.054 (3) | −0.001 (3) | −0.029 (3) |
| C109 | 0.069 (3) | 0.079 (3) | 0.051 (2) | −0.034 (2) | −0.023 (2) | 0.007 (2) |
| C110 | 0.100 (4) | 0.103 (4) | 0.060 (3) | −0.052 (4) | −0.040 (3) | 0.013 (3) |
| C111 | 0.115 (4) | 0.106 (4) | 0.040 (2) | −0.071 (4) | −0.027 (3) | 0.004 (2) |
| C112 | 0.061 (3) | 0.058 (2) | 0.051 (2) | −0.033 (2) | −0.0010 (19) | −0.0078 (18) |
| C113 | 0.061 (3) | 0.065 (3) | 0.061 (3) | −0.035 (2) | 0.012 (2) | −0.013 (2) |
| C114 | 0.079 (3) | 0.063 (3) | 0.051 (2) | −0.040 (2) | 0.012 (2) | −0.015 (2) |
| C115 | 0.296 (11) | 0.352 (12) | 0.286 (11) | −0.188 (9) | −0.010 (8) | 0.009 (8) |
| C116 | 0.161 (7) | 0.187 (7) | 0.188 (7) | −0.118 (6) | −0.036 (6) | 0.003 (6) |
| C117 | 0.140 (6) | 0.133 (5) | 0.225 (8) | −0.075 (5) | −0.063 (6) | −0.037 (5) |
| C118 | 0.177 (8) | 0.219 (8) | 0.246 (9) | −0.103 (7) | −0.035 (7) | −0.096 (7) |
| C119 | 0.178 (7) | 0.212 (8) | 0.177 (7) | −0.123 (6) | −0.039 (6) | −0.038 (6) |
| C120 | 0.206 (8) | 0.175 (7) | 0.219 (8) | −0.115 (6) | −0.072 (7) | −0.011 (6) |
| C121 | 0.154 (6) | 0.137 (6) | 0.186 (7) | −0.070 (5) | −0.060 (6) | −0.006 (5) |
| C122 | 0.195 (7) | 0.117 (5) | 0.129 (5) | −0.096 (5) | 0.003 (5) | −0.008 (4) |
| C123 | 0.142 (5) | 0.083 (4) | 0.095 (4) | −0.051 (4) | −0.012 (4) | −0.019 (3) |
| C124 | 0.075 (3) | 0.109 (4) | 0.124 (5) | −0.044 (3) | −0.012 (3) | −0.042 (4) |

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|---|---|---|---|---|---|---|
| C125 | 0.117 (5) | 0.129 (5) | 0.132 (6) | −0.058 (4) | −0.001 (4) | −0.029 (4) |
| C126 | 0.144 (6) | 0.108 (5) | 0.113 (5) | −0.073 (4) | 0.015 (4) | −0.013 (4) |
| C127 | 0.132 (5) | 0.112 (5) | 0.118 (5) | −0.055 (4) | −0.017 (4) | −0.023 (4) |
| C128 | 0.107 (4) | 0.085 (4) | 0.100 (4) | −0.044 (3) | −0.032 (3) | −0.006 (3) |
| C129 | 0.170 (6) | 0.116 (5) | 0.134 (6) | −0.042 (5) | −0.028 (5) | −0.005 (4) |
| C130 | 0.131 (5) | 0.096 (4) | 0.071 (3) | −0.051 (4) | −0.016 (3) | −0.017 (3) |
| C131 | 0.137 (5) | 0.121 (5) | 0.110 (4) | −0.088 (4) | −0.016 (4) | −0.008 (4) |
| C132 | 0.155 (6) | 0.125 (5) | 0.118 (5) | −0.082 (5) | −0.028 (4) | −0.011 (4) |
| C133 | 0.156 (6) | 0.114 (5) | 0.096 (4) | −0.051 (4) | −0.035 (4) | −0.012 (4) |
| C134 | 0.116 (5) | 0.152 (6) | 0.108 (5) | −0.070 (5) | −0.006 (4) | −0.021 (4) |
| C135 | 0.112 (4) | 0.117 (4) | 0.087 (4) | −0.073 (4) | −0.005 (3) | −0.010 (3) |
| C136 | 0.58 (4) | 0.090 (10) | 0.193 (13) | 0.028 (14) | −0.003 (16) | −0.013 (8) |
| C137 | 0.58 (4) | 0.090 (10) | 0.193 (13) | 0.028 (14) | −0.003 (16) | −0.013 (8) |
| C138 | 0.58 (4) | 0.090 (10) | 0.193 (13) | 0.028 (14) | −0.003 (16) | −0.013 (8) |
| C139 | 0.58 (4) | 0.090 (10) | 0.193 (13) | 0.028 (14) | −0.003 (16) | −0.013 (8) |
| C140 | 0.58 (4) | 0.090 (10) | 0.193 (13) | 0.028 (14) | −0.003 (16) | −0.013 (8) |
| C141 | 0.58 (4) | 0.090 (10) | 0.193 (13) | 0.028 (14) | −0.003 (16) | −0.013 (8) |
| C142 | 0.58 (4) | 0.090 (10) | 0.193 (13) | 0.028 (14) | −0.003 (16) | −0.013 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Sm1—N4 | 2.409 (3) | C58—C59 | 1.439 (5) |
| Sm1—N1 | 2.411 (3) | C59—C60 | 1.350 (5) |
| Sm1—N3 | 2.425 (2) | C59—H59 | 0.9300 |
| Sm1—N2 | 2.438 (3) | C60—C61 | 1.433 (5) |
| Sm1—N5 | 2.572 (3) | C60—H60 | 0.9300 |
| Sm1—N9 | 2.585 (3) | C61—C62 | 1.405 (5) |
| Sm1—N7 | 2.598 (3) | C62—C63 | 1.399 (5) |
| Sm1—B1 | 3.690 (4) | C62—C78 | 1.523 (4) |
| Sm2—N11 | 2.400 (3) | C63—C64 | 1.435 (5) |
| Sm2—N13 | 2.401 (3) | C64—C65 | 1.337 (6) |
| Sm2—N12 | 2.410 (3) | C64—H64 | 0.9300 |
| Sm2—N14 | 2.448 (3) | C65—C66 | 1.444 (5) |
| Sm2—N17 | 2.584 (3) | C65—H65 | 0.9300 |
| Sm2—N19 | 2.600 (3) | C66—C67 | 1.402 (5) |
| Sm2—N15 | 2.606 (3) | C67—C68 | 1.424 (5) |
| Sm2—B2 | 3.677 (4) | C67—C85 | 1.503 (4) |
| N1—C4 | 1.373 (4) | C68—C69 | 1.436 (5) |
| N1—C1 | 1.379 (4) | C69—C70 | 1.345 (5) |
| N2—C6 | 1.373 (4) | C69—H69 | 0.9300 |
| N2—C9 | 1.374 (4) | C70—C71 | 1.430 (5) |
| N3—C11 | 1.366 (4) | C70—H70 | 0.9300 |
| N3—C14 | 1.381 (4) | C71—C72 | 1.418 (5) |
| N4—C19 | 1.370 (4) | C72—C73 | 1.400 (5) |
| N4—C16 | 1.374 (4) | C72—C92 | 1.528 (4) |
| N5—C49 | 1.328 (5) | C73—C74 | 1.444 (5) |
| N5—N6 | 1.355 (4) | C74—C75 | 1.341 (5) |
| N6—C51 | 1.345 (5) | C74—H74 | 0.9300 |
| N6—B1 | 1.535 (5) | C75—C76 | 1.438 (5) |

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|---|---|---|---|
| N7—C52 | 1.318 (5) | C75—H75 | 0.9300 |
| N7—N8 | 1.363 (4) | C76—C77 | 1.406 (5) |
| N8—C54 | 1.335 (5) | C77—C99 | 1.509 (4) |
| N8—B1 | 1.526 (5) | C78—C79 | 1.3900 |
| N9—C55 | 1.322 (5) | C78—C83 | 1.3900 |
| N9—N10 | 1.373 (4) | C79—C80 | 1.3900 |
| N10—C57 | 1.329 (5) | C79—H79 | 0.9300 |
| N10—B1 | 1.541 (5) | C80—C81 | 1.3900 |
| N11—C58 | 1.380 (4) | C80—H80 | 0.9300 |
| N11—C61 | 1.380 (4) | C81—C82 | 1.3900 |
| N12—C66 | 1.377 (4) | C81—C84 | 1.534 (4) |
| N12—C63 | 1.381 (4) | C82—C83 | 1.3900 |
| N13—C71 | 1.377 (4) | C82—H82 | 0.9300 |
| N13—C68 | 1.381 (4) | C83—H83 | 0.9300 |
| N14—C73 | 1.376 (4) | C84—H84A | 0.9600 |
| N14—C76 | 1.384 (4) | C84—H84B | 0.9600 |
| N15—C106 | 1.331 (5) | C84—H84C | 0.9600 |
| N15—N16 | 1.356 (4) | C85—C86 | 1.3900 |
| N16—C108 | 1.331 (5) | C85—C90 | 1.3900 |
| N16—B2 | 1.533 (6) | C86—C87 | 1.3900 |
| N17—C109 | 1.343 (5) | C86—H86 | 0.9300 |
| N17—N18 | 1.355 (5) | C87—C88 | 1.3900 |
| N18—C111 | 1.355 (5) | C87—H87 | 0.9300 |
| N18—B2 | 1.524 (6) | C88—C89 | 1.3900 |
| N19—C112 | 1.335 (5) | C88—C91 | 1.539 (5) |
| N19—N20 | 1.369 (4) | C89—C90 | 1.3900 |
| N20—C114 | 1.334 (5) | C89—H89 | 0.9300 |
| N20—B2 | 1.542 (6) | C90—H90 | 0.9300 |
| B1—H1 | 0.9800 | C91—H91A | 0.9600 |
| B2—H2B1 | 0.9800 | C91—H91B | 0.9600 |
| C1—C20 | 1.404 (4) | C91—H91C | 0.9600 |
| C1—C2 | 1.432 (5) | C92—C93 | 1.3900 |
| C2—C3 | 1.340 (5) | C92—C97 | 1.3900 |
| C2—H2 | 0.9300 | C93—C94 | 1.3900 |
| C3—C4 | 1.438 (4) | C93—H93 | 0.9300 |
| C3—H3 | 0.9300 | C94—C95 | 1.3900 |
| C4—C5 | 1.398 (4) | C94—H94 | 0.9300 |
| C5—C6 | 1.402 (4) | C95—C96 | 1.3900 |
| C5—C21 | 1.523 (4) | C95—C98 | 1.533 (5) |
| C6—C7 | 1.442 (4) | C96—C97 | 1.3900 |
| C7—C8 | 1.334 (5) | C96—H96 | 0.9300 |
| C7—H7 | 0.9300 | C97—H97 | 0.9300 |
| C8—C9 | 1.435 (5) | C98—H98A | 0.9600 |
| C8—H8 | 0.9300 | C98—H98B | 0.9600 |
| C9—C10 | 1.398 (5) | C98—H98C | 0.9600 |
| C10—C11 | 1.409 (4) | C99—C100 | 1.3900 |
| C10—C28 | 1.505 (3) | C99—C104 | 1.3900 |
| C11—C12 | 1.433 (4) | C100—C101 | 1.3900 |
| C12—C13 | 1.339 (5) | C100—H100 | 0.9300 |

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| C12—H12D | 0.9300 | C101—C102 | 1.3900 |
| C13—C14 | 1.433 (4) | C101—H101 | 0.9300 |
| C13—H13 | 0.9300 | C102—C103 | 1.3900 |
| C14—C15 | 1.402 (4) | C102—C105 | 1.536 (5) |
| C15—C16 | 1.408 (4) | C103—C104 | 1.3900 |
| C15—C35 | 1.520 (3) | C103—H103 | 0.9300 |
| C16—C17 | 1.437 (4) | C104—H104 | 0.9300 |
| C17—C18 | 1.346 (5) | C105—H10A | 0.9600 |
| C17—H17 | 0.9300 | C105—H10B | 0.9600 |
| C18—C19 | 1.445 (5) | C105—H10C | 0.9600 |
| C18—H18 | 0.9300 | C106—C107 | 1.369 (7) |
| C19—C20 | 1.407 (4) | C106—H106 | 0.9300 |
| C20—C42 | 1.501 (3) | C107—C108 | 1.359 (7) |
| C21—C22 | 1.3900 | C107—H107 | 0.9300 |
| C21—C26 | 1.3900 | C108—H108 | 0.9300 |
| C22—C23 | 1.3900 | C109—C110 | 1.372 (6) |
| C22—H22 | 0.9300 | C109—H109 | 0.9300 |
| C23—C24 | 1.3900 | C110—C111 | 1.366 (7) |
| C23—H23 | 0.9300 | C110—H110 | 0.9300 |
| C24—C25 | 1.3900 | C111—H111 | 0.9300 |
| C24—C27 | 1.538 (4) | C112—C113 | 1.380 (5) |
| C25—C26 | 1.3900 | C112—H112 | 0.9300 |
| C25—H25 | 0.9300 | C113—C114 | 1.349 (6) |
| C26—H26 | 0.9300 | C113—H113 | 0.9300 |
| C27—H27A | 0.9600 | C114—H114 | 0.9300 |
| C27—H27B | 0.9600 | C115—C116 | 1.465 (6) |
| C27—H27C | 0.9600 | C115—H11A | 0.9600 |
| C28—C29 | 1.3900 | C115—H11B | 0.9600 |
| C28—C33 | 1.3900 | C115—H11C | 0.9600 |
| C29—C30 | 1.3900 | C116—C117 | 1.3900 |
| C29—H29 | 0.9300 | C116—C121 | 1.3900 |
| C30—C31 | 1.3900 | C117—C118 | 1.3900 |
| C30—H30 | 0.9300 | C117—H117 | 0.9300 |
| C31—C32 | 1.3900 | C118—C119 | 1.3900 |
| C31—C34 | 1.511 (4) | C118—H18A | 0.9300 |
| C32—C33 | 1.3900 | C119—C120 | 1.3900 |
| C32—H32 | 0.9300 | C119—H119 | 0.9300 |
| C33—H33 | 0.9300 | C120—C121 | 1.3900 |
| C34—H34A | 0.9600 | C120—H120 | 0.9300 |
| C34—H34B | 0.9600 | C121—H121 | 0.9300 |
| C34—H34C | 0.9600 | C122—C123 | 1.464 (6) |
| C35—C36 | 1.3900 | C122—H12A | 0.9600 |
| C35—C40 | 1.3900 | C122—H12B | 0.9600 |
| C36—C37 | 1.3900 | C122—H12C | 0.9600 |
| C36—H36 | 0.9300 | C123—C128 | 1.347 (8) |
| C37—C38 | 1.3900 | C123—C124 | 1.426 (8) |
| C37—H37 | 0.9300 | C124—C125 | 1.322 (9) |
| C38—C39 | 1.3900 | C124—H12F | 0.9300 |
| C38—C41 | 1.538 (4) | C125—C126 | 1.488 (10) |

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| C39—C40 | 1.3900 | C125—H125 | 0.9300 |
| C39—H39 | 0.9300 | C126—C127 | 1.290 (9) |
| C40—H40 | 0.9300 | C126—H126 | 0.9300 |
| C41—H41A | 0.9600 | C127—C128 | 1.414 (9) |
| C41—H41B | 0.9600 | C127—H127 | 0.9300 |
| C41—H41C | 0.9600 | C128—H128 | 0.9300 |
| C42—C43 | 1.3900 | C129—C130 | 1.483 (5) |
| C42—C47 | 1.3900 | C129—H12H | 0.9600 |
| C43—C44 | 1.3900 | C129—H12I | 0.9600 |
| C43—H43 | 0.9300 | C129—H12J | 0.9600 |
| C44—C45 | 1.3900 | C130—C131 | 1.3900 |
| C44—H44 | 0.9300 | C130—C135 | 1.3900 |
| C45—C46 | 1.3900 | C131—C132 | 1.3900 |
| C45—C48 | 1.516 (4) | C131—H131 | 0.9300 |
| C46—C47 | 1.3900 | C132—C133 | 1.3900 |
| C46—H46 | 0.9300 | C132—H132 | 0.9300 |
| C47—H47 | 0.9300 | C133—C134 | 1.3900 |
| C48—H48A | 0.9600 | C133—H133 | 0.9300 |
| C48—H48B | 0.9600 | C134—C135 | 1.3900 |
| C48—H48C | 0.9600 | C134—H124 | 0.9300 |
| C49—C50 | 1.385 (6) | C135—H135 | 0.9300 |
| C49—H49 | 0.9300 | C136—C137 | 1.521 (10) |
| C50—C51 | 1.349 (6) | C136—H13A | 0.9600 |
| C50—H50 | 0.9300 | C136—H13B | 0.9600 |
| C51—H51 | 0.9300 | C136—H13C | 0.9600 |
| C52—C53 | 1.378 (6) | C137—C138 | 1.3900 |
| C52—H52 | 0.9300 | C137—C142 | 1.3900 |
| C53—C54 | 1.347 (7) | C138—C139 | 1.3900 |
| C53—H53 | 0.9300 | C138—H138 | 0.9300 |
| C54—H54 | 0.9300 | C139—C140 | 1.3900 |
| C55—C56 | 1.381 (6) | C139—H139 | 0.9300 |
| C55—H55 | 0.9300 | C140—C141 | 1.3900 |
| C56—C57 | 1.370 (6) | C140—H140 | 0.9300 |
| C56—H56 | 0.9300 | C141—C142 | 1.3900 |
| C57—H57 | 0.9300 | C141—H141 | 0.9300 |
| C58—C77 | 1.407 (5) | C142—H142 | 0.9300 |
| N4—Sm1—N1 | 75.30 (9) | N6—C51—H51 | 125.4 |
| N4—Sm1—N3 | 73.80 (8) | C50—C51—H51 | 125.4 |
| N1—Sm1—N3 | 116.82 (9) | N7—C52—C53 | 111.7 (4) |
| N4—Sm1—N2 | 117.18 (9) | N7—C52—H52 | 124.2 |
| N1—Sm1—N2 | 73.65 (8) | C53—C52—H52 | 124.2 |
| N3—Sm1—N2 | 73.88 (8) | C54—C53—C52 | 104.7 (4) |
| N4—Sm1—N5 | 129.53 (9) | C54—C53—H53 | 127.6 |
| N1—Sm1—N5 | 80.75 (9) | C52—C53—H53 | 127.6 |
| N3—Sm1—N5 | 155.49 (9) | N8—C54—C53 | 108.7 (4) |
| N2—Sm1—N5 | 96.97 (9) | N8—C54—H54 | 125.6 |
| N4—Sm1—N9 | 77.72 (9) | C53—C54—H54 | 125.6 |
| N1—Sm1—N9 | 114.80 (9) | N9—C55—C56 | 111.0 (4) |
| N3—Sm1—N9 | 110.39 (9) | N9—C55—H55 | 124.5 |

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| N2—Sm1—N9 | 164.91 (9) | C56—C55—H55 | 124.5 |
| N5—Sm1—N9 | 73.15 (10) | C57—C56—C55 | 104.8 (4) |
| N4—Sm1—N7 | 132.95 (10) | C57—C56—H56 | 127.6 |
| N1—Sm1—N7 | 150.81 (10) | C55—C56—H56 | 127.6 |
| N3—Sm1—N7 | 83.44 (9) | N10—C57—C56 | 108.8 (4) |
| N2—Sm1—N7 | 94.11 (9) | N10—C57—H57 | 125.6 |
| N5—Sm1—N7 | 74.45 (10) | C56—C57—H57 | 125.6 |
| N9—Sm1—N7 | 72.48 (10) | N11—C58—C77 | 125.2 (3) |
| N4—Sm1—B1 | 121.69 (9) | N11—C58—C59 | 108.9 (3) |
| N1—Sm1—B1 | 121.12 (9) | C77—C58—C59 | 125.8 (3) |
| N3—Sm1—B1 | 122.05 (9) | C60—C59—C58 | 107.9 (3) |
| N2—Sm1—B1 | 121.12 (9) | C60—C59—H59 | 126.1 |
| N5—Sm1—B1 | 43.45 (10) | C58—C59—H59 | 126.1 |
| N9—Sm1—B1 | 44.03 (9) | C59—C60—C61 | 107.0 (3) |
| N7—Sm1—B1 | 43.39 (9) | C59—C60—H60 | 126.5 |
| N11—Sm2—N13 | 117.64 (10) | C61—C60—H60 | 126.5 |
| N11—Sm2—N12 | 74.22 (10) | N11—C61—C62 | 125.6 (3) |
| N13—Sm2—N12 | 74.87 (9) | N11—C61—C60 | 109.7 (3) |
| N11—Sm2—N14 | 74.56 (9) | C62—C61—C60 | 124.2 (3) |
| N13—Sm2—N14 | 73.67 (9) | C63—C62—C61 | 124.8 (3) |
| N12—Sm2—N14 | 117.10 (9) | C63—C62—C78 | 117.5 (3) |
| N11—Sm2—N17 | 106.81 (10) | C61—C62—C78 | 117.5 (3) |
| N13—Sm2—N17 | 116.77 (10) | N12—C63—C62 | 126.0 (3) |
| N12—Sm2—N17 | 76.86 (10) | N12—C63—C64 | 109.3 (3) |
| N14—Sm2—N17 | 165.25 (10) | C62—C63—C64 | 124.6 (3) |
| N11—Sm2—N19 | 153.93 (10) | C65—C64—C63 | 107.4 (3) |
| N13—Sm2—N19 | 82.68 (9) | C65—C64—H64 | 126.3 |
| N12—Sm2—N19 | 129.73 (10) | C63—C64—H64 | 126.3 |
| N14—Sm2—N19 | 97.99 (10) | C64—C65—C66 | 108.0 (3) |
| N17—Sm2—N19 | 74.24 (11) | C64—C65—H65 | 126.0 |
| N11—Sm2—N15 | 82.32 (10) | C66—C65—H65 | 126.0 |
| N13—Sm2—N15 | 150.23 (10) | N12—C66—C67 | 125.8 (3) |
| N12—Sm2—N15 | 134.27 (10) | N12—C66—C65 | 108.6 (3) |
| N14—Sm2—N15 | 92.68 (10) | C67—C66—C65 | 125.5 (3) |
| N17—Sm2—N15 | 73.17 (11) | C66—C67—C68 | 125.5 (3) |
| N19—Sm2—N15 | 72.99 (10) | C66—C67—C85 | 117.3 (3) |
| N11—Sm2—B2 | 119.12 (11) | C68—C67—C85 | 117.1 (3) |
| N13—Sm2—B2 | 123.23 (10) | N13—C68—C67 | 125.2 (3) |
| N12—Sm2—B2 | 120.21 (11) | N13—C68—C69 | 109.4 (3) |
| N14—Sm2—B2 | 122.65 (11) | C67—C68—C69 | 125.3 (3) |
| N17—Sm2—B2 | 43.44 (12) | C70—C69—C68 | 107.3 (3) |
| N19—Sm2—B2 | 44.05 (11) | C70—C69—H69 | 126.3 |
| N15—Sm2—B2 | 43.56 (10) | C68—C69—H69 | 126.3 |
| C4—N1—C1 | 106.3 (3) | C69—C70—C71 | 107.5 (3) |
| C4—N1—Sm1 | 128.4 (2) | C69—C70—H70 | 126.3 |
| C1—N1—Sm1 | 122.6 (2) | C71—C70—H70 | 126.3 |
| C6—N2—C9 | 106.5 (3) | N13—C71—C72 | 124.7 (3) |
| C6—N2—Sm1 | 126.04 (19) | N13—C71—C70 | 109.7 (3) |
| C9—N2—Sm1 | 123.7 (2) | C72—C71—C70 | 125.5 (3) |

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| C11—N3—C14 | 106.2 (3) | C73—C72—C71 | 125.3 (3) |
| C11—N3—Sm1 | 124.1 (2) | C73—C72—C92 | 117.1 (3) |
| C14—N3—Sm1 | 122.70 (19) | C71—C72—C92 | 117.5 (3) |
| C19—N4—C16 | 106.7 (3) | N14—C73—C72 | 126.0 (3) |
| C19—N4—Sm1 | 122.9 (2) | N14—C73—C74 | 109.2 (3) |
| C16—N4—Sm1 | 125.7 (2) | C72—C73—C74 | 124.7 (3) |
| C49—N5—N6 | 105.4 (3) | C75—C74—C73 | 107.3 (3) |
| C49—N5—Sm1 | 131.7 (3) | C75—C74—H74 | 126.3 |
| N6—N5—Sm1 | 122.9 (2) | C73—C74—H74 | 126.3 |
| C51—N6—N5 | 109.6 (3) | C74—C75—C76 | 107.9 (3) |
| C51—N6—B1 | 127.4 (3) | C74—C75—H75 | 126.1 |
| N5—N6—B1 | 122.9 (3) | C76—C75—H75 | 126.1 |
| C52—N7—N8 | 105.0 (3) | N14—C76—C77 | 125.7 (3) |
| C52—N7—Sm1 | 132.8 (3) | N14—C76—C75 | 109.0 (3) |
| N8—N7—Sm1 | 122.2 (2) | C77—C76—C75 | 125.2 (3) |
| C54—N8—N7 | 109.8 (3) | C76—C77—C58 | 126.3 (3) |
| C54—N8—B1 | 127.2 (3) | C76—C77—C99 | 117.3 (3) |
| N7—N8—B1 | 122.7 (3) | C58—C77—C99 | 116.3 (3) |
| C55—N9—N10 | 106.0 (3) | C79—C78—C83 | 120.0 |
| C55—N9—Sm1 | 132.1 (3) | C79—C78—C62 | 120.1 (2) |
| N10—N9—Sm1 | 121.6 (2) | C83—C78—C62 | 119.8 (2) |
| C57—N10—N9 | 109.5 (3) | C78—C79—C80 | 120.0 |
| C57—N10—B1 | 127.2 (3) | C78—C79—H79 | 120.0 |
| N9—N10—B1 | 123.3 (3) | C80—C79—H79 | 120.0 |
| C58—N11—C61 | 106.4 (3) | C79—C80—C81 | 120.0 |
| C58—N11—Sm2 | 125.1 (2) | C79—C80—H80 | 120.0 |
| C61—N11—Sm2 | 120.9 (2) | C81—C80—H80 | 120.0 |
| C66—N12—C63 | 106.7 (3) | C82—C81—C80 | 120.0 |
| C66—N12—Sm2 | 125.5 (2) | C82—C81—C84 | 119.0 (3) |
| C63—N12—Sm2 | 124.7 (2) | C80—C81—C84 | 120.9 (3) |
| C71—N13—C68 | 106.0 (3) | C81—C82—C83 | 120.0 |
| C71—N13—Sm2 | 122.5 (2) | C81—C82—H82 | 120.0 |
| C68—N13—Sm2 | 121.4 (2) | C83—C82—H82 | 120.0 |
| C73—N14—C76 | 106.5 (3) | C82—C83—C78 | 120.0 |
| C73—N14—Sm2 | 125.2 (2) | C82—C83—H83 | 120.0 |
| C76—N14—Sm2 | 126.6 (2) | C78—C83—H83 | 120.0 |
| C106—N15—N16 | 105.8 (3) | C81—C84—H84A | 109.5 |
| C106—N15—Sm2 | 132.1 (3) | C81—C84—H84B | 109.5 |
| N16—N15—Sm2 | 122.0 (2) | H84A—C84—H84B | 109.5 |
| C108—N16—N15 | 109.6 (4) | C81—C84—H84C | 109.5 |
| C108—N16—B2 | 127.9 (4) | H84A—C84—H84C | 109.5 |
| N15—N16—B2 | 122.5 (3) | H84B—C84—H84C | 109.5 |
| C109—N17—N18 | 105.6 (3) | C86—C85—C90 | 120.0 |
| C109—N17—Sm2 | 132.0 (3) | C86—C85—C67 | 120.3 (2) |
| N18—N17—Sm2 | 122.3 (2) | C90—C85—C67 | 119.7 (2) |
| N17—N18—C111 | 109.1 (4) | C85—C86—C87 | 120.0 |
| N17—N18—B2 | 122.9 (3) | C85—C86—H86 | 120.0 |
| C111—N18—B2 | 128.0 (4) | C87—C86—H86 | 120.0 |
| C112—N19—N20 | 104.8 (3) | C88—C87—C86 | 120.0 |

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| C112—N19—Sm2 | 133.7 (3) | C88—C87—H87 | 120.0 |
| N20—N19—Sm2 | 121.4 (2) | C86—C87—H87 | 120.0 |
| C114—N20—N19 | 109.1 (3) | C87—C88—C89 | 120.0 |
| C114—N20—B2 | 128.0 (3) | C87—C88—C91 | 118.5 (4) |
| N19—N20—B2 | 122.8 (3) | C89—C88—C91 | 121.5 (4) |
| N8—B1—N6 | 110.8 (3) | C90—C89—C88 | 120.0 |
| N8—B1—N10 | 108.6 (3) | C90—C89—H89 | 120.0 |
| N6—B1—N10 | 110.6 (3) | C88—C89—H89 | 120.0 |
| N8—B1—Sm1 | 71.52 (18) | C89—C90—C85 | 120.0 |
| N6—B1—Sm1 | 70.72 (18) | C89—C90—H90 | 120.0 |
| N10—B1—Sm1 | 71.00 (18) | C85—C90—H90 | 120.0 |
| N8—B1—H1 | 108.9 | C88—C91—H91A | 109.5 |
| N6—B1—H1 | 108.9 | C88—C91—H91B | 109.5 |
| N10—B1—H1 | 108.9 | H91A—C91—H91B | 109.5 |
| Sm1—B1—H1 | 179.5 | C88—C91—H91C | 109.5 |
| N18—B2—N16 | 110.7 (4) | H91A—C91—H91C | 109.5 |
| N18—B2—N20 | 112.0 (3) | H91B—C91—H91C | 109.5 |
| N16—B2—N20 | 109.0 (4) | C93—C92—C97 | 120.0 |
| N18—B2—Sm2 | 71.4 (2) | C93—C92—C72 | 120.88 (19) |
| N16—B2—Sm2 | 71.9 (2) | C97—C92—C72 | 119.11 (19) |
| N20—B2—Sm2 | 71.72 (19) | C94—C93—C92 | 120.0 |
| N18—B2—H2B1 | 108.3 | C94—C93—H93 | 120.0 |
| N16—B2—H2B1 | 108.3 | C92—C93—H93 | 120.0 |
| N20—B2—H2B1 | 108.3 | C93—C94—C95 | 120.0 |
| Sm2—B2—H2B1 | 179.7 | C93—C94—H94 | 120.0 |
| N1—C1—C20 | 125.8 (3) | C95—C94—H94 | 120.0 |
| N1—C1—C2 | 109.2 (3) | C96—C95—C94 | 120.0 |
| C20—C1—C2 | 124.3 (3) | C96—C95—C98 | 120.8 (3) |
| C3—C2—C1 | 107.8 (3) | C94—C95—C98 | 119.2 (3) |
| C3—C2—H2 | 126.1 | C95—C96—C97 | 120.0 |
| C1—C2—H2 | 126.1 | C95—C96—H96 | 120.0 |
| C2—C3—C4 | 107.2 (3) | C97—C96—H96 | 120.0 |
| C2—C3—H3 | 126.4 | C96—C97—C92 | 120.0 |
| C4—C3—H3 | 126.4 | C96—C97—H97 | 120.0 |
| N1—C4—C5 | 126.1 (3) | C92—C97—H97 | 120.0 |
| N1—C4—C3 | 109.5 (3) | C95—C98—H98A | 109.5 |
| C5—C4—C3 | 124.4 (3) | C95—C98—H98B | 109.5 |
| C4—C5—C6 | 125.4 (3) | H98A—C98—H98B | 109.5 |
| C4—C5—C21 | 116.7 (3) | C95—C98—H98C | 109.5 |
| C6—C5—C21 | 117.7 (3) | H98A—C98—H98C | 109.5 |
| N2—C6—C5 | 125.9 (3) | H98B—C98—H98C | 109.5 |
| N2—C6—C7 | 109.4 (3) | C100—C99—C104 | 120.0 |
| C5—C6—C7 | 124.4 (3) | C100—C99—C77 | 119.1 (2) |
| C8—C7—C6 | 106.8 (3) | C104—C99—C77 | 120.9 (2) |
| C8—C7—H7 | 126.6 | C101—C100—C99 | 120.0 |
| C6—C7—H7 | 126.6 | C101—C100—H100 | 120.0 |
| C7—C8—C9 | 108.2 (3) | C99—C100—H100 | 120.0 |
| C7—C8—H8 | 125.9 | C100—C101—C102 | 120.0 |
| C9—C8—H8 | 125.9 | C100—C101—H101 | 120.0 |

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| N2—C9—C10 | 125.7 (3) | C102—C101—H101 | 120.0 |
| N2—C9—C8 | 108.9 (3) | C103—C102—C101 | 120.0 |
| C10—C9—C8 | 125.0 (3) | C103—C102—C105 | 120.1 (3) |
| C9—C10—C11 | 126.6 (3) | C101—C102—C105 | 119.9 (3) |
| C9—C10—C28 | 117.1 (3) | C102—C103—C104 | 120.0 |
| C11—C10—C28 | 116.1 (3) | C102—C103—H103 | 120.0 |
| N3—C11—C10 | 125.1 (3) | C104—C103—H103 | 120.0 |
| N3—C11—C12 | 109.4 (3) | C103—C104—C99 | 120.0 |
| C10—C11—C12 | 125.5 (3) | C103—C104—H104 | 120.0 |
| C13—C12—C11 | 107.9 (3) | C99—C104—H104 | 120.0 |
| C13—C12—H12D | 126.0 | C102—C105—H10A | 109.5 |
| C11—C12—H12D | 126.0 | C102—C105—H10B | 109.5 |
| C12—C13—C14 | 106.9 (3) | H10A—C105—H10B | 109.5 |
| C12—C13—H13 | 126.6 | C102—C105—H10C | 109.5 |
| C14—C13—H13 | 126.6 | H10A—C105—H10C | 109.5 |
| N3—C14—C15 | 126.1 (3) | H10B—C105—H10C | 109.5 |
| N3—C14—C13 | 109.5 (3) | N15—C106—C107 | 110.9 (4) |
| C15—C14—C13 | 124.2 (3) | N15—C106—H106 | 124.6 |
| C14—C15—C16 | 124.9 (3) | C107—C106—H106 | 124.6 |
| C14—C15—C35 | 117.6 (3) | C108—C107—C106 | 105.0 (4) |
| C16—C15—C35 | 117.4 (3) | C108—C107—H107 | 127.5 |
| N4—C16—C15 | 125.9 (3) | C106—C107—H107 | 127.5 |
| N4—C16—C17 | 109.8 (3) | N16—C108—C107 | 108.8 (4) |
| C15—C16—C17 | 124.2 (3) | N16—C108—H108 | 125.6 |
| C18—C17—C16 | 106.8 (3) | C107—C108—H108 | 125.6 |
| C18—C17—H17 | 126.6 | N17—C109—C110 | 112.0 (5) |
| C16—C17—H17 | 126.6 | N17—C109—H109 | 124.0 |
| C17—C18—C19 | 107.8 (3) | C110—C109—H109 | 124.0 |
| C17—C18—H18 | 126.1 | C111—C110—C109 | 104.0 (4) |
| C19—C18—H18 | 126.1 | C111—C110—H110 | 128.0 |
| N4—C19—C20 | 125.6 (3) | C109—C110—H110 | 128.0 |
| N4—C19—C18 | 108.9 (3) | N18—C111—C110 | 109.4 (4) |
| C20—C19—C18 | 125.3 (3) | N18—C111—H111 | 125.3 |
| C1—C20—C19 | 126.3 (3) | C110—C111—H111 | 125.3 |
| C1—C20—C42 | 116.4 (3) | N19—C112—C113 | 111.9 (4) |
| C19—C20—C42 | 116.9 (3) | N19—C112—H112 | 124.0 |
| C22—C21—C26 | 120.0 | C113—C112—H112 | 124.0 |
| C22—C21—C5 | 120.69 (18) | C114—C113—C112 | 103.8 (4) |
| C26—C21—C5 | 119.29 (18) | C114—C113—H113 | 128.1 |
| C23—C22—C21 | 120.0 | C112—C113—H113 | 128.1 |
| C23—C22—H22 | 120.0 | N20—C114—C113 | 110.3 (4) |
| C21—C22—H22 | 120.0 | N20—C114—H114 | 124.8 |
| C24—C23—C22 | 120.0 | C113—C114—H114 | 124.8 |
| C24—C23—H23 | 120.0 | C116—C115—H11A | 109.5 |
| C22—C23—H23 | 120.0 | C116—C115—H11B | 109.5 |
| C23—C24—C25 | 120.0 | H11A—C115—H11B | 109.5 |
| C23—C24—C27 | 119.9 (3) | C116—C115—H11C | 109.5 |
| C25—C24—C27 | 120.1 (3) | H11A—C115—H11C | 109.5 |
| C24—C25—C26 | 120.0 | H11B—C115—H11C | 109.5 |

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| C24—C25—H25 | 120.0 | C117—C116—C121 | 120.0 |
| C26—C25—H25 | 120.0 | C117—C116—C115 | 120.2 (5) |
| C25—C26—C21 | 120.0 | C121—C116—C115 | 119.8 (5) |
| C25—C26—H26 | 120.0 | C118—C117—C116 | 120.0 |
| C21—C26—H26 | 120.0 | C118—C117—H117 | 120.0 |
| C24—C27—H27A | 109.5 | C116—C117—H117 | 120.0 |
| C24—C27—H27B | 109.5 | C119—C118—C117 | 120.0 |
| H27A—C27—H27B | 109.5 | C119—C118—H18A | 120.0 |
| C24—C27—H27C | 109.5 | C117—C118—H18A | 120.0 |
| H27A—C27—H27C | 109.5 | C120—C119—C118 | 120.0 |
| H27B—C27—H27C | 109.5 | C120—C119—H119 | 120.0 |
| C29—C28—C33 | 120.0 | C118—C119—H119 | 120.0 |
| C29—C28—C10 | 118.67 (18) | C119—C120—C121 | 120.0 |
| C33—C28—C10 | 121.30 (18) | C119—C120—H120 | 120.0 |
| C28—C29—C30 | 120.0 | C121—C120—H120 | 120.0 |
| C28—C29—H29 | 120.0 | C120—C121—C116 | 120.0 |
| C30—C29—H29 | 120.0 | C120—C121—H121 | 120.0 |
| C31—C30—C29 | 120.0 | C116—C121—H121 | 120.0 |
| C31—C30—H30 | 120.0 | C123—C122—H12A | 109.5 |
| C29—C30—H30 | 120.0 | C123—C122—H12B | 109.5 |
| C32—C31—C30 | 120.0 | H12A—C122—H12B | 109.5 |
| C32—C31—C34 | 119.9 (3) | C123—C122—H12C | 109.5 |
| C30—C31—C34 | 120.1 (3) | H12A—C122—H12C | 109.5 |
| C31—C32—C33 | 120.0 | H12B—C122—H12C | 109.5 |
| C31—C32—H32 | 120.0 | C128—C123—C124 | 119.2 (6) |
| C33—C32—H32 | 120.0 | C128—C123—C122 | 123.2 (7) |
| C32—C33—C28 | 120.0 | C124—C123—C122 | 117.6 (6) |
| C32—C33—H33 | 120.0 | C125—C124—C123 | 119.2 (7) |
| C28—C33—H33 | 120.0 | C125—C124—H12F | 120.4 |
| C31—C34—H34A | 109.5 | C123—C124—H12F | 120.4 |
| C31—C34—H34B | 109.5 | C124—C125—C126 | 121.8 (7) |
| H34A—C34—H34B | 109.5 | C124—C125—H125 | 119.1 |
| C31—C34—H34C | 109.5 | C126—C125—H125 | 119.1 |
| H34A—C34—H34C | 109.5 | C127—C126—C125 | 116.3 (7) |
| H34B—C34—H34C | 109.5 | C127—C126—H126 | 121.9 |
| C36—C35—C40 | 120.0 | C125—C126—H126 | 121.9 |
| C36—C35—C15 | 120.02 (18) | C126—C127—C128 | 123.2 (8) |
| C40—C35—C15 | 119.93 (18) | C126—C127—H127 | 118.4 |
| C35—C36—C37 | 120.0 | C128—C127—H127 | 118.4 |
| C35—C36—H36 | 120.0 | C123—C128—C127 | 120.3 (7) |
| C37—C36—H36 | 120.0 | C123—C128—H128 | 119.8 |
| C36—C37—C38 | 120.0 | C127—C128—H128 | 119.8 |
| C36—C37—H37 | 120.0 | C130—C129—H12H | 109.5 |
| C38—C37—H37 | 120.0 | C130—C129—H12I | 109.5 |
| C39—C38—C37 | 120.0 | H12H—C129—H12I | 109.5 |
| C39—C38—C41 | 120.7 (3) | C130—C129—H12J | 109.5 |
| C37—C38—C41 | 119.3 (3) | H12H—C129—H12J | 109.5 |
| C38—C39—C40 | 120.0 | H12I—C129—H12J | 109.5 |
| C38—C39—H39 | 120.0 | C131—C130—C135 | 120.0 |

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|---|---|---|---|
| C40—C39—H39 | 120.0 | C131—C130—C129 | 118.9 (4) |
| C39—C40—C35 | 120.0 | C135—C130—C129 | 121.1 (4) |
| C39—C40—H40 | 120.0 | C130—C131—C132 | 120.0 |
| C35—C40—H40 | 120.0 | C130—C131—H131 | 120.0 |
| C38—C41—H41A | 109.5 | C132—C131—H131 | 120.0 |
| C38—C41—H41B | 109.5 | C133—C132—C131 | 120.0 |
| H41A—C41—H41B | 109.5 | C133—C132—H132 | 120.0 |
| C38—C41—H41C | 109.5 | C131—C132—H132 | 120.0 |
| H41A—C41—H41C | 109.5 | C134—C133—C132 | 120.0 |
| H41B—C41—H41C | 109.5 | C134—C133—H133 | 120.0 |
| C43—C42—C47 | 120.0 | C132—C133—H133 | 120.0 |
| C43—C42—C20 | 119.71 (18) | C133—C134—C135 | 120.0 |
| C47—C42—C20 | 120.27 (18) | C133—C134—H124 | 120.0 |
| C42—C43—C44 | 120.0 | C135—C134—H124 | 120.0 |
| C42—C43—H43 | 120.0 | C134—C135—C130 | 120.0 |
| C44—C43—H43 | 120.0 | C134—C135—H135 | 120.0 |
| C45—C44—C43 | 120.0 | C130—C135—H135 | 120.0 |
| C45—C44—H44 | 120.0 | C137—C136—H13A | 109.5 |
| C43—C44—H44 | 120.0 | C137—C136—H13B | 109.5 |
| C46—C45—C44 | 120.0 | H13A—C136—H13B | 109.5 |
| C46—C45—C48 | 119.0 (3) | C137—C136—H13C | 109.5 |
| C44—C45—C48 | 121.0 (3) | H13A—C136—H13C | 109.5 |
| C47—C46—C45 | 120.0 | H13B—C136—H13C | 109.5 |
| C47—C46—H46 | 120.0 | C138—C137—C142 | 120.0 |
| C45—C46—H46 | 120.0 | C138—C137—C136 | 117.5 (10) |
| C46—C47—C42 | 120.0 | C142—C137—C136 | 122.5 (10) |
| C46—C47—H47 | 120.0 | C137—C138—C139 | 120.0 |
| C42—C47—H47 | 120.0 | C137—C138—H138 | 120.0 |
| C45—C48—H48A | 109.5 | C139—C138—H138 | 120.0 |
| C45—C48—H48B | 109.5 | C140—C139—C138 | 120.0 |
| H48A—C48—H48B | 109.5 | C140—C139—H139 | 120.0 |
| C45—C48—H48C | 109.5 | C138—C139—H139 | 120.0 |
| H48A—C48—H48C | 109.5 | C139—C140—C141 | 120.0 |
| H48B—C48—H48C | 109.5 | C139—C140—H140 | 120.0 |
| N5—C49—C50 | 111.5 (4) | C141—C140—H140 | 120.0 |
| N5—C49—H49 | 124.2 | C142—C141—C140 | 120.0 |
| C50—C49—H49 | 124.2 | C142—C141—H141 | 120.0 |
| C51—C50—C49 | 104.3 (4) | C140—C141—H141 | 120.0 |
| C51—C50—H50 | 127.9 | C141—C142—C137 | 120.0 |
| C49—C50—H50 | 127.9 | C141—C142—H142 | 120.0 |
| N6—C51—C50 | 109.2 (4) | C137—C142—H142 | 120.0 |

**Fig. 1**

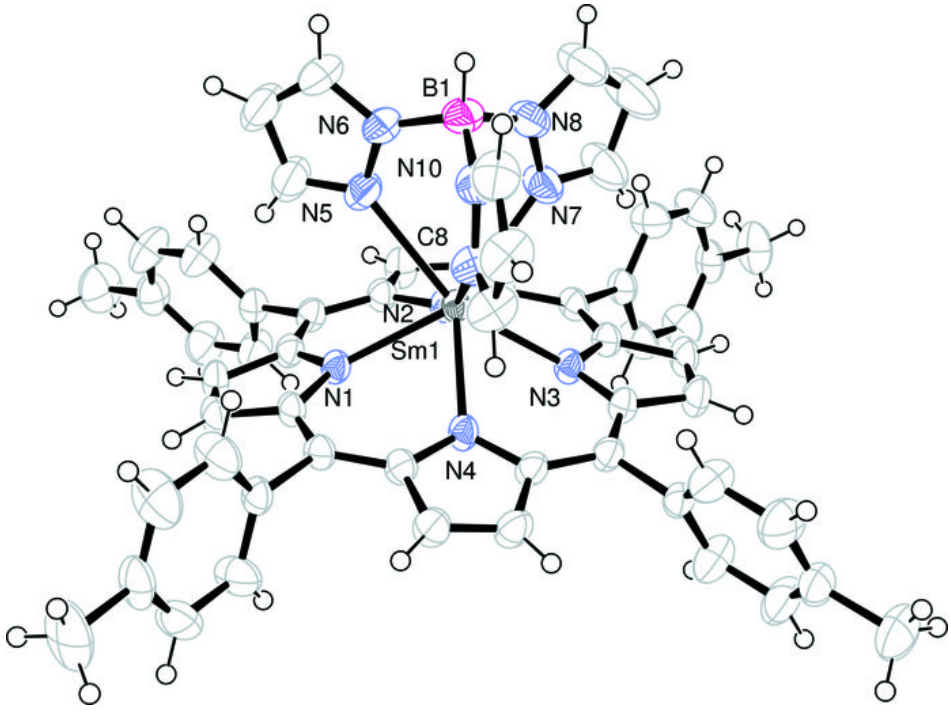

**Fig. 2**

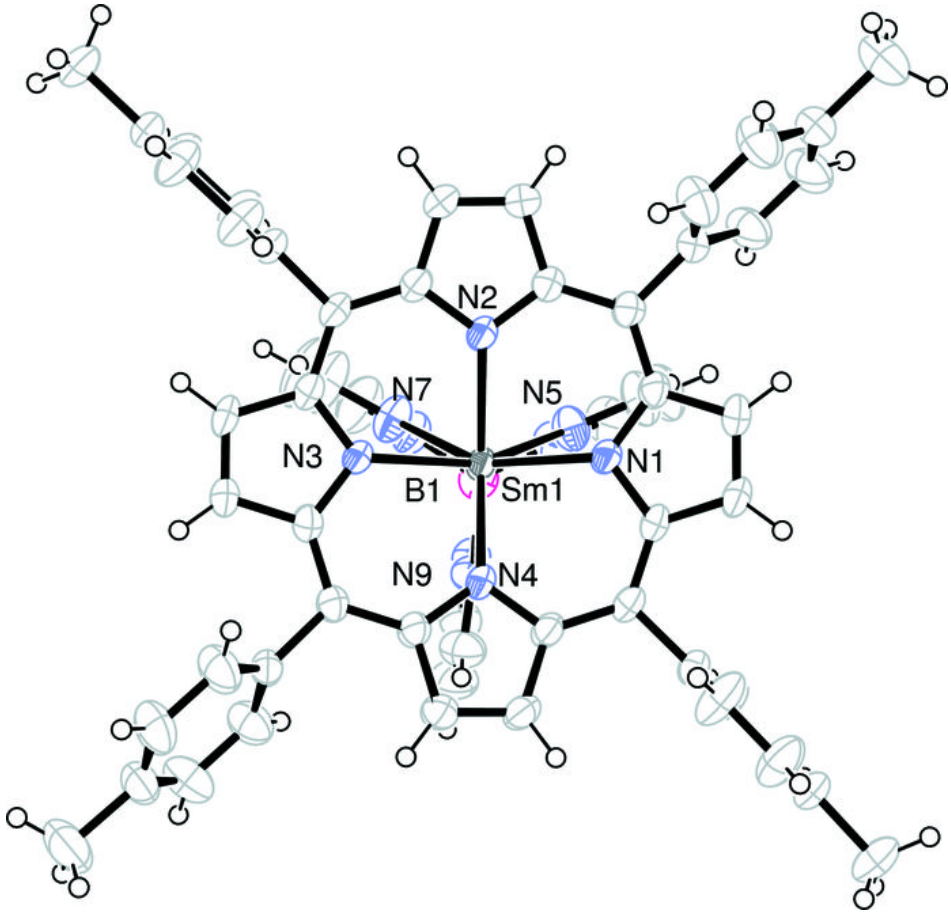

**Fig. 3**