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{μ-6,6′-Dimethoxy-2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocopper(II)samarium(III) acetone solvate

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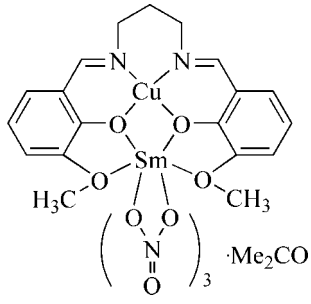
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.026; wR factor = 0.062; data-to-parameter ratio = 16.3.

In the title complex, $[CuSm(C_{19}H_{20}N_2O_4)(NO_3)_3]\cdot CH_3COCH_3$, the Cu^{II} atom is four-coordinated in a square-planar geometry by two O atoms and two N atoms of the deprotonated Schiff base. The Sm^{III} atom is ten-coordinate, chelated by three nitrate groups and linked to the four O atoms of the deprotonated Schiff base.

Related literature

See Elmali & Elerman (2003, 2004) for similar copper–lanthanum complexes of the same Schiff base.



Experimental

Crystal data

$[CuSm(C_{19}H_{20}N_2O_4)(NO_3)_3]\cdot C_3H_6O$
M_r = 798.37
Triclinic, $P\overline{1}$
a = 9.384 (5) Å
b = 12.111 (5) Å
c = 13.529 (6) Å
α = 73.071 (18)°
β = 86.984 (19)°
γ = 72.346 (18)°
V = 1400.5 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.91 mm^{-1}
T = 295 (2) K
0.33 × 0.30 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.446, T_{max} = 0.610
(expected range = 0.420–0.575)
13938 measured reflections
6381 independent reflections
5692 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.062
S = 1.09
6381 reflections
392 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2393).

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supporting information

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{μ-6,6′-Dimethoxy-2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}trinitratocopper(II)samarium(III) acetone solvate

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S1. Comment

As shown in Fig. 1, the octodentate Schiff base ligand links Cu and Sm atoms into a dinuclear complex through two phenolate O atoms, which is similar with the bonding reported for another copper-lanthanum complex of the same ligand (Elmali & Elerman, 2003, 2004). The Sm^{III} centre in (I) is ten-coordinated by four oxygen atoms from the ligand and six oxygen atoms from three nitrate ions. The Cu^{II} center is four-coordinate by two nitrogen atoms and two oxygen atoms from the ligand. And one molecular acetone is dissociative in the complex.

S2. Experimental

The title complex was obtained by the treatment of copper(II) acetate monohydrate with the Schiff base in methanol/acetone (4:1) at room temperature. Then the mixture was refluxed for 3 h after the addition of samarium (III) nitrate hexahydrate. The reaction mixture was cooled and filtered; diethyl ether was allowed to diffuse slowly into the solution of the filtrate. Single crystals were obtained after several days. Analysis calculated for $C_{22}H_{26}CuN_5O_{14}Sm$: C, 33.28; H, 3.12; Cu, 7.91; N, 8.88; Sm, 18.86; found: C, 33.10; H, 3.28; Cu, 7.96; N, 8.77; Sm, 18.83%.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C), C—H = 0.97 Å (methylene C), C—H = 0.98 Å (methine C), and with U_{iso}(H) = 1.2Ueq(C) or C—H = 0.96 Å (methly C) and with U_{iso}(H) = 1.5Ueq(C). In complex (I), the diaminopropane is disordered and was refined with a split model over two positions, and with an occupancy of 0.289 (11) for C8, C9, C10, and 0.711 (11) for C8′, C9′, C10′.

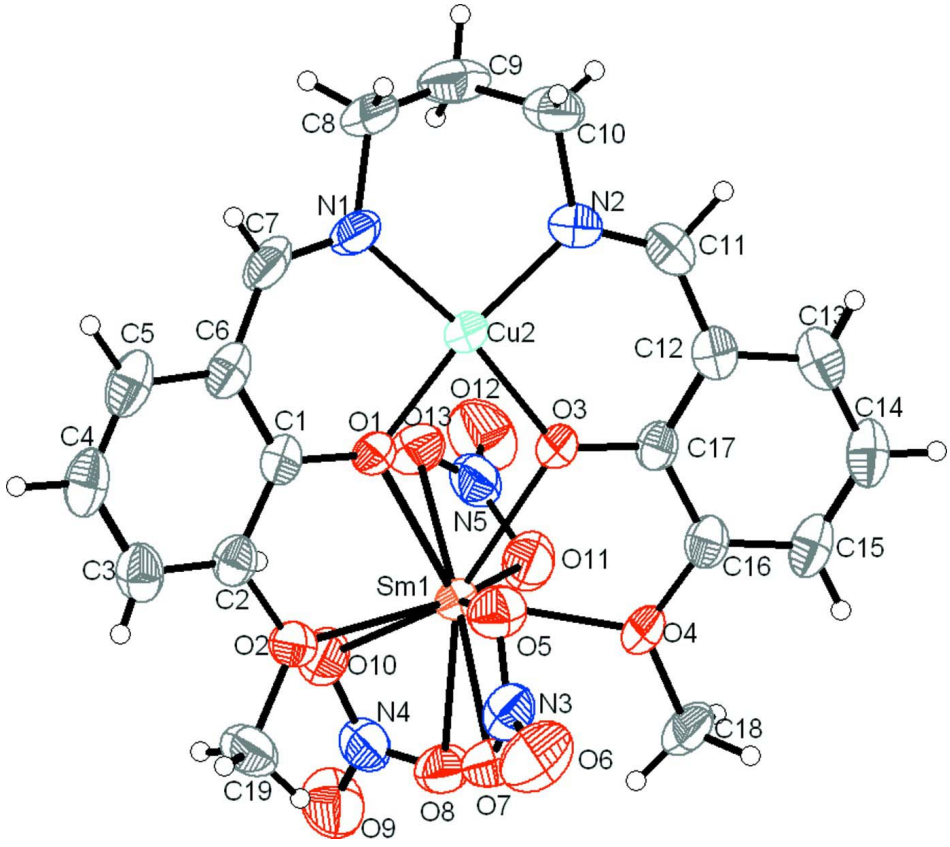

Figure 1

The molecular structure of (I), showing 40% probability displacement ellipsoids. All H atoms and actone molecule have been omitted for clarity.

{*μ*-6,6′-Dimethoxy-2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}*τ*rinitratocopper(II)samarium(III) acetone solvate

Crystal data

$[CuSm(C_{19}H_{20}N_2O_4)(NO_3)_3]\cdot C_3H_6O$
$M_r = 798.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.384\ (5)$ Å
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$c = 13.529\ (6)$ Å
$\alpha = 73.071\ (18)°$
$\beta = 86.984\ (19)°$
$\gamma = 72.346\ (18)°$
$V = 1400.5\ (11)$ Å^3
$Z = 2$
$F(000) = 792$
$D_x = 1.893$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 12555 reflections
$\theta = 6.3–55.0°$
$\mu = 2.91$ mm^{-1}
$T = 295$ K
Block, green
0.33 × 0.30 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.446$, $T_{max} = 0.610$
13938 measured reflections
6381 independent reflections

5692 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.7°$, $\theta_{min} = 3.2°$
$h = -12 \rightarrow 12$
$k = -15 \rightarrow 15$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.062$
$S = 1.09$
6381 reflections
392 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0234P)^2 + 0.9589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5501 (3)	0.7332 (2)	0.4170 (2)	0.0360 (6)
C2	0.6420 (3)	0.7711 (2)	0.3375 (2)	0.0380 (6)
C3	0.7936 (3)	0.7349 (3)	0.3504 (3)	0.0465 (7)
H1	0.8522	0.7622	0.2969	0.056*
C4	0.8598 (4)	0.6566 (3)	0.4449 (3)	0.0537 (9)
H2	0.9634	0.6310	0.4546	0.064*
C5	0.7740 (4)	0.6175 (3)	0.5226 (3)	0.0527 (8)
H3	0.8195	0.5648	0.5852	0.063*
C6	0.6162 (3)	0.6554 (3)	0.5105 (2)	0.0422 (7)
C7	0.5318 (4)	0.6060 (3)	0.5936 (2)	0.0490 (8)
H4	0.5879	0.5478	0.6504	0.059*
C8	0.3395 (5)	0.5602 (4)	0.6970 (3)	0.0819 (14)
H5	0.3455	0.5953	0.7520	0.098*
H6	0.4067	0.4780	0.7162	0.098*
C9	0.1820 (5)	0.5565 (3)	0.6872 (3)	0.0663 (11)
H7	0.1718	0.5328	0.6260	0.080*
H8	0.1627	0.4960	0.7468	0.080*
C10	0.0698 (4)	0.6750 (3)	0.6799 (2)	0.0538 (8)
H9	−0.0281	0.6636	0.6933	0.065*
H10	0.0937	0.7071	0.7326	0.065*
C11	−0.0655 (3)	0.8406 (3)	0.5481 (2)	0.0424 (7)
H11	−0.1403	0.8359	0.5956	0.051*

C12	−0.1089 (3)	0.9324 (3)	0.4522 (2)	0.0384 (6)
C13	−0.2583 (4)	1.0074 (3)	0.4383 (3)	0.0497 (8)
H12	−0.3221	0.9999	0.4932	0.060*
C14	−0.3108 (4)	1.0906 (3)	0.3460 (3)	0.0533 (8)
H13	−0.4098	1.1394	0.3381	0.064*
C15	−0.2161 (3)	1.1026 (3)	0.2633 (3)	0.0470 (7)
H14	−0.2519	1.1588	0.1998	0.056*
C16	−0.0682 (3)	1.0303 (2)	0.2762 (2)	0.0376 (6)
C17	−0.0128 (3)	0.9440 (2)	0.3701 (2)	0.0340 (6)
C18	−0.0188 (4)	1.1099 (3)	0.0970 (3)	0.0576 (9)
H15	−0.0858	1.0772	0.0718	0.086*
H16	0.0640	1.1107	0.0523	0.086*
H17	−0.0709	1.1909	0.0983	0.086*
C19	0.6504 (4)	0.8849 (4)	0.1599 (3)	0.0568 (9)
H18	0.7168	0.9218	0.1802	0.085*
H19	0.5843	0.9427	0.1042	0.085*
H20	0.7078	0.8167	0.1376	0.085*
C20	0.1935 (7)	0.3884 (5)	−0.0090 (5)	0.1100 (19)
H21	0.1201	0.4099	−0.0636	0.165*
H22	0.1525	0.3581	0.0562	0.165*
H23	0.2805	0.3270	−0.0197	0.165*
C21	0.2360 (6)	0.4971 (4)	−0.0088 (4)	0.0800 (13)
C22	0.3365 (7)	0.4818 (5)	0.0816 (4)	0.1022 (18)
H24	0.3632	0.5547	0.0722	0.153*
H25	0.4256	0.4154	0.0852	0.153*
H26	0.2844	0.4658	0.1447	0.153*
Cu2	0.24465 (4)	0.75758 (3)	0.49629 (3)	0.03670 (8)
N1	0.3895 (3)	0.6310 (2)	0.60036 (19)	0.0498 (7)
N2	0.0646 (3)	0.7631 (2)	0.57760 (18)	0.0402 (5)
N3	0.3263 (3)	1.1105 (2)	0.2284 (2)	0.0510 (7)
N4	0.3808 (3)	0.8126 (3)	0.0426 (2)	0.0478 (6)
N5	0.1427 (3)	0.6889 (3)	0.2369 (2)	0.0528 (7)
O1	0.4021 (2)	0.77107 (19)	0.39863 (15)	0.0439 (5)
O2	0.5643 (2)	0.84507 (19)	0.24634 (16)	0.0447 (5)
O3	0.1281 (2)	0.87450 (18)	0.37652 (15)	0.0411 (5)
O4	0.0358 (2)	1.03583 (18)	0.20020 (16)	0.0436 (5)
O5	0.3167 (3)	1.0333 (2)	0.31093 (18)	0.0543 (6)
O6	0.3339 (4)	1.2091 (2)	0.2275 (2)	0.0787 (9)
O7	0.3255 (3)	1.0798 (2)	0.14667 (18)	0.0535 (6)
O8	0.3018 (3)	0.9182 (2)	0.04383 (17)	0.0524 (5)
O9	0.4101 (3)	0.7863 (3)	−0.0366 (2)	0.0736 (8)
O10	0.4267 (3)	0.7385 (2)	0.12933 (19)	0.0545 (6)
O11	0.0985 (3)	0.7954 (2)	0.1774 (2)	0.0568 (6)
O12	0.0852 (4)	0.6118 (3)	0.2345 (3)	0.0822 (9)
O13	0.2480 (3)	0.6667 (2)	0.2982 (2)	0.0590 (6)
O14	0.2011 (5)	0.5883 (3)	−0.0775 (3)	0.1208 (15)
Sm1	0.286846 (16)	0.877380 (13)	0.233252 (11)	0.03533 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0338 (14)	0.0327 (13)	0.0389 (14)	−0.0044 (11)	−0.0040 (11)	−0.0115 (12)
C2	0.0372 (15)	0.0340 (13)	0.0426 (15)	−0.0094 (11)	−0.0013 (12)	−0.0117 (12)
C3	0.0372 (16)	0.0438 (16)	0.063 (2)	−0.0129 (13)	0.0002 (14)	−0.0205 (16)
C4	0.0359 (16)	0.0490 (18)	0.075 (2)	−0.0042 (14)	−0.0133 (16)	−0.0223 (18)
C5	0.0488 (19)	0.0469 (17)	0.055 (2)	0.0011 (14)	−0.0207 (16)	−0.0163 (16)
C6	0.0437 (16)	0.0355 (14)	0.0418 (16)	−0.0010 (12)	−0.0114 (13)	−0.0120 (13)
C7	0.054 (2)	0.0409 (15)	0.0349 (15)	0.0064 (14)	−0.0118 (14)	−0.0049 (13)
C8	0.084 (3)	0.067 (2)	0.045 (2)	0.009 (2)	0.012 (2)	0.0240 (18)
C9	0.112 (4)	0.0417 (17)	0.0437 (19)	−0.033 (2)	0.014 (2)	−0.0017 (15)
C10	0.060 (2)	0.065 (2)	0.0346 (16)	−0.0272 (17)	0.0042 (14)	−0.0029 (15)
C11	0.0416 (16)	0.0494 (16)	0.0441 (16)	−0.0206 (13)	0.0115 (13)	−0.0198 (14)
C12	0.0362 (15)	0.0393 (14)	0.0442 (16)	−0.0129 (12)	0.0015 (12)	−0.0174 (13)
C13	0.0403 (17)	0.0566 (19)	0.059 (2)	−0.0135 (14)	0.0077 (15)	−0.0286 (17)
C14	0.0332 (16)	0.0585 (19)	0.067 (2)	−0.0022 (14)	−0.0076 (15)	−0.0275 (18)
C15	0.0414 (17)	0.0416 (15)	0.0527 (18)	0.0004 (13)	−0.0143 (14)	−0.0164 (14)
C16	0.0365 (15)	0.0346 (13)	0.0420 (15)	−0.0074 (11)	−0.0021 (12)	−0.0144 (12)
C17	0.0315 (13)	0.0328 (13)	0.0378 (14)	−0.0079 (10)	−0.0037 (11)	−0.0115 (11)
C18	0.061 (2)	0.0499 (18)	0.0401 (17)	0.0023 (16)	−0.0113 (15)	0.0023 (15)
C19	0.051 (2)	0.070 (2)	0.052 (2)	−0.0303 (17)	0.0147 (16)	−0.0114 (18)
C20	0.117 (5)	0.084 (3)	0.109 (4)	−0.019 (3)	−0.038 (4)	−0.003 (3)
C21	0.099 (4)	0.056 (2)	0.063 (3)	−0.003 (2)	0.019 (2)	−0.010 (2)
C22	0.153 (6)	0.071 (3)	0.081 (3)	−0.034 (3)	0.015 (3)	−0.022 (3)
Cu2	0.03880 (19)	0.03451 (16)	0.02912 (16)	−0.00780 (14)	−0.00024 (14)	−0.00084 (14)
N1	0.0625 (18)	0.0373 (13)	0.0317 (13)	−0.0001 (12)	0.0018 (12)	0.0014 (11)
N2	0.0490 (15)	0.0431 (13)	0.0323 (12)	−0.0213 (11)	0.0042 (11)	−0.0092 (11)
N3	0.0517 (16)	0.0426 (14)	0.0546 (17)	−0.0123 (12)	−0.0041 (13)	−0.0090 (13)
N4	0.0424 (15)	0.0607 (17)	0.0417 (15)	−0.0184 (13)	0.0044 (12)	−0.0147 (13)
N5	0.0500 (17)	0.0454 (15)	0.0623 (18)	−0.0177 (13)	0.0185 (14)	−0.0138 (14)
O1	0.0326 (10)	0.0514 (12)	0.0324 (10)	−0.0059 (9)	−0.0036 (8)	0.0044 (9)
O2	0.0373 (11)	0.0522 (12)	0.0375 (11)	−0.0141 (9)	0.0013 (9)	−0.0015 (9)
O3	0.0360 (11)	0.0396 (10)	0.0342 (10)	−0.0018 (8)	0.0006 (8)	−0.0005 (9)
O4	0.0397 (11)	0.0387 (10)	0.0376 (11)	−0.0001 (8)	−0.0067 (9)	0.0004 (9)
O5	0.0666 (16)	0.0520 (13)	0.0429 (12)	−0.0183 (11)	0.0025 (11)	−0.0113 (11)
O6	0.105 (2)	0.0482 (14)	0.085 (2)	−0.0268 (15)	−0.0138 (18)	−0.0155 (14)
O7	0.0694 (16)	0.0457 (12)	0.0414 (12)	−0.0210 (11)	0.0005 (11)	−0.0025 (10)
O8	0.0641 (15)	0.0494 (12)	0.0365 (11)	−0.0139 (11)	0.0023 (10)	−0.0052 (10)
O9	0.0754 (19)	0.098 (2)	0.0495 (15)	−0.0150 (16)	0.0049 (13)	−0.0367 (16)
O10	0.0538 (14)	0.0500 (13)	0.0507 (14)	−0.0041 (10)	−0.0009 (11)	−0.0126 (11)
O11	0.0489 (14)	0.0500 (13)	0.0649 (16)	−0.0132 (10)	−0.0024 (11)	−0.0077 (12)
O12	0.085 (2)	0.0648 (17)	0.115 (3)	−0.0453 (16)	0.0311 (19)	−0.0355 (18)
O13	0.0676 (17)	0.0407 (12)	0.0568 (15)	−0.0125 (11)	0.0042 (13)	−0.0008 (11)
O14	0.180 (4)	0.069 (2)	0.076 (2)	−0.009 (2)	−0.003 (2)	0.0073 (18)
Sm1	0.03475 (8)	0.03416 (8)	0.02833 (8)	−0.00614 (5)	−0.00093 (5)	0.00000 (5)

Geometric parameters (Å, º)

C1—O1	1.335 (3)	C18—H15	0.9600
C1—C6	1.381 (4)	C18—H16	0.9600
C1—C2	1.402 (4)	C18—H17	0.9600
C2—C3	1.360 (4)	C19—O2	1.436 (4)
C2—O2	1.382 (4)	C19—H18	0.9600
C3—C4	1.393 (5)	C19—H19	0.9600
C3—H1	0.9300	C19—H20	0.9600
C4—C5	1.353 (5)	C20—C21	1.488 (7)
C4—H2	0.9300	C20—H21	0.9600
C5—C6	1.414 (4)	C20—H22	0.9600
C5—H3	0.9300	C20—H23	0.9600
C6—C7	1.433 (5)	C21—O14	1.186 (5)
C7—N1	1.281 (4)	C21—C22	1.518 (7)
C7—H4	0.9300	C22—H24	0.9600
C8—N1	1.481 (4)	C22—H25	0.9600
C8—C9	1.506 (6)	C22—H26	0.9600
C8—H5	0.9700	Cu2—O3	1.933 (2)
C8—H6	0.9700	Cu2—O1	1.942 (2)
C9—C10	1.479 (5)	Cu2—N2	1.962 (3)
C9—H7	0.9700	Cu2—N1	1.965 (3)
C9—H8	0.9700	N3—O6	1.215 (4)
C10—N2	1.474 (4)	N3—O5	1.249 (4)
C10—H9	0.9700	N3—O7	1.265 (4)
C10—H10	0.9700	N4—O9	1.201 (3)
C11—N2	1.291 (4)	N4—O10	1.254 (3)
C11—C12	1.424 (4)	N4—O8	1.274 (3)
C11—H11	0.9300	N5—O12	1.221 (4)
C12—C17	1.395 (4)	N5—O13	1.238 (4)
C12—C13	1.407 (4)	N5—O11	1.261 (4)
C13—C14	1.359 (5)	O1—Sm1	2.359 (2)
C13—H12	0.9300	O2—Sm1	2.520 (2)
C14—C15	1.393 (5)	O3—Sm1	2.380 (2)
C14—H13	0.9300	O4—Sm1	2.510 (2)
C15—C16	1.386 (4)	O5—Sm1	2.501 (2)
C15—H14	0.9300	O7—Sm1	2.517 (2)
C16—O4	1.381 (4)	O8—Sm1	2.469 (2)
C16—C17	1.394 (4)	O10—Sm1	2.525 (2)
C17—O3	1.326 (3)	O11—Sm1	2.515 (3)
C18—O4	1.443 (4)	O13—Sm1	2.577 (3)
O1—C1—C6	122.4 (3)	H25—C22—H26	109.5
O1—C1—C2	118.8 (3)	O3—Cu2—O1	79.81 (9)
C6—C1—C2	118.7 (3)	O3—Cu2—N2	91.27 (10)
C3—C2—O2	124.3 (3)	O1—Cu2—N2	171.07 (9)
C3—C2—C1	121.9 (3)	O3—Cu2—N1	169.89 (10)
O2—C2—C1	113.8 (2)	O1—Cu2—N1	90.75 (11)

C2—C3—C4	119.1 (3)	N2—Cu2—N1	98.18 (12)
C2—C3—H1	120.4	C7—N1—C8	114.6 (3)
C4—C3—H1	120.4	C7—N1—Cu2	124.2 (2)
C5—C4—C3	120.2 (3)	C8—N1—Cu2	121.2 (2)
C5—C4—H2	119.9	C11—N2—C10	114.6 (3)
C3—C4—H2	119.9	C11—N2—Cu2	124.6 (2)
C4—C5—C6	121.2 (3)	C10—N2—Cu2	120.8 (2)
C4—C5—H3	119.4	O6—N3—O5	121.5 (3)
C6—C5—H3	119.4	O6—N3—O7	122.7 (3)
C1—C6—C5	118.8 (3)	O5—N3—O7	115.9 (3)
C1—C6—C7	122.5 (3)	O9—N4—O10	122.3 (3)
C5—C6—C7	118.6 (3)	O9—N4—O8	122.0 (3)
N1—C7—C6	128.8 (3)	O10—N4—O8	115.7 (2)
N1—C7—H4	115.6	O12—N5—O13	121.7 (3)
C6—C7—H4	115.6	O12—N5—O11	122.0 (3)
N1—C8—C9	112.9 (3)	O13—N5—O11	116.3 (3)
N1—C8—H5	109.0	C1—O1—Cu2	128.75 (18)
C9—C8—H5	109.0	C1—O1—Sm1	123.53 (18)
N1—C8—H6	109.0	Cu2—O1—Sm1	107.68 (9)
C9—C8—H6	109.0	C2—O2—C19	117.3 (2)
H5—C8—H6	107.8	C2—O2—Sm1	118.50 (17)
C10—C9—C8	112.1 (3)	C19—O2—Sm1	123.5 (2)
C10—C9—H7	109.2	C17—O3—Cu2	129.08 (18)
C8—C9—H7	109.2	C17—O3—Sm1	123.76 (17)
C10—C9—H8	109.2	Cu2—O3—Sm1	107.15 (9)
C8—C9—H8	109.2	C16—O4—C18	117.2 (2)
H7—C9—H8	107.9	C16—O4—Sm1	118.80 (16)
N2—C10—C9	112.3 (3)	C18—O4—Sm1	121.66 (19)
N2—C10—H9	109.2	N3—O5—Sm1	97.49 (18)
C9—C10—H9	109.2	N3—O7—Sm1	96.27 (18)
N2—C10—H10	109.2	N4—O8—Sm1	97.71 (17)
C9—C10—H10	109.2	N4—O10—Sm1	95.60 (17)
H9—C10—H10	107.9	N5—O11—Sm1	98.4 (2)
N2—C11—C12	128.3 (3)	N5—O13—Sm1	96.02 (18)
N2—C11—H11	115.9	O1—Sm1—O3	63.27 (8)
C12—C11—H11	115.9	O1—Sm1—O8	148.32 (8)
C17—C12—C13	119.5 (3)	O3—Sm1—O8	146.44 (8)
C17—C12—C11	122.5 (3)	O1—Sm1—O5	73.64 (8)
C13—C12—C11	117.8 (3)	O3—Sm1—O5	73.43 (8)
C14—C13—C12	121.1 (3)	O8—Sm1—O5	117.84 (8)
C14—C13—H12	119.5	O1—Sm1—O4	124.51 (7)
C12—C13—H12	119.5	O3—Sm1—O4	64.03 (7)
C13—C14—C15	119.9 (3)	O8—Sm1—O4	87.13 (8)
C13—C14—H13	120.0	O5—Sm1—O4	76.07 (8)
C15—C14—H13	120.0	O1—Sm1—O11	115.72 (8)
C16—C15—C14	119.6 (3)	O3—Sm1—O11	80.42 (8)
C16—C15—H14	120.2	O8—Sm1—O11	73.58 (9)
C14—C15—H14	120.2	O5—Sm1—O11	144.02 (8)

O4—C16—C15	124.5 (3)	O4—Sm1—O11	70.38 (8)
O4—C16—C17	114.3 (2)	O1—Sm1—O7	117.15 (8)
C15—C16—C17	121.2 (3)	O3—Sm1—O7	114.49 (8)
O3—C17—C16	118.4 (3)	O8—Sm1—O7	67.60 (8)
O3—C17—C12	123.0 (3)	O5—Sm1—O7	50.26 (8)
C16—C17—C12	118.6 (3)	O4—Sm1—O7	71.58 (8)
O4—C18—H15	109.5	O11—Sm1—O7	125.99 (8)
O4—C18—H16	109.5	O1—Sm1—O2	64.43 (7)
H15—C18—H16	109.5	O3—Sm1—O2	123.87 (7)
O4—C18—H17	109.5	O8—Sm1—O2	89.45 (8)
H15—C18—H17	109.5	O5—Sm1—O2	73.80 (8)
H16—C18—H17	109.5	O4—Sm1—O2	143.74 (7)
O2—C19—H18	109.5	O11—Sm1—O2	142.17 (8)
O2—C19—H19	109.5	O7—Sm1—O2	73.77 (8)
H18—C19—H19	109.5	O1—Sm1—O10	100.83 (8)
O2—C19—H20	109.5	O3—Sm1—O10	139.45 (8)
H18—C19—H20	109.5	O8—Sm1—O10	50.74 (8)
H19—C19—H20	109.5	O5—Sm1—O10	141.10 (8)
C21—C20—H21	109.5	O4—Sm1—O10	130.89 (7)
C21—C20—H22	109.5	O11—Sm1—O10	73.75 (9)
H21—C20—H22	109.5	O7—Sm1—O10	105.97 (8)
C21—C20—H23	109.5	O2—Sm1—O10	69.44 (8)
H21—C20—H23	109.5	O1—Sm1—O13	69.00 (8)
H22—C20—H23	109.5	O3—Sm1—O13	71.58 (8)
O14—C21—C20	122.5 (5)	O8—Sm1—O13	104.97 (8)
O14—C21—C22	121.5 (5)	O5—Sm1—O13	137.17 (8)
C20—C21—C22	115.9 (4)	O4—Sm1—O13	108.91 (9)
C21—C22—H24	109.5	O11—Sm1—O13	49.23 (8)
C21—C22—H25	109.5	O7—Sm1—O13	172.57 (8)
H24—C22—H25	109.5	O2—Sm1—O13	106.84 (8)
C21—C22—H26	109.5	O10—Sm1—O13	67.87 (9)
H24—C22—H26	109.5		