

Bis(3-methyl-1-propyl-1,3-dihydro-1*H*-imidazol-2-ylidene)silver(I) chlorido(5,10,15,20-tetraphenylporphinato)cadmate(II)

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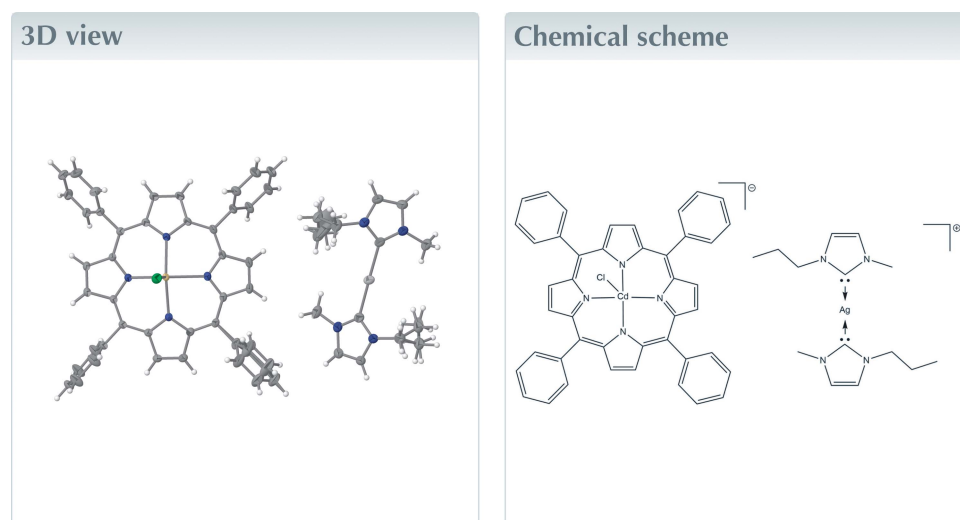
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Keywords: crystal structure; cadmium(II) porphyrin; silver(I)carbene.

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Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title salt, $[\text{Ag}(\text{C}_7\text{H}_{12}\text{N}_2)_2][\text{CdCl}(\text{C}_{44}\text{H}_{28}\text{N}_4)]$, at 150 K has triclinic symmetry. One of the phenyl rings bonded to the porphyrin molecule and the propyl groups of both ylidene molecules coordinating to silver are disordered over two positions.



Structure description

The structures of various cadmium(II) porphyrins have been determined previously. However, this exact combination of the chloride apical ligand and porphyrin structure has not been obtained before. In the absence of an apical ligand (Byrn *et al.* 1991), the cadmium porphyrin is planar and the cadmium atom resides in the mean plane through the porphyrin atoms. In the presence of an apical ligand like chloride (Zhang, Zhang, Wojtas *et al.*, 2012; Zhang, Gao *et al.*, 2012) or water (Toumi *et al.*, 2013), the cadmium centre is pulled 0.84–1.07 Å out of the mean porphyrin plane, which is similar to the distance in the title salt (Fig. 1) of 0.89 (12) Å. The dihedral angle between the imidazol-2-ylidene planes is 41.49 (13)°, which is similar to the angle of 52.0° reported previously for a similar silver(I) carbene compound (Achar *et al.*, 2017). The angle between the Ag–C bonds in the title salt is close to linear at 179.14 (9)°, which is close to the angle of 170.6° reported by Achar *et al.* (2017).

The porphyrin planes show an offset stacked geometry (Fig. 2).

Synthesis and crystallization

The title salt was obtained as a single crystal during an attempt to prepare and grow single crystals of a cadmium(II) tetraphenylporphyrin carbene by mixing cadmium(II)–5,10,15,20-tetraphenylporphyrin, 3-methyl-1-propylimidazolium chloride and silver(I)

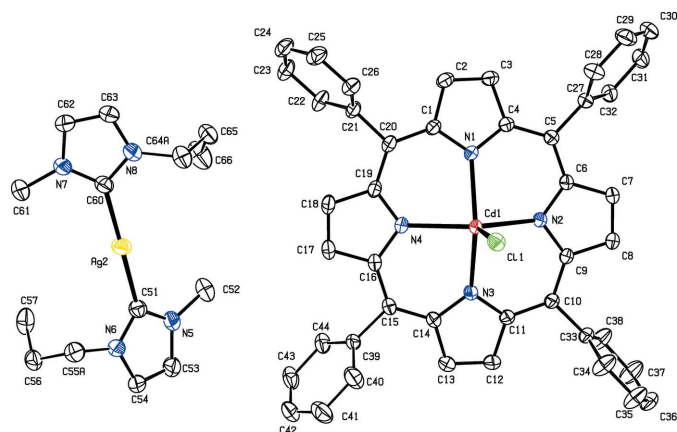


Figure 1

The structures of the molecular entities in the title salt. Displacement ellipsoids are drawn at the 50% probability level. The minor-occupied sites of the disordered atoms have been omitted for clarity.

oxide in a 1:1:1 molar ratio in dichloromethane/*n*-heptane (1:1 *v/v*). The mixture was stored in the dark at 298 K, resulting in the formation of blue needle-shaped crystals after 72 h.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed in calculated positions and refined with a riding model, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ otherwise. One of the phenyl rings of the porphyrin molecule and the ethyl groups of both ylide molecules coordinating to silver are disordered over two positions. The major conformation of the disordered phenyl ring has an occupancy of 0.703 (13). Bond lengths and angles of the minor fraction of the disordered benzene ring were restrained to be similar to those of the major-occupied fraction using the SAME instruction. The terminal ethyl groups of the propyl groups of both carbenes are disordered, with the occupancies of the major conformations being 0.679 (7) and 0.786 (11). The displacement parameters of bonded atoms were restrained to be similar using SIMU and RIGU instructions.

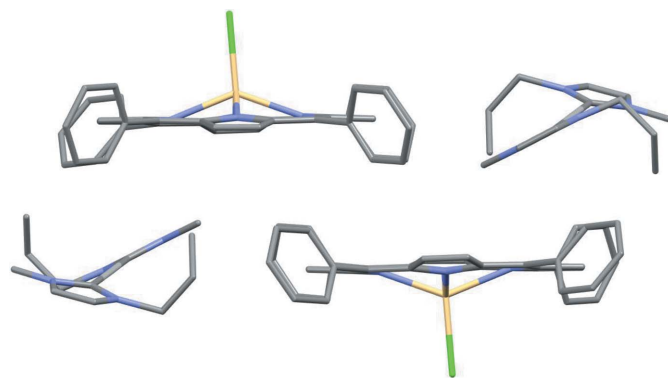


Figure 2

Two units of the stacked title salt, showing the offset stack alignment of the porphyrin planes relative to each other. H atoms and the minor-occupied sites of the disordered atoms have been omitted for clarity.

Table 1

Experimental details.

| | |
|--|---|
| Crystal data | |
| Chemical formula | $[\text{Ag}(\text{C}_7\text{H}_{12}\text{N}_2)_2][\text{CdCl}(\text{C}_{44}\text{H}_{28}\text{N}_4)]$ |
| M_r | 1116.79 |
| Crystal system, space group | Triclinic, $P\bar{1}$ |
| Temperature (K) | 150 |
| a, b, c (Å) | 11.1004 (4), 13.1655 (5), 18.3723 (7) |
| α, β, γ (°) | 84.0191 (17), 86.6707 (15), 70.0762 (14) |
| V (Å ³) | 2509.79 (16) |
| Z | 2 |
| Radiation type | Mo $K\alpha$ |
| μ (mm ⁻¹) | 0.91 |
| Crystal size (mm) | 0.31 × 0.29 × 0.13 |
| Data collection | |
| Diffractometer | Bruker D8 Quest APEX3 |
| Absorption correction | Numerical (SADABS; Krause <i>et al.</i> , 2015) |
| $T_{\text{min}}, T_{\text{max}}$ | 0.811, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 213430, 19237, 17410 |
| R_{int} | 0.034 |
| $(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹) | 0.771 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.036, 0.108, 1.06 |
| No. of reflections | 19237 |
| No. of parameters | 721 |
| No. of restraints | 1420 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³) | 1.99, -2.60 |

Computer programs: APEX3 (Bruker, 2017), SAINT (Bruker, 2003), SHELXT2014 (Sheldrick, 2015a), SHELXL2018 (Sheldrick, 2015b), PLATON (Spek, 2020) and shelxtle (Hübschle *et al.*, 2011).

Funding information

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full crystallographic data

IUCrData (2022). 7, x220489 [https://doi.org/10.1107/S2414314622004898]

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chlorido(5,10,15,20-tetraphenylporphinato)cadmate(II)**

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Crystal data

[Ag(C₇H₁₂N₂)₂][CdCl(C₄₄H₂₈N₄)]

$M_r = 1116.79$

Triclinic, $P\bar{1}$

$a = 11.1004$ (4) Å

$b = 13.1655$ (5) Å

$c = 18.3723$ (7) Å

$\alpha = 84.0191$ (17)°

$\beta = 86.6707$ (15)°

$\gamma = 70.0762$ (14)°

$V = 2509.79$ (16) Å³

$Z = 2$

$F(000) = 1136$

$D_x = 1.478$ Mg m⁻³

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

Cell parameters from 9319 reflections

$\theta = 2.9$ – 33.1 °

$\mu = 0.91$ mm⁻¹

$T = 150$ K

Block, blue

$0.31 \times 0.29 \times 0.13$ mm

Data collection

Bruker D8 Quest APEX3

diffractometer

Radiation source: sealed tube

Graphite monochromator

Detector resolution: 7.41 pixels mm⁻¹

φ and ω scans

Absorption correction: numerical

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.811$, $T_{\max} = 1.000$

213430 measured reflections

19237 independent reflections

17410 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 33.3$ °, $\theta_{\min} = 2.1$ °

$h = -17 \rightarrow 17$

$k = -20 \rightarrow 20$

$l = -28 \rightarrow 28$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.108$

$S = 1.06$

19237 reflections

721 parameters

1420 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 3.5802P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.005$

$\Delta\rho_{\max} = 1.99$ e Å⁻³

$\Delta\rho_{\min} = -2.60$ e Å⁻³

Special details

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

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|--------------|--------------|--------------|----------------------------------|-----------|
| Cd1 | 0.42416 (2) | 0.69550 (2) | 0.71225 (2) | 0.01906 (4) | |
| Cl1 | 0.55041 (5) | 0.77535 (4) | 0.78143 (3) | 0.02852 (9) | |
| N1 | 0.24983 (15) | 0.82356 (13) | 0.66660 (8) | 0.0214 (3) | |
| N2 | 0.27992 (15) | 0.65635 (13) | 0.79048 (9) | 0.0220 (3) | |
| N3 | 0.51854 (16) | 0.51550 (13) | 0.72081 (9) | 0.0223 (3) | |
| N4 | 0.48437 (16) | 0.67998 (14) | 0.59490 (8) | 0.0242 (3) | |
| C1 | 0.24569 (18) | 0.88289 (15) | 0.60036 (10) | 0.0227 (3) | |
| C2 | 0.12384 (19) | 0.97021 (17) | 0.59480 (11) | 0.0281 (4) | |
| H2 | 0.096041 | 1.023256 | 0.554521 | 0.034* | |
| C3 | 0.05671 (19) | 0.96205 (17) | 0.65802 (12) | 0.0279 (4) | |
| H3 | -0.026842 | 1.008457 | 0.670278 | 0.033* | |
| C4 | 0.13636 (17) | 0.86923 (15) | 0.70338 (10) | 0.0224 (3) | |
| C5 | 0.09997 (17) | 0.83000 (15) | 0.77306 (10) | 0.0218 (3) | |
| C6 | 0.16882 (17) | 0.73126 (15) | 0.81346 (10) | 0.0214 (3) | |
| C7 | 0.13225 (19) | 0.69220 (17) | 0.88490 (10) | 0.0264 (3) | |
| H7 | 0.059414 | 0.728673 | 0.913683 | 0.032* | |
| C8 | 0.22172 (19) | 0.59322 (17) | 0.90336 (11) | 0.0266 (3) | |
| H8 | 0.222797 | 0.547761 | 0.947187 | 0.032* | |
| C9 | 0.31451 (18) | 0.57088 (15) | 0.84341 (10) | 0.0220 (3) | |
| C10 | 0.42052 (17) | 0.47453 (14) | 0.83970 (10) | 0.0219 (3) | |
| C11 | 0.51128 (18) | 0.44772 (14) | 0.78126 (10) | 0.0219 (3) | |
| C12 | 0.6092 (2) | 0.34284 (16) | 0.77501 (11) | 0.0263 (3) | |
| H12 | 0.625068 | 0.280969 | 0.809445 | 0.032* | |
| C13 | 0.6740 (2) | 0.34948 (16) | 0.71070 (11) | 0.0281 (4) | |
| H13 | 0.743640 | 0.293168 | 0.691602 | 0.034* | |
| C14 | 0.61667 (18) | 0.45887 (15) | 0.67670 (10) | 0.0232 (3) | |
| C15 | 0.65374 (19) | 0.49959 (16) | 0.60806 (10) | 0.0250 (3) | |
| C16 | 0.59096 (19) | 0.60177 (16) | 0.57051 (10) | 0.0250 (3) | |
| C17 | 0.6272 (2) | 0.63886 (19) | 0.49831 (11) | 0.0307 (4) | |
| H17 | 0.698553 | 0.600706 | 0.469122 | 0.037* | |
| C18 | 0.5403 (2) | 0.73832 (18) | 0.48013 (11) | 0.0297 (4) | |
| H18 | 0.539124 | 0.782733 | 0.435789 | 0.036* | |
| C19 | 0.44944 (19) | 0.76401 (16) | 0.54134 (10) | 0.0236 (3) | |
| C20 | 0.34025 (19) | 0.85861 (16) | 0.54385 (10) | 0.0236 (3) | |
| C21 | 0.31851 (19) | 0.93785 (16) | 0.47740 (10) | 0.0245 (3) | |
| C22 | 0.2886 (2) | 0.9100 (2) | 0.41127 (11) | 0.0312 (4) | |
| H22 | 0.279346 | 0.841334 | 0.408858 | 0.037* | |
| C23 | 0.2721 (2) | 0.9825 (2) | 0.34867 (12) | 0.0352 (5) | |
| H23 | 0.251782 | 0.962891 | 0.303810 | 0.042* | |

| | | | | | |
|-----|---------------|--------------|--------------|-------------|------------|
| C24 | 0.2852 (2) | 1.0825 (2) | 0.35148 (13) | 0.0360 (5) | |
| H24 | 0.274342 | 1.131483 | 0.308613 | 0.043* | |
| C25 | 0.3142 (2) | 1.1114 (2) | 0.41687 (14) | 0.0358 (5) | |
| H25 | 0.322973 | 1.180289 | 0.419000 | 0.043* | |
| C26 | 0.3305 (2) | 1.03930 (18) | 0.47953 (12) | 0.0300 (4) | |
| H26 | 0.350123 | 1.059644 | 0.524319 | 0.036* | |
| C27 | -0.02434 (18) | 0.89793 (16) | 0.80617 (10) | 0.0234 (3) | |
| C28 | -0.0439 (2) | 1.00464 (18) | 0.82000 (14) | 0.0319 (4) | |
| H28 | 0.022507 | 1.034355 | 0.808452 | 0.038* | |
| C29 | -0.1595 (2) | 1.0684 (2) | 0.85054 (15) | 0.0379 (5) | |
| H29 | -0.170638 | 1.140649 | 0.860055 | 0.046* | |
| C30 | -0.2580 (2) | 1.0272 (2) | 0.86705 (14) | 0.0385 (5) | |
| H30 | -0.336711 | 1.070749 | 0.887798 | 0.046* | |
| C31 | -0.2405 (2) | 0.9222 (2) | 0.85301 (13) | 0.0347 (4) | |
| H31 | -0.307945 | 0.893528 | 0.863727 | 0.042* | |
| C32 | -0.12453 (19) | 0.85777 (18) | 0.82320 (11) | 0.0274 (3) | |
| H32 | -0.113749 | 0.785321 | 0.814379 | 0.033* | |
| C33 | 0.43734 (18) | 0.38888 (15) | 0.90240 (10) | 0.0226 (3) | |
| C34 | 0.5279 (3) | 0.3731 (2) | 0.95519 (14) | 0.0397 (5) | |
| H34 | 0.578828 | 0.418681 | 0.952273 | 0.048* | |
| C35 | 0.5455 (3) | 0.2917 (2) | 1.01234 (15) | 0.0437 (6) | |
| H35 | 0.607545 | 0.282703 | 1.048190 | 0.052* | |
| C36 | 0.4739 (2) | 0.22448 (19) | 1.01725 (13) | 0.0350 (4) | |
| H36 | 0.485747 | 0.169074 | 1.056381 | 0.042* | |
| C37 | 0.3847 (3) | 0.2381 (2) | 0.96481 (15) | 0.0444 (6) | |
| H37 | 0.336226 | 0.190659 | 0.967048 | 0.053* | |
| C38 | 0.3649 (3) | 0.3212 (2) | 0.90847 (14) | 0.0379 (5) | |
| H38 | 0.300713 | 0.331431 | 0.873732 | 0.045* | |
| C39 | 0.7664 (6) | 0.4246 (11) | 0.5690 (8) | 0.0266 (11) | 0.703 (13) |
| C40 | 0.8885 (4) | 0.3961 (6) | 0.5985 (3) | 0.0500 (15) | 0.703 (13) |
| H40 | 0.899224 | 0.426459 | 0.641337 | 0.060* | 0.703 (13) |
| C41 | 0.9947 (5) | 0.3230 (7) | 0.5649 (3) | 0.0631 (19) | 0.703 (13) |
| H41 | 1.077755 | 0.305016 | 0.584177 | 0.076* | 0.703 (13) |
| C42 | 0.9781 (8) | 0.2773 (6) | 0.5037 (5) | 0.0490 (15) | 0.703 (13) |
| H42 | 1.050146 | 0.228812 | 0.480216 | 0.059* | 0.703 (13) |
| C43 | 0.8592 (6) | 0.3012 (4) | 0.4768 (3) | 0.0370 (11) | 0.703 (13) |
| H43 | 0.848613 | 0.268296 | 0.435128 | 0.044* | 0.703 (13) |
| C44 | 0.7524 (6) | 0.3737 (5) | 0.5098 (3) | 0.0290 (9) | 0.703 (13) |
| H44 | 0.669510 | 0.388009 | 0.491285 | 0.035* | 0.703 (13) |
| C45 | 0.7777 (16) | 0.426 (3) | 0.5760 (19) | 0.030 (3) | 0.297 (13) |
| C46 | 0.8887 (9) | 0.4532 (15) | 0.5746 (8) | 0.050 (3) | 0.297 (13) |
| H46 | 0.888475 | 0.516328 | 0.595476 | 0.060* | 0.297 (13) |
| C47 | 1.0000 (9) | 0.3861 (17) | 0.5421 (10) | 0.064 (4) | 0.297 (13) |
| H47 | 1.077399 | 0.401519 | 0.543295 | 0.077* | 0.297 (13) |
| C48 | 0.9993 (15) | 0.2978 (18) | 0.5082 (14) | 0.051 (4) | 0.297 (13) |
| H48 | 1.077187 | 0.247226 | 0.491606 | 0.061* | 0.297 (13) |
| C49 | 0.8863 (14) | 0.2841 (11) | 0.4989 (9) | 0.040 (3) | 0.297 (13) |
| H49 | 0.883799 | 0.227406 | 0.471690 | 0.048* | 0.297 (13) |

| | | | | | |
|------|--------------|--------------|--------------|-------------|------------|
| C50 | 0.7716 (13) | 0.3535 (10) | 0.5293 (8) | 0.030 (2) | 0.297 (13) |
| H50 | 0.691105 | 0.349908 | 0.517396 | 0.036* | 0.297 (13) |
| Ag2 | 0.90698 (2) | 0.69473 (2) | 0.19974 (2) | 0.03222 (4) | |
| N5 | 0.9319 (2) | 0.47300 (16) | 0.28850 (11) | 0.0327 (4) | |
| N6 | 1.10727 (19) | 0.46983 (15) | 0.23211 (10) | 0.0296 (3) | |
| N7 | 0.8462 (2) | 0.89703 (17) | 0.08714 (11) | 0.0347 (4) | |
| N8 | 0.7516 (2) | 0.94014 (16) | 0.18960 (11) | 0.0339 (4) | |
| C51 | 0.9846 (2) | 0.53447 (18) | 0.24251 (12) | 0.0299 (4) | |
| C52 | 0.7997 (3) | 0.5085 (2) | 0.31683 (16) | 0.0436 (6) | |
| H52A | 0.799411 | 0.510836 | 0.369982 | 0.065* | |
| H52B | 0.758031 | 0.457415 | 0.305608 | 0.065* | |
| H52C | 0.753102 | 0.580921 | 0.293897 | 0.065* | |
| C53 | 1.0214 (3) | 0.3723 (2) | 0.30666 (14) | 0.0403 (5) | |
| H53 | 1.007855 | 0.314947 | 0.338064 | 0.048* | |
| C54 | 1.1317 (3) | 0.37092 (19) | 0.27135 (13) | 0.0370 (5) | |
| H54 | 1.211037 | 0.312658 | 0.273296 | 0.044* | |
| C55A | 1.2013 (2) | 0.4974 (2) | 0.18115 (14) | 0.0355 (4) | 0.679 (7) |
| H55A | 1.284834 | 0.476254 | 0.205256 | 0.043* | 0.679 (7) |
| H55B | 1.171940 | 0.576699 | 0.167993 | 0.043* | 0.679 (7) |
| C56 | 1.2179 (4) | 0.4372 (3) | 0.1102 (2) | 0.0369 (9) | 0.679 (7) |
| H56A | 1.285406 | 0.453047 | 0.078216 | 0.044* | 0.679 (7) |
| H56B | 1.246697 | 0.357971 | 0.123815 | 0.044* | 0.679 (7) |
| C57 | 1.0955 (4) | 0.4699 (4) | 0.0677 (2) | 0.0460 (11) | 0.679 (7) |
| H57A | 1.028228 | 0.454223 | 0.098999 | 0.069* | 0.679 (7) |
| H57B | 1.110633 | 0.429061 | 0.024527 | 0.069* | 0.679 (7) |
| H57C | 1.068313 | 0.547779 | 0.052266 | 0.069* | 0.679 (7) |
| C55B | 1.2013 (2) | 0.4974 (2) | 0.18115 (14) | 0.0355 (4) | 0.321 (7) |
| H55C | 1.208910 | 0.566394 | 0.193314 | 0.043* | 0.321 (7) |
| H55D | 1.286053 | 0.440193 | 0.188227 | 0.043* | 0.321 (7) |
| C58 | 1.1682 (8) | 0.5084 (6) | 0.1047 (4) | 0.0360 (17) | 0.321 (7) |
| H58A | 1.232833 | 0.530031 | 0.073635 | 0.043* | 0.321 (7) |
| H58B | 1.083771 | 0.565747 | 0.096845 | 0.043* | 0.321 (7) |
| C59 | 1.1632 (8) | 0.4017 (7) | 0.0830 (4) | 0.0375 (18) | 0.321 (7) |
| H59A | 1.241617 | 0.342881 | 0.098216 | 0.056* | 0.321 (7) |
| H59B | 1.155892 | 0.406156 | 0.029773 | 0.056* | 0.321 (7) |
| H59C | 1.088690 | 0.387368 | 0.107013 | 0.056* | 0.321 (7) |
| C60 | 0.8317 (2) | 0.85473 (18) | 0.15588 (13) | 0.0314 (4) | |
| C61 | 0.9308 (3) | 0.8367 (3) | 0.03077 (15) | 0.0485 (7) | |
| H61A | 0.887730 | 0.856493 | -0.016301 | 0.073* | |
| H61B | 0.951391 | 0.758683 | 0.044072 | 0.073* | |
| H61C | 1.009948 | 0.854364 | 0.026752 | 0.073* | |
| C62 | 0.7750 (3) | 1.0062 (2) | 0.07772 (14) | 0.0409 (5) | |
| H62 | 0.769901 | 1.053167 | 0.034218 | 0.049* | |
| C63 | 0.7144 (2) | 1.0330 (2) | 0.14213 (14) | 0.0384 (5) | |
| H63 | 0.657282 | 1.102383 | 0.152815 | 0.046* | |
| C64A | 0.7133 (3) | 0.9366 (2) | 0.26848 (15) | 0.0384 (5) | 0.787 (11) |
| H64A | 0.716891 | 1.002339 | 0.288668 | 0.046* | 0.787 (11) |
| H64B | 0.775791 | 0.872783 | 0.294963 | 0.046* | 0.787 (11) |

| | | | | | |
|------|-------------|-------------|--------------|-------------|------------|
| C65 | 0.5796 (3) | 0.9302 (3) | 0.28222 (19) | 0.0360 (8) | 0.787 (11) |
| H65A | 0.517840 | 0.992348 | 0.253920 | 0.043* | 0.787 (11) |
| H65B | 0.556495 | 0.937222 | 0.334773 | 0.043* | 0.787 (11) |
| C66 | 0.5659 (5) | 0.8245 (4) | 0.2613 (3) | 0.0526 (12) | 0.787 (11) |
| H66A | 0.581207 | 0.819865 | 0.208527 | 0.079* | 0.787 (11) |
| H66B | 0.479217 | 0.824132 | 0.274395 | 0.079* | 0.787 (11) |
| H66C | 0.628670 | 0.762285 | 0.287815 | 0.079* | 0.787 (11) |
| C64B | 0.7133 (3) | 0.9366 (2) | 0.26848 (15) | 0.0384 (5) | 0.213 (11) |
| H64C | 0.787953 | 0.897820 | 0.299636 | 0.046* | 0.213 (11) |
| H64D | 0.670942 | 1.010409 | 0.284185 | 0.046* | 0.213 (11) |
| C67 | 0.6288 (19) | 0.8800 (18) | 0.2704 (13) | 0.077 (5) | 0.213 (11) |
| H67A | 0.685793 | 0.803314 | 0.271973 | 0.093* | 0.213 (11) |
| H67B | 0.588774 | 0.888877 | 0.319925 | 0.093* | 0.213 (11) |
| C68 | 0.542 (3) | 0.882 (4) | 0.233 (2) | 0.107 (9) | 0.213 (11) |
| H68A | 0.464223 | 0.940521 | 0.246321 | 0.160* | 0.213 (11) |
| H68B | 0.527391 | 0.812534 | 0.241062 | 0.160* | 0.213 (11) |
| H68C | 0.564434 | 0.895184 | 0.181331 | 0.160* | 0.213 (11) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|---------------|---------------|---------------|
| Cd1 | 0.02000 (6) | 0.01896 (6) | 0.01589 (5) | -0.00464 (4) | 0.00228 (4) | 0.00067 (4) |
| Cl1 | 0.0272 (2) | 0.0300 (2) | 0.0290 (2) | -0.00941 (17) | -0.00066 (16) | -0.00654 (17) |
| N1 | 0.0215 (6) | 0.0222 (6) | 0.0177 (6) | -0.0050 (5) | 0.0002 (5) | 0.0019 (5) |
| N2 | 0.0214 (6) | 0.0205 (6) | 0.0210 (6) | -0.0047 (5) | 0.0036 (5) | 0.0020 (5) |
| N3 | 0.0241 (7) | 0.0198 (6) | 0.0204 (6) | -0.0052 (5) | 0.0042 (5) | -0.0010 (5) |
| N4 | 0.0258 (7) | 0.0263 (7) | 0.0169 (6) | -0.0049 (6) | 0.0016 (5) | -0.0004 (5) |
| C1 | 0.0235 (8) | 0.0238 (8) | 0.0192 (7) | -0.0071 (6) | -0.0021 (6) | 0.0032 (6) |
| C2 | 0.0247 (8) | 0.0287 (9) | 0.0263 (8) | -0.0057 (7) | -0.0040 (7) | 0.0076 (7) |
| C3 | 0.0219 (8) | 0.0274 (9) | 0.0287 (9) | -0.0030 (7) | -0.0017 (6) | 0.0045 (7) |
| C4 | 0.0202 (7) | 0.0228 (7) | 0.0221 (7) | -0.0054 (6) | -0.0002 (6) | 0.0013 (6) |
| C5 | 0.0202 (7) | 0.0215 (7) | 0.0222 (7) | -0.0055 (6) | 0.0010 (6) | -0.0012 (6) |
| C6 | 0.0214 (7) | 0.0214 (7) | 0.0199 (7) | -0.0062 (6) | 0.0026 (6) | -0.0006 (5) |
| C7 | 0.0248 (8) | 0.0290 (9) | 0.0207 (7) | -0.0045 (7) | 0.0057 (6) | -0.0001 (6) |
| C8 | 0.0263 (8) | 0.0287 (9) | 0.0207 (7) | -0.0063 (7) | 0.0046 (6) | 0.0028 (6) |
| C9 | 0.0225 (7) | 0.0217 (7) | 0.0201 (7) | -0.0072 (6) | 0.0029 (6) | 0.0021 (6) |
| C10 | 0.0219 (7) | 0.0205 (7) | 0.0217 (7) | -0.0067 (6) | 0.0010 (6) | 0.0021 (6) |
| C11 | 0.0222 (7) | 0.0189 (7) | 0.0228 (7) | -0.0055 (6) | 0.0015 (6) | 0.0002 (6) |
| C12 | 0.0267 (8) | 0.0199 (7) | 0.0280 (8) | -0.0034 (6) | 0.0003 (7) | 0.0003 (6) |
| C13 | 0.0288 (9) | 0.0225 (8) | 0.0277 (9) | -0.0018 (7) | 0.0023 (7) | -0.0037 (6) |
| C14 | 0.0243 (8) | 0.0218 (7) | 0.0213 (7) | -0.0046 (6) | 0.0028 (6) | -0.0042 (6) |
| C15 | 0.0253 (8) | 0.0274 (8) | 0.0197 (7) | -0.0052 (7) | 0.0038 (6) | -0.0055 (6) |
| C16 | 0.0269 (8) | 0.0285 (8) | 0.0174 (7) | -0.0067 (7) | 0.0036 (6) | -0.0030 (6) |
| C17 | 0.0342 (10) | 0.0343 (10) | 0.0207 (8) | -0.0088 (8) | 0.0089 (7) | -0.0036 (7) |
| C18 | 0.0363 (10) | 0.0329 (9) | 0.0183 (7) | -0.0112 (8) | 0.0061 (7) | -0.0001 (7) |
| C19 | 0.0271 (8) | 0.0274 (8) | 0.0160 (7) | -0.0096 (7) | 0.0007 (6) | 0.0005 (6) |
| C20 | 0.0271 (8) | 0.0263 (8) | 0.0173 (7) | -0.0102 (7) | -0.0016 (6) | 0.0026 (6) |
| C21 | 0.0254 (8) | 0.0295 (8) | 0.0182 (7) | -0.0102 (7) | -0.0022 (6) | 0.0045 (6) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C22 | 0.0382 (11) | 0.0406 (11) | 0.0190 (8) | -0.0204 (9) | -0.0067 (7) | 0.0062 (7) |
| C23 | 0.0347 (10) | 0.0508 (13) | 0.0214 (8) | -0.0186 (10) | -0.0060 (7) | 0.0084 (8) |
| C24 | 0.0317 (10) | 0.0432 (12) | 0.0303 (10) | -0.0141 (9) | -0.0042 (8) | 0.0158 (9) |
| C25 | 0.0368 (11) | 0.0321 (10) | 0.0376 (11) | -0.0139 (9) | -0.0039 (9) | 0.0106 (8) |
| C26 | 0.0328 (10) | 0.0290 (9) | 0.0273 (9) | -0.0106 (8) | -0.0040 (7) | 0.0041 (7) |
| C27 | 0.0203 (7) | 0.0248 (8) | 0.0223 (7) | -0.0042 (6) | 0.0002 (6) | -0.0016 (6) |
| C28 | 0.0251 (9) | 0.0268 (9) | 0.0407 (11) | -0.0037 (7) | -0.0007 (8) | -0.0065 (8) |
| C29 | 0.0317 (10) | 0.0311 (10) | 0.0431 (12) | 0.0018 (8) | -0.0013 (9) | -0.0104 (9) |
| C30 | 0.0256 (9) | 0.0441 (12) | 0.0334 (11) | 0.0042 (8) | 0.0028 (8) | -0.0057 (9) |
| C31 | 0.0224 (9) | 0.0460 (12) | 0.0316 (10) | -0.0082 (8) | 0.0054 (7) | -0.0011 (9) |
| C32 | 0.0245 (8) | 0.0317 (9) | 0.0244 (8) | -0.0082 (7) | 0.0022 (6) | -0.0019 (7) |
| C33 | 0.0238 (8) | 0.0215 (7) | 0.0213 (7) | -0.0073 (6) | 0.0001 (6) | 0.0026 (6) |
| C34 | 0.0454 (13) | 0.0411 (12) | 0.0390 (12) | -0.0257 (11) | -0.0167 (10) | 0.0147 (9) |
| C35 | 0.0510 (15) | 0.0481 (14) | 0.0356 (12) | -0.0243 (12) | -0.0191 (11) | 0.0168 (10) |
| C36 | 0.0397 (11) | 0.0319 (10) | 0.0291 (10) | -0.0105 (9) | -0.0018 (8) | 0.0111 (8) |
| C37 | 0.0559 (15) | 0.0446 (13) | 0.0418 (13) | -0.0332 (12) | -0.0145 (11) | 0.0194 (11) |
| C38 | 0.0449 (12) | 0.0418 (12) | 0.0341 (11) | -0.0269 (10) | -0.0146 (9) | 0.0148 (9) |
| C39 | 0.0227 (16) | 0.033 (3) | 0.018 (3) | -0.0007 (14) | -0.0005 (13) | -0.0039 (15) |
| C40 | 0.0305 (17) | 0.075 (4) | 0.0333 (19) | 0.0015 (19) | -0.0013 (14) | -0.019 (2) |
| C41 | 0.033 (2) | 0.086 (4) | 0.046 (2) | 0.012 (2) | 0.0029 (17) | -0.014 (3) |
| C42 | 0.049 (3) | 0.040 (3) | 0.041 (3) | 0.004 (2) | 0.019 (3) | -0.0058 (18) |
| C43 | 0.053 (3) | 0.0253 (19) | 0.034 (2) | -0.0155 (19) | 0.0191 (18) | -0.0101 (17) |
| C44 | 0.038 (2) | 0.027 (2) | 0.025 (2) | -0.0144 (16) | 0.0078 (15) | -0.0068 (15) |
| C45 | 0.035 (5) | 0.036 (6) | 0.018 (6) | -0.009 (5) | 0.006 (5) | -0.013 (5) |
| C46 | 0.030 (4) | 0.077 (8) | 0.047 (6) | -0.017 (4) | 0.009 (4) | -0.038 (6) |
| C47 | 0.022 (4) | 0.104 (10) | 0.066 (8) | -0.009 (5) | 0.005 (4) | -0.048 (7) |
| C48 | 0.028 (4) | 0.065 (9) | 0.049 (6) | 0.000 (4) | 0.014 (4) | -0.020 (6) |
| C49 | 0.043 (5) | 0.030 (5) | 0.042 (7) | -0.005 (4) | 0.014 (4) | -0.009 (4) |
| C50 | 0.035 (4) | 0.024 (4) | 0.033 (6) | -0.011 (3) | 0.011 (4) | -0.006 (4) |
| Ag2 | 0.03106 (8) | 0.02611 (7) | 0.03577 (8) | -0.00444 (6) | -0.00168 (6) | -0.00369 (6) |
| N5 | 0.0353 (9) | 0.0324 (9) | 0.0283 (8) | -0.0085 (7) | 0.0053 (7) | -0.0072 (7) |
| N6 | 0.0317 (8) | 0.0266 (8) | 0.0276 (8) | -0.0058 (6) | -0.0001 (6) | -0.0032 (6) |
| N7 | 0.0344 (9) | 0.0330 (9) | 0.0288 (8) | 0.0001 (7) | -0.0008 (7) | -0.0062 (7) |
| N8 | 0.0327 (9) | 0.0298 (8) | 0.0348 (9) | -0.0047 (7) | 0.0042 (7) | -0.0056 (7) |
| C51 | 0.0319 (9) | 0.0284 (9) | 0.0283 (9) | -0.0074 (7) | -0.0014 (7) | -0.0062 (7) |
| C52 | 0.0404 (13) | 0.0481 (14) | 0.0411 (13) | -0.0127 (11) | 0.0127 (10) | -0.0136 (11) |
| C53 | 0.0491 (14) | 0.0311 (10) | 0.0336 (11) | -0.0071 (9) | 0.0101 (10) | 0.0003 (8) |
| C54 | 0.0426 (12) | 0.0287 (10) | 0.0305 (10) | -0.0024 (9) | 0.0055 (9) | 0.0012 (8) |
| C55A | 0.0313 (10) | 0.0373 (11) | 0.0395 (11) | -0.0147 (9) | -0.0010 (8) | -0.0001 (9) |
| C56 | 0.0365 (17) | 0.0366 (19) | 0.0347 (16) | -0.0110 (14) | 0.0108 (13) | -0.0014 (13) |
| C57 | 0.047 (2) | 0.067 (3) | 0.0311 (17) | -0.029 (2) | 0.0061 (15) | -0.0055 (17) |
| C55B | 0.0313 (10) | 0.0373 (11) | 0.0395 (11) | -0.0147 (9) | -0.0010 (8) | -0.0001 (9) |
| C58 | 0.037 (4) | 0.034 (4) | 0.035 (3) | -0.012 (3) | 0.008 (3) | 0.002 (3) |
| C59 | 0.038 (4) | 0.040 (4) | 0.033 (3) | -0.011 (3) | -0.001 (3) | -0.005 (3) |
| C60 | 0.0295 (9) | 0.0281 (9) | 0.0330 (10) | -0.0043 (7) | 0.0007 (7) | -0.0062 (7) |
| C61 | 0.0499 (15) | 0.0497 (15) | 0.0320 (11) | 0.0018 (12) | 0.0068 (10) | -0.0096 (10) |
| C62 | 0.0429 (13) | 0.0337 (11) | 0.0338 (11) | 0.0020 (9) | -0.0019 (9) | 0.0013 (9) |
| C63 | 0.0359 (11) | 0.0309 (10) | 0.0383 (11) | 0.0019 (9) | 0.0004 (9) | -0.0039 (8) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|-------------|--------------|
| C64A | 0.0387 (12) | 0.0400 (12) | 0.0390 (11) | -0.0154 (10) | 0.0065 (9) | -0.0116 (9) |
| C65 | 0.0312 (15) | 0.0344 (16) | 0.0406 (16) | -0.0092 (12) | 0.0085 (11) | -0.0078 (12) |
| C66 | 0.049 (2) | 0.049 (2) | 0.072 (3) | -0.0312 (19) | 0.022 (2) | -0.023 (2) |
| C64B | 0.0387 (12) | 0.0400 (12) | 0.0390 (11) | -0.0154 (10) | 0.0065 (9) | -0.0116 (9) |
| C67 | 0.050 (7) | 0.072 (10) | 0.119 (12) | -0.024 (7) | 0.039 (7) | -0.060 (8) |
| C68 | 0.074 (13) | 0.15 (3) | 0.125 (18) | -0.078 (16) | 0.033 (10) | -0.050 (17) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|------------|
| Cd1—N1 | 2.2273 (15) | C41—C42 | 1.379 (9) |
| Cd1—N4 | 2.2289 (16) | C41—H41 | 0.9500 |
| Cd1—N3 | 2.2333 (16) | C42—C43 | 1.358 (8) |
| Cd1—N2 | 2.2440 (15) | C42—H42 | 0.9500 |
| Cd1—C11 | 2.4847 (5) | C43—C44 | 1.396 (6) |
| N1—C4 | 1.369 (2) | C43—H43 | 0.9500 |
| N1—C1 | 1.370 (2) | C44—H44 | 0.9500 |
| N2—C6 | 1.367 (2) | C45—C50 | 1.367 (13) |
| N2—C9 | 1.371 (2) | C45—C46 | 1.394 (17) |
| N3—C11 | 1.367 (2) | C46—C47 | 1.395 (11) |
| N3—C14 | 1.367 (2) | C46—H46 | 0.9500 |
| N4—C16 | 1.366 (2) | C47—C48 | 1.378 (15) |
| N4—C19 | 1.367 (2) | C47—H47 | 0.9500 |
| C1—C20 | 1.413 (3) | C48—C49 | 1.348 (14) |
| C1—C2 | 1.447 (3) | C48—H48 | 0.9500 |
| C2—C3 | 1.358 (3) | C49—C50 | 1.414 (12) |
| C2—H2 | 0.9500 | C49—H49 | 0.9500 |
| C3—C4 | 1.451 (3) | C50—H50 | 0.9500 |
| C3—H3 | 0.9500 | Ag2—C51 | 2.075 (2) |
| C4—C5 | 1.419 (3) | Ag2—C60 | 2.076 (2) |
| C5—C6 | 1.419 (3) | N5—C51 | 1.354 (3) |
| C5—C27 | 1.500 (3) | N5—C53 | 1.380 (3) |
| C6—C7 | 1.446 (3) | N5—C52 | 1.462 (3) |
| C7—C8 | 1.365 (3) | N6—C51 | 1.353 (3) |
| C7—H7 | 0.9500 | N6—C54 | 1.369 (3) |
| C8—C9 | 1.446 (3) | N6—C55B | 1.473 (3) |
| C8—H8 | 0.9500 | N6—C55A | 1.473 (3) |
| C9—C10 | 1.411 (3) | N7—C60 | 1.350 (3) |
| C10—C11 | 1.415 (3) | N7—C62 | 1.382 (3) |
| C10—C33 | 1.498 (2) | N7—C61 | 1.461 (3) |
| C11—C12 | 1.448 (3) | N8—C60 | 1.356 (3) |
| C12—C13 | 1.358 (3) | N8—C63 | 1.379 (3) |
| C12—H12 | 0.9500 | N8—C64B | 1.487 (3) |
| C13—C14 | 1.450 (3) | N8—C64A | 1.487 (3) |
| C13—H13 | 0.9500 | C52—H52A | 0.9800 |
| C14—C15 | 1.413 (3) | C52—H52B | 0.9800 |
| C15—C16 | 1.412 (3) | C52—H52C | 0.9800 |
| C15—C39 | 1.502 (7) | C53—C54 | 1.347 (4) |
| C15—C45 | 1.516 (17) | C53—H53 | 0.9500 |

| | | | |
|-----------|------------|-------------|------------|
| C16—C17 | 1.448 (3) | C54—H54 | 0.9500 |
| C17—C18 | 1.357 (3) | C55A—C56 | 1.566 (5) |
| C17—H17 | 0.9500 | C55A—H55A | 0.9900 |
| C18—C19 | 1.453 (3) | C55A—H55B | 0.9900 |
| C18—H18 | 0.9500 | C56—C57 | 1.514 (6) |
| C19—C20 | 1.414 (3) | C56—H56A | 0.9900 |
| C20—C21 | 1.495 (3) | C56—H56B | 0.9900 |
| C21—C26 | 1.392 (3) | C57—H57A | 0.9800 |
| C21—C22 | 1.394 (3) | C57—H57B | 0.9800 |
| C22—C23 | 1.394 (3) | C57—H57C | 0.9800 |
| C22—H22 | 0.9500 | C55B—C58 | 1.452 (8) |
| C23—C24 | 1.380 (4) | C55B—H55C | 0.9900 |
| C23—H23 | 0.9500 | C55B—H55D | 0.9900 |
| C24—C25 | 1.384 (4) | C58—C59 | 1.518 (12) |
| C24—H24 | 0.9500 | C58—H58A | 0.9900 |
| C25—C26 | 1.392 (3) | C58—H58B | 0.9900 |
| C25—H25 | 0.9500 | C59—H59A | 0.9800 |
| C26—H26 | 0.9500 | C59—H59B | 0.9800 |
| C27—C32 | 1.393 (3) | C59—H59C | 0.9800 |
| C27—C28 | 1.395 (3) | C61—H61A | 0.9800 |
| C28—C29 | 1.395 (3) | C61—H61B | 0.9800 |
| C28—H28 | 0.9500 | C61—H61C | 0.9800 |
| C29—C30 | 1.383 (4) | C62—C63 | 1.346 (4) |
| C29—H29 | 0.9500 | C62—H62 | 0.9500 |
| C30—C31 | 1.379 (4) | C63—H63 | 0.9500 |
| C30—H30 | 0.9500 | C64A—C65 | 1.521 (4) |
| C31—C32 | 1.396 (3) | C64A—H64A | 0.9900 |
| C31—H31 | 0.9500 | C64A—H64B | 0.9900 |
| C32—H32 | 0.9500 | C65—C66 | 1.539 (5) |
| C33—C38 | 1.382 (3) | C65—H65A | 0.9900 |
| C33—C34 | 1.387 (3) | C65—H65B | 0.9900 |
| C34—C35 | 1.391 (3) | C66—H66A | 0.9800 |
| C34—H34 | 0.9500 | C66—H66B | 0.9800 |
| C35—C36 | 1.370 (4) | C66—H66C | 0.9800 |
| C35—H35 | 0.9500 | C64B—C67 | 1.380 (18) |
| C36—C37 | 1.377 (4) | C64B—H64C | 0.9900 |
| C36—H36 | 0.9500 | C64B—H64D | 0.9900 |
| C37—C38 | 1.394 (3) | C67—C68 | 1.20 (4) |
| C37—H37 | 0.9500 | C67—H67A | 0.9900 |
| C38—H38 | 0.9500 | C67—H67B | 0.9900 |
| C39—C44 | 1.378 (7) | C68—H68A | 0.9800 |
| C39—C40 | 1.403 (9) | C68—H68B | 0.9800 |
| C40—C41 | 1.401 (6) | C68—H68C | 0.9800 |
| C40—H40 | 0.9500 | | |
| N1—Cd1—N4 | 83.78 (6) | C43—C42—C41 | 120.3 (5) |
| N1—Cd1—N3 | 140.24 (6) | C43—C42—H42 | 119.8 |
| N4—Cd1—N3 | 82.65 (6) | C41—C42—H42 | 119.8 |

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| N1—Cd1—N2 | 82.44 (6) | C42—C43—C44 | 120.7 (5) |
| N4—Cd1—N2 | 138.19 (6) | C42—C43—H43 | 119.7 |
| N3—Cd1—N2 | 83.25 (6) | C44—C43—H43 | 119.7 |
| N1—Cd1—Cl1 | 110.89 (4) | C39—C44—C43 | 120.5 (5) |
| N4—Cd1—Cl1 | 114.15 (5) | C39—C44—H44 | 119.8 |
| N3—Cd1—Cl1 | 108.78 (5) | C43—C44—H44 | 119.8 |
| N2—Cd1—Cl1 | 107.65 (5) | C50—C45—C46 | 118.3 (15) |
| C4—N1—C1 | 107.80 (15) | C50—C45—C15 | 118.6 (11) |
| C4—N1—Cd1 | 126.55 (12) | C46—C45—C15 | 120.0 (15) |
| C1—N1—Cd1 | 124.81 (12) | C45—C46—C47 | 118.7 (12) |
| C6—N2—C9 | 108.04 (15) | C45—C46—H46 | 120.6 |
| C6—N2—Cd1 | 124.43 (12) | C47—C46—H46 | 120.6 |
| C9—N2—Cd1 | 121.99 (12) | C48—C47—C46 | 121.0 (11) |
| C11—N3—C14 | 107.76 (15) | C48—C47—H47 | 119.5 |
| C11—N3—Cd1 | 124.51 (12) | C46—C47—H47 | 119.5 |
| C14—N3—Cd1 | 125.73 (12) | C49—C48—C47 | 119.0 (12) |
| C16—N4—C19 | 108.05 (16) | C49—C48—H48 | 120.5 |
| C16—N4—Cd1 | 124.54 (13) | C47—C48—H48 | 120.5 |
| C19—N4—Cd1 | 123.88 (13) | C48—C49—C50 | 120.6 (12) |
| N1—C1—C20 | 125.89 (17) | C48—C49—H49 | 119.7 |
| N1—C1—C2 | 109.09 (16) | C50—C49—H49 | 119.7 |
| C20—C1—C2 | 124.85 (17) | C45—C50—C49 | 119.3 (12) |
| C3—C2—C1 | 107.07 (17) | C45—C50—H50 | 120.3 |
| C3—C2—H2 | 126.5 | C49—C50—H50 | 120.3 |
| C1—C2—H2 | 126.5 | C51—Ag2—C60 | 179.14 (9) |
| C2—C3—C4 | 107.26 (17) | C51—N5—C53 | 110.6 (2) |
| C2—C3—H3 | 126.4 | C51—N5—C52 | 125.1 (2) |
| C4—C3—H3 | 126.4 | C53—N5—C52 | 124.3 (2) |
| N1—C4—C5 | 125.81 (16) | C51—N6—C54 | 111.3 (2) |
| N1—C4—C3 | 108.78 (16) | C51—N6—C55B | 125.16 (19) |
| C5—C4—C3 | 125.36 (17) | C54—N6—C55B | 123.4 (2) |
| C6—C5—C4 | 126.01 (16) | C51—N6—C55A | 125.16 (19) |
| C6—C5—C27 | 117.04 (16) | C54—N6—C55A | 123.4 (2) |
| C4—C5—C27 | 116.93 (16) | C60—N7—C62 | 111.3 (2) |
| N2—C6—C5 | 125.40 (16) | C60—N7—C61 | 124.5 (2) |
| N2—C6—C7 | 108.75 (16) | C62—N7—C61 | 124.1 (2) |
| C5—C6—C7 | 125.85 (16) | C60—N8—C63 | 111.3 (2) |
| C8—C7—C6 | 107.37 (16) | C60—N8—C64B | 124.8 (2) |
| C8—C7—H7 | 126.3 | C63—N8—C64B | 123.8 (2) |
| C6—C7—H7 | 126.3 | C60—N8—C64A | 124.8 (2) |
| C7—C8—C9 | 106.83 (16) | C63—N8—C64A | 123.8 (2) |
| C7—C8—H8 | 126.6 | N6—C51—N5 | 104.55 (19) |
| C9—C8—H8 | 126.6 | N6—C51—Ag2 | 125.11 (17) |
| N2—C9—C10 | 126.12 (16) | N5—C51—Ag2 | 130.24 (17) |
| N2—C9—C8 | 109.00 (16) | N5—C52—H52A | 109.5 |
| C10—C9—C8 | 124.85 (16) | N5—C52—H52B | 109.5 |
| C9—C10—C11 | 126.81 (16) | H52A—C52—H52B | 109.5 |
| C9—C10—C33 | 117.40 (16) | N5—C52—H52C | 109.5 |

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| C11—C10—C33 | 115.74 (16) | H52A—C52—H52C | 109.5 |
| N3—C11—C10 | 125.60 (16) | H52B—C52—H52C | 109.5 |
| N3—C11—C12 | 109.05 (16) | C54—C53—N5 | 106.9 (2) |
| C10—C11—C12 | 125.32 (17) | C54—C53—H53 | 126.6 |
| C13—C12—C11 | 107.16 (17) | N5—C53—H53 | 126.6 |
| C13—C12—H12 | 126.4 | C53—C54—N6 | 106.7 (2) |
| C11—C12—H12 | 126.4 | C53—C54—H54 | 126.7 |
| C12—C13—C14 | 106.97 (17) | N6—C54—H54 | 126.7 |
| C12—C13—H13 | 126.5 | N6—C55A—C56 | 110.5 (2) |
| C14—C13—H13 | 126.5 | N6—C55A—H55A | 109.6 |
| N3—C14—C15 | 125.39 (17) | C56—C55A—H55A | 109.6 |
| N3—C14—C13 | 109.05 (16) | N6—C55A—H55B | 109.6 |
| C15—C14—C13 | 125.54 (17) | C56—C55A—H55B | 109.6 |
| C16—C15—C14 | 126.43 (17) | H55A—C55A—H55B | 108.1 |
| C16—C15—C39 | 116.5 (7) | C57—C56—C55A | 112.8 (3) |
| C14—C15—C39 | 116.9 (7) | C57—C56—H56A | 109.0 |
| C16—C15—C45 | 119.1 (17) | C55A—C56—H56A | 109.0 |
| C14—C15—C45 | 114.4 (17) | C57—C56—H56B | 109.0 |
| N4—C16—C15 | 125.92 (17) | C55A—C56—H56B | 109.0 |
| N4—C16—C17 | 108.93 (17) | H56A—C56—H56B | 107.8 |
| C15—C16—C17 | 125.12 (18) | C56—C57—H57A | 109.5 |
| C18—C17—C16 | 107.21 (18) | C56—C57—H57B | 109.5 |
| C18—C17—H17 | 126.4 | H57A—C57—H57B | 109.5 |
| C16—C17—H17 | 126.4 | C56—C57—H57C | 109.5 |
| C17—C18—C19 | 107.02 (17) | H57A—C57—H57C | 109.5 |
| C17—C18—H18 | 126.5 | H57B—C57—H57C | 109.5 |
| C19—C18—H18 | 126.5 | C58—C55B—N6 | 113.6 (3) |
| N4—C19—C20 | 125.68 (17) | C58—C55B—H55C | 108.8 |
| N4—C19—C18 | 108.77 (17) | N6—C55B—H55C | 108.8 |
| C20—C19—C18 | 125.52 (17) | C58—C55B—H55D | 108.8 |
| C1—C20—C19 | 126.96 (16) | N6—C55B—H55D | 108.8 |
| C1—C20—C21 | 116.68 (17) | H55C—C55B—H55D | 107.7 |
| C19—C20—C21 | 116.23 (16) | C55B—C58—C59 | 110.2 (6) |
| C26—C21—C22 | 118.65 (18) | C55B—C58—H58A | 109.6 |
| C26—C21—C20 | 121.13 (18) | C59—C58—H58A | 109.6 |
| C22—C21—C20 | 120.21 (18) | C55B—C58—H58B | 109.6 |
| C21—C22—C23 | 120.3 (2) | C59—C58—H58B | 109.6 |
| C21—C22—H22 | 119.8 | H58A—C58—H58B | 108.1 |
| C23—C22—H22 | 119.8 | C58—C59—H59A | 109.5 |
| C24—C23—C22 | 120.4 (2) | C58—C59—H59B | 109.5 |
| C24—C23—H23 | 119.8 | H59A—C59—H59B | 109.5 |
| C22—C23—H23 | 119.8 | C58—C59—H59C | 109.5 |
| C23—C24—C25 | 119.8 (2) | H59A—C59—H59C | 109.5 |
| C23—C24—H24 | 120.1 | H59B—C59—H59C | 109.5 |
| C25—C24—H24 | 120.1 | N7—C60—N8 | 104.14 (19) |
| C24—C25—C26 | 119.9 (2) | N7—C60—Ag2 | 128.48 (16) |
| C24—C25—H25 | 120.0 | N8—C60—Ag2 | 127.32 (17) |
| C26—C25—H25 | 120.0 | N7—C61—H61A | 109.5 |

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| C21—C26—C25 | 120.8 (2) | N7—C61—H61B | 109.5 |
| C21—C26—H26 | 119.6 | H61A—C61—H61B | 109.5 |
| C25—C26—H26 | 119.6 | N7—C61—H61C | 109.5 |
| C32—C27—C28 | 117.72 (18) | H61A—C61—H61C | 109.5 |
| C32—C27—C5 | 121.56 (18) | H61B—C61—H61C | 109.5 |
| C28—C27—C5 | 120.72 (18) | C63—C62—N7 | 106.7 (2) |
| C27—C28—C29 | 121.0 (2) | C63—C62—H62 | 126.7 |
| C27—C28—H28 | 119.5 | N7—C62—H62 | 126.7 |
| C29—C28—H28 | 119.5 | C62—C63—N8 | 106.5 (2) |
| C30—C29—C28 | 120.5 (2) | C62—C63—H63 | 126.7 |
| C30—C29—H29 | 119.8 | N8—C63—H63 | 126.7 |
| C28—C29—H29 | 119.8 | N8—C64A—C65 | 113.2 (2) |
| C31—C30—C29 | 119.1 (2) | N8—C64A—H64A | 108.9 |
| C31—C30—H30 | 120.4 | C65—C64A—H64A | 108.9 |
| C29—C30—H30 | 120.4 | N8—C64A—H64B | 108.9 |
| C30—C31—C32 | 120.6 (2) | C65—C64A—H64B | 108.9 |
| C30—C31—H31 | 119.7 | H64A—C64A—H64B | 107.8 |
| C32—C31—H31 | 119.7 | C64A—C65—C66 | 114.0 (3) |
| C27—C32—C31 | 121.1 (2) | C64A—C65—H65A | 108.8 |
| C27—C32—H32 | 119.5 | C66—C65—H65A | 108.8 |
| C31—C32—H32 | 119.5 | C64A—C65—H65B | 108.8 |
| C38—C33—C34 | 117.84 (18) | C66—C65—H65B | 108.8 |
| C38—C33—C10 | 120.88 (18) | H65A—C65—H65B | 107.7 |
| C34—C33—C10 | 121.26 (18) | C65—C66—H66A | 109.5 |
| C33—C34—C35 | 121.1 (2) | C65—C66—H66B | 109.5 |
| C33—C34—H34 | 119.4 | H66A—C66—H66B | 109.5 |
| C35—C34—H34 | 119.4 | C65—C66—H66C | 109.5 |
| C36—C35—C34 | 120.4 (2) | H66A—C66—H66C | 109.5 |
| C36—C35—H35 | 119.8 | H66B—C66—H66C | 109.5 |
| C34—C35—H35 | 119.8 | C67—C64B—N8 | 101.6 (10) |
| C35—C36—C37 | 119.2 (2) | C67—C64B—H64C | 111.5 |
| C35—C36—H36 | 120.4 | N8—C64B—H64C | 111.4 |
| C37—C36—H36 | 120.4 | C67—C64B—H64D | 111.4 |
| C36—C37—C38 | 120.4 (2) | N8—C64B—H64D | 111.4 |
| C36—C37—H37 | 119.8 | H64C—C64B—H64D | 109.3 |
| C38—C37—H37 | 119.8 | C68—C67—C64B | 135 (3) |
| C33—C38—C37 | 121.0 (2) | C68—C67—H67A | 103.4 |
| C33—C38—H38 | 119.5 | C64B—C67—H67A | 103.4 |
| C37—C38—H38 | 119.5 | C68—C67—H67B | 103.4 |
| C44—C39—C40 | 118.6 (6) | C64B—C67—H67B | 103.4 |
| C44—C39—C15 | 122.3 (5) | H67A—C67—H67B | 105.2 |
| C40—C39—C15 | 118.8 (6) | C67—C68—H68A | 109.5 |
| C41—C40—C39 | 120.2 (5) | C67—C68—H68B | 109.5 |
| C41—C40—H40 | 119.9 | H68A—C68—H68B | 109.5 |
| C39—C40—H40 | 119.9 | C67—C68—H68C | 109.5 |
| C42—C41—C40 | 119.6 (5) | H68A—C68—H68C | 109.5 |
| C42—C41—H41 | 120.2 | H68B—C68—H68C | 109.5 |
| C40—C41—H41 | 120.2 | | |

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| C4—N1—C1—C20 | -175.51 (19) | C23—C24—C25—C26 | 0.2 (4) |
| Cd1—N1—C1—C20 | 14.4 (3) | C22—C21—C26—C25 | -0.6 (3) |
| C4—N1—C1—C2 | -0.1 (2) | C20—C21—C26—C25 | 177.9 (2) |
| Cd1—N1—C1—C2 | -170.14 (13) | C24—C25—C26—C21 | 0.2 (4) |
| N1—C1—C2—C3 | 0.1 (2) | C6—C5—C27—C32 | -58.8 (3) |
| C20—C1—C2—C3 | 175.6 (2) | C4—C5—C27—C32 | 119.8 (2) |
| C1—C2—C3—C4 | -0.1 (2) | C6—C5—C27—C28 | 122.1 (2) |
| C1—N1—C4—C5 | 177.60 (19) | C4—C5—C27—C28 | -59.3 (3) |
| Cd1—N1—C4—C5 | -12.6 (3) | C32—C27—C28—C29 | 0.6 (3) |
| C1—N1—C4—C3 | 0.0 (2) | C5—C27—C28—C29 | 179.8 (2) |
| Cd1—N1—C4—C3 | 169.83 (13) | C27—C28—C29—C30 | -0.7 (4) |
| C2—C3—C4—N1 | 0.1 (2) | C28—C29—C30—C31 | 0.1 (4) |
| C2—C3—C4—C5 | -177.5 (2) | C29—C30—C31—C32 | 0.6 (4) |
| N1—C4—C5—C6 | -6.6 (3) | C28—C27—C32—C31 | 0.1 (3) |
| C3—C4—C5—C6 | 170.6 (2) | C5—C27—C32—C31 | -179.05 (19) |
| N1—C4—C5—C27 | 174.96 (18) | C30—C31—C32—C27 | -0.7 (3) |
| C3—C4—C5—C27 | -7.8 (3) | C9—C10—C33—C38 | 78.7 (3) |
| C9—N2—C6—C5 | -178.04 (18) | C11—C10—C33—C38 | -99.0 (2) |
| Cd1—N2—C6—C5 | 28.0 (3) | C9—C10—C33—C34 | -102.9 (3) |
| C9—N2—C6—C7 | 0.9 (2) | C11—C10—C33—C34 | 79.4 (3) |
| Cd1—N2—C6—C7 | -153.07 (14) | C38—C33—C34—C35 | 0.1 (4) |
| C4—C5—C6—N2 | -2.0 (3) | C10—C33—C34—C35 | -178.4 (3) |
| C27—C5—C6—N2 | 176.36 (18) | C33—C34—C35—C36 | 0.6 (5) |
| C4—C5—C6—C7 | 179.2 (2) | C34—C35—C36—C37 | 0.2 (5) |
| C27—C5—C6—C7 | -2.4 (3) | C35—C36—C37—C38 | -1.7 (5) |
| N2—C6—C7—C8 | -0.7 (2) | C34—C33—C38—C37 | -1.6 (4) |
| C5—C6—C7—C8 | 178.22 (19) | C10—C33—C38—C37 | 176.9 (3) |
| C6—C7—C8—C9 | 0.3 (2) | C36—C37—C38—C33 | 2.4 (5) |
| C6—N2—C9—C10 | 177.15 (19) | C16—C15—C39—C44 | -72.0 (13) |
| Cd1—N2—C9—C10 | -28.1 (3) | C14—C15—C39—C44 | 104.5 (13) |
| C6—N2—C9—C8 | -0.8 (2) | C16—C15—C39—C40 | 115.1 (11) |
| Cd1—N2—C9—C8 | 153.99 (14) | C14—C15—C39—C40 | -68.3 (12) |
| C7—C8—C9—N2 | 0.3 (2) | C44—C39—C40—C41 | 4.4 (17) |
| C7—C8—C9—C10 | -177.6 (2) | C15—C39—C40—C41 | 177.5 (8) |
| N2—C9—C10—C11 | 0.2 (3) | C39—C40—C41—C42 | -1.5 (13) |
| C8—C9—C10—C11 | 177.8 (2) | C40—C41—C42—C43 | -1.3 (12) |
| N2—C9—C10—C33 | -177.15 (18) | C41—C42—C43—C44 | 1.1 (11) |
| C8—C9—C10—C33 | 0.5 (3) | C40—C39—C44—C43 | -4.6 (16) |
| C14—N3—C11—C10 | -178.68 (19) | C15—C39—C44—C43 | -177.4 (8) |
| Cd1—N3—C11—C10 | 16.6 (3) | C42—C43—C44—C39 | 1.9 (11) |
| C14—N3—C11—C12 | -0.3 (2) | C16—C15—C45—C50 | -90 (3) |
| Cd1—N3—C11—C12 | -164.99 (13) | C14—C15—C45—C50 | 93 (3) |
| C9—C10—C11—N3 | 6.5 (3) | C16—C15—C45—C46 | 69 (3) |
| C33—C10—C11—N3 | -176.04 (18) | C14—C15—C45—C46 | -107 (3) |
| C9—C10—C11—C12 | -171.6 (2) | C50—C45—C46—C47 | -17 (4) |
| C33—C10—C11—C12 | 5.8 (3) | C15—C45—C46—C47 | -177 (2) |
| N3—C11—C12—C13 | 0.1 (2) | C45—C46—C47—C48 | 4 (3) |

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| C10—C11—C12—C13 | 178.5 (2) | C46—C47—C48—C49 | 8 (3) |
| C11—C12—C13—C14 | 0.1 (2) | C47—C48—C49—C50 | -6 (3) |
| C11—N3—C14—C15 | 178.69 (19) | C46—C45—C50—C49 | 20 (4) |
| Cd1—N3—C14—C15 | -16.9 (3) | C15—C45—C50—C49 | 180 (2) |
| C11—N3—C14—C13 | 0.4 (2) | C48—C49—C50—C45 | -8 (3) |
| Cd1—N3—C14—C13 | 164.82 (14) | C54—N6—C51—N5 | -0.9 (3) |
| C12—C13—C14—N3 | -0.3 (2) | C55B—N6—C51—N5 | 174.7 (2) |
| C12—C13—C14—C15 | -178.6 (2) | C55A—N6—C51—N5 | 174.7 (2) |
| N3—C14—C15—C16 | -5.2 (3) | C54—N6—C51—Ag2 | 175.85 (17) |
| C13—C14—C15—C16 | 172.9 (2) | C55B—N6—C51—Ag2 | -8.5 (3) |
| N3—C14—C15—C39 | 178.7 (3) | C55A—N6—C51—Ag2 | -8.5 (3) |
| C13—C14—C15—C39 | -3.3 (4) | C53—N5—C51—N6 | 0.6 (3) |
| N3—C14—C15—C45 | 171.2 (7) | C52—N5—C51—N6 | 179.1 (2) |
| C13—C14—C15—C45 | -10.8 (7) | C53—N5—C51—Ag2 | -175.94 (18) |
| C19—N4—C16—C15 | -176.8 (2) | C52—N5—C51—Ag2 | 2.6 (3) |
| Cd1—N4—C16—C15 | 23.8 (3) | C51—N5—C53—C54 | -0.1 (3) |
| C19—N4—C16—C17 | 1.2 (2) | C52—N5—C53—C54 | -178.6 (2) |
| Cd1—N4—C16—C17 | -158.20 (15) | N5—C53—C54—N6 | -0.5 (3) |
| C14—C15—C16—N4 | 1.3 (4) | C51—N6—C54—C53 | 0.9 (3) |
| C39—C15—C16—N4 | 177.5 (3) | C55B—N6—C54—C53 | -174.8 (2) |
| C45—C15—C16—N4 | -174.9 (7) | C55A—N6—C54—C53 | -174.8 (2) |
| C14—C15—C16—C17 | -176.4 (2) | C51—N6—C55A—C56 | -102.6 (3) |
| C39—C15—C16—C17 | -0.2 (4) | C54—N6—C55A—C56 | 72.5 (3) |
| C45—C15—C16—C17 | 7.4 (8) | N6—C55A—C56—C57 | 62.4 (4) |
| N4—C16—C17—C18 | -0.9 (3) | C51—N6—C55B—C58 | -65.1 (4) |
| C15—C16—C17—C18 | 177.1 (2) | C54—N6—C55B—C58 | 110.1 (4) |
| C16—C17—C18—C19 | 0.3 (3) | N6—C55B—C58—C59 | -61.8 (6) |
| C16—N4—C19—C20 | 176.82 (19) | C62—N7—C60—N8 | -0.9 (3) |
| Cd1—N4—C19—C20 | -23.6 (3) | C61—N7—C60—N8 | 176.4 (3) |
| C16—N4—C19—C18 | -1.0 (2) | C62—N7—C60—Ag2 | 176.5 (2) |
| Cd1—N4—C19—C18 | 158.55 (14) | C61—N7—C60—Ag2 | -6.2 (4) |
| C17—C18—C19—N4 | 0.4 (3) | C63—N8—C60—N7 | 1.5 (3) |
| C17—C18—C19—C20 | -177.4 (2) | C64B—N8—C60—N7 | -175.5 (2) |
| N1—C1—C20—C19 | 7.1 (3) | C64A—N8—C60—N7 | -175.5 (2) |
| C2—C1—C20—C19 | -167.7 (2) | C63—N8—C60—Ag2 | -175.95 (19) |
| N1—C1—C20—C21 | -177.19 (18) | C64B—N8—C60—Ag2 | 7.0 (4) |
| C2—C1—C20—C21 | 8.1 (3) | C64A—N8—C60—Ag2 | 7.0 (4) |
| N4—C19—C20—C1 | -1.9 (3) | C60—N7—C62—C63 | 0.0 (3) |
| C18—C19—C20—C1 | 175.6 (2) | C61—N7—C62—C63 | -177.3 (3) |
| N4—C19—C20—C21 | -177.64 (19) | N7—C62—C63—N8 | 0.9 (3) |
| C18—C19—C20—C21 | -0.1 (3) | C60—N8—C63—C62 | -1.6 (3) |
| C1—C20—C21—C26 | 71.7 (3) | C64B—N8—C63—C62 | 175.5 (2) |
| C19—C20—C21—C26 | -112.1 (2) | C64A—N8—C63—C62 | 175.5 (2) |
| C1—C20—C21—C22 | -109.8 (2) | C60—N8—C64A—C65 | -102.4 (3) |
| C19—C20—C21—C22 | 66.4 (3) | C63—N8—C64A—C65 | 81.0 (3) |
| C26—C21—C22—C23 | 0.5 (3) | N8—C64A—C65—C66 | 65.4 (4) |
| C20—C21—C22—C23 | -178.0 (2) | C60—N8—C64B—C67 | -74.2 (10) |
| C21—C22—C23—C24 | 0.0 (4) | C63—N8—C64B—C67 | 109.2 (10) |

C22—C23—C24—C25

-0.3 (4)

N8—C64B—C67—C68

-44 (3)
