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Supporting Information

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Voltammetric Characterization of Redox-Inactive Guest Binding to Ln^{III}[15-Metallacrown-5] Hosts Based on Competition with a Redox Probe

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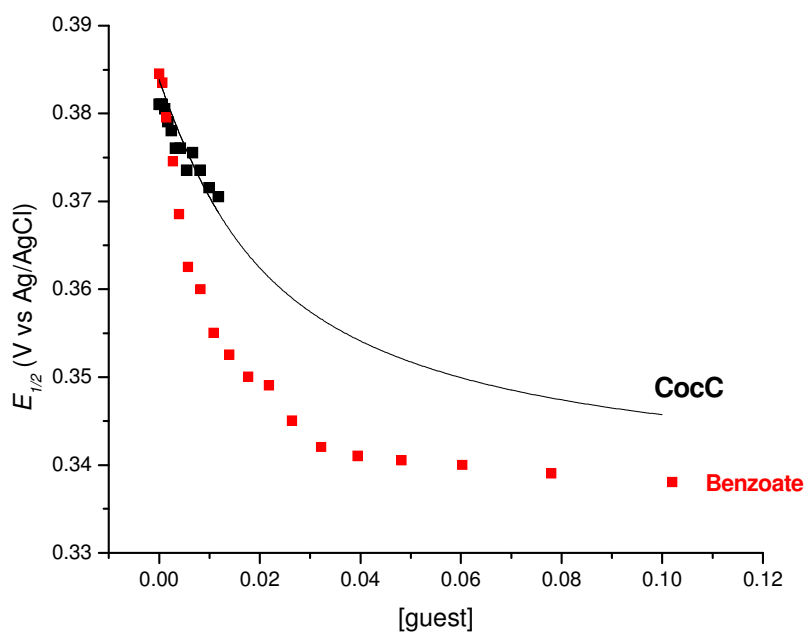


Figure S1: Plots showing competitive binding curves for benzoate (red squares) and CocC (black squares). The limited solubility of CocC allows only a small portion of the competition curve to be generated, so the accuracy of these fits is uncertain. In contrast, the complete displacement of FcC^- was achieved with benzoate, so the full curve could be generated. The displayed fit is for CocC, and was determined using K_{red} values calculated under the assumption that K_{ox} is zero.

S2

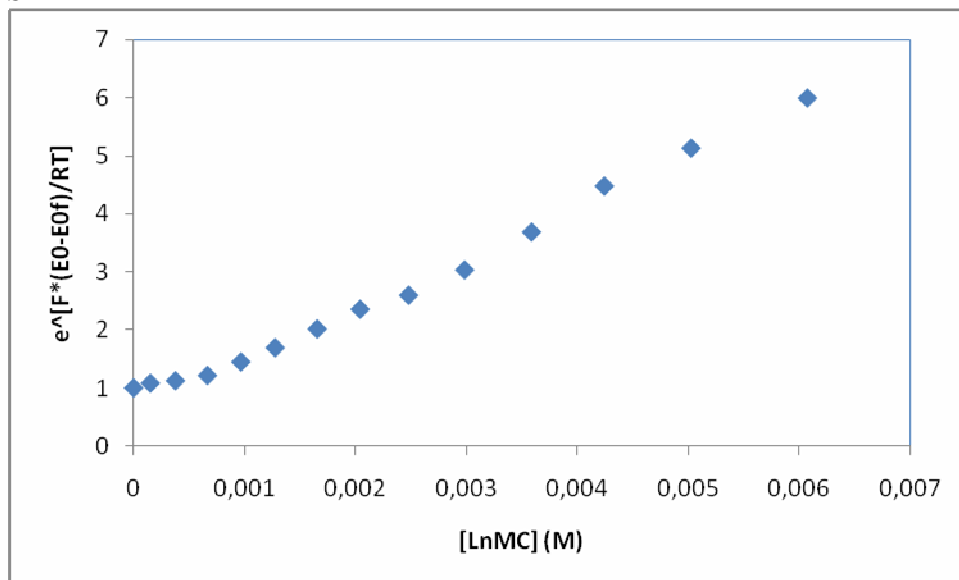


Figure S2: Plot of $e^{[F^*(E_0-E_{0f})/RT]}$ vs. $[DyMC]$. This plot helps assess the influence of K_{ox} on the observed electrochemical behaviour during the titration of DyMC to FcC^+ . If K_{ox} were negligible, the plot would be linear. However, a slight curvature is evident, which reveals the significant influence of K_{ox} .

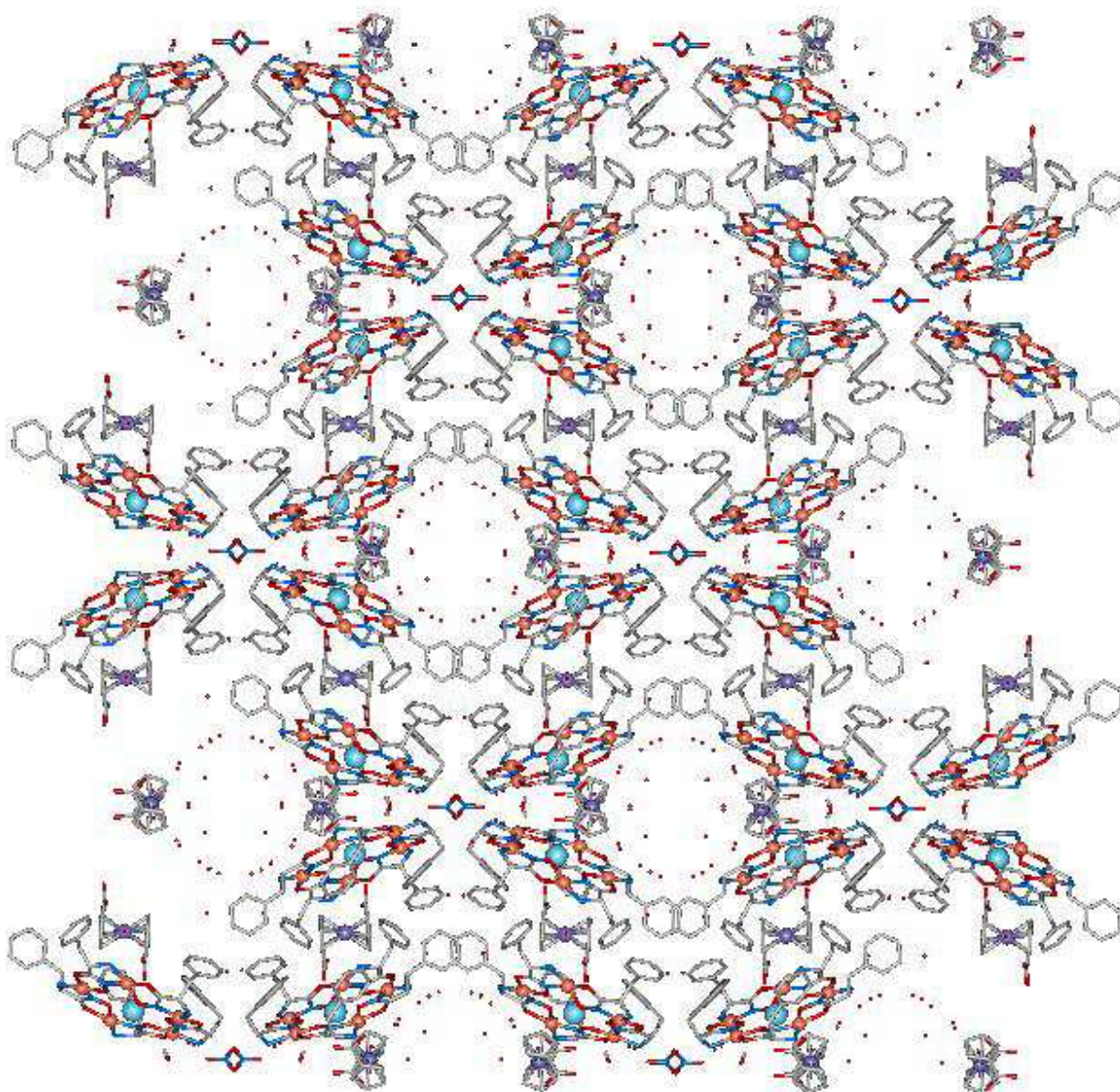
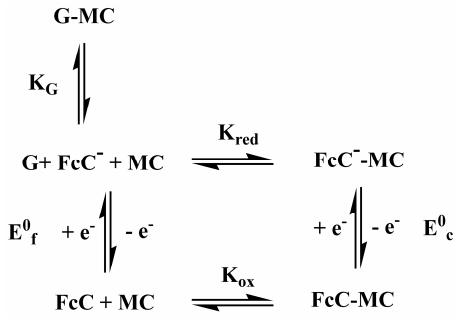


Figure S3- Packing diagram for $\text{La}^{\text{III}}(\text{FcDC}^{2-})[\text{15-MC}_{\text{Cu}^{\text{II}}, \text{N}, \text{L-phHA-5}}] (\text{NO}_3)_{0.5}(\text{HO}^-)_{0.5}$ that displays the continuous chains of LaMC compartments containing FcDC^{2-} bridged by FcDC^{2-} . An unbound nitrate and hydroxide achieve charge balance. An 11.14 Å distance separates the La^{III} central metals across the hydrophobic faces. A 9.74 Å La-La distance is observed on the hydrophilic face. Solvent filled channels are observed with a diameter of 12.4-14.6 Å depending on where the measurement is taken. Hydrogen atoms were removed for clarity. Color scheme: Red, oxygen; blue, nitrogen; grey, carbon; orange, copper, turquoise, lanthanum; purple, iron.

S5: Derivation of the CV competition titration fitting.



For the binding equilibrium between a guest molecule or FcC^- to a MC, the dissociation constants can be written as:

$$(1) K_{Dox} = \frac{[\text{FcC}^-]_f [\text{MC}]_f}{[\text{FcC}^- \text{-MC}]}$$

$$(2) K_{DG} = \frac{[\text{G}]_f [\text{MC}]_f}{[\text{G-MC}]}$$

where $[\text{FcC}^-]_f$, $[\text{MC}]_f$, $[\text{FcC}^- \text{-MC}]$ are the concentrations of unbound FcC^- , unbound MC, and the $\text{FcC}^- \text{-MC}$ complex respectively. The same nomenclature applies to equation 2.

Rearrangement of equation 2 gives:

$$(3) [\text{FcC}^-]_f = \frac{K_{D1} [\text{FcC}^- \text{-MC}]}{[\text{MC}]_f}$$

Mass balance for FcC^- gives:

$$(4) [\text{FcC}^-]_0 = [\text{FcC}^-]_f + [\text{FcC}^- \text{-MC}]$$

where $[\text{FcC}^-]_0$ is the overall concentration of FcC^- added to the solution.

Replacing $[\text{FcC}^-]_f$ with eq 4 and rearranging gives:

$$(5) [\text{FcC}^- \text{-MC}] = \frac{[\text{FcC}^-]_0 [\text{MC}]_f}{K_{D1} + [\text{MC}]_f}$$

A similar treatment for the mass balance for G gives:

$$(6) [\text{G-MC}] = \frac{[\text{G}]_0 [\text{MC}]_f}{K_{DG} + [\text{MC}]_f}$$

Mass balance for MC gives:

$$(7) [\text{MC}]_0 = [\text{MC}]_f + [\text{FcC}^- \text{-MC}] + [\text{G-MC}]$$

Inputting equation 5 and 6 into equation 7 gives

$$(8) \quad [MC]_0 = [MC]_f + \frac{[FcC^-]_0 [MC]_f}{K_{D1} + [MC]_f} + \frac{[G]_0 [MC]_f}{K_{DG} + [MC]_f}$$

Rearranging equation 8 to solve for $[MC]_f$ gives :

$$(9) \quad [MC]_f^3 + a[MC]_f^2 + [MC]_f b + c = 0$$

$$(10) \quad a = K_{D1} + K_{DG} + [FcC^-]_0 + [G]_0 - [MC]_0$$

$$(11) \quad b = K_{DG}([FcC^-]_0 - [MC]_0) + K_{D1}([G]_0 - [MC]_0) + K_{D1} \cdot K_{DG}$$

$$(12) \quad c = -K_{D1} \cdot K_{DG} [MC]_0$$

$[MC]_f$ can be solved for using the solution to this cubic equation that was reported by Wang^[104]:

$$(13) \quad [MC]_f = \frac{-a}{3} + \frac{2}{3} \sqrt{(a^2 - 3b)} \cdot \cos \left(\frac{1}{3} \arccos \left(\frac{-2a^3 + 9ab - 27c}{2 * \sqrt{(a^2 - 3b)^3}} \right) \right)$$

This allows $[MC]_f$ to be solved for explicitly using all known quantities: the overall concentration of FcC^- , G, and MC in solution, and the dissociation constant of the FcC^- -MC complex. Inputting the solution for $[MC]_f$ into equation 14 allows for the determination of K_{DG} based on the electrochemical potential of FcC^- in the presence of MC and G.

$$(14) \quad E^0 = E^0_f + \frac{RT}{F} \ln \left(\frac{1 + K_{red} [MC]_f}{1 + K_{ox} [MC]_f} \right)$$

The derivation of equation 14 has been previously reported.^[11d]

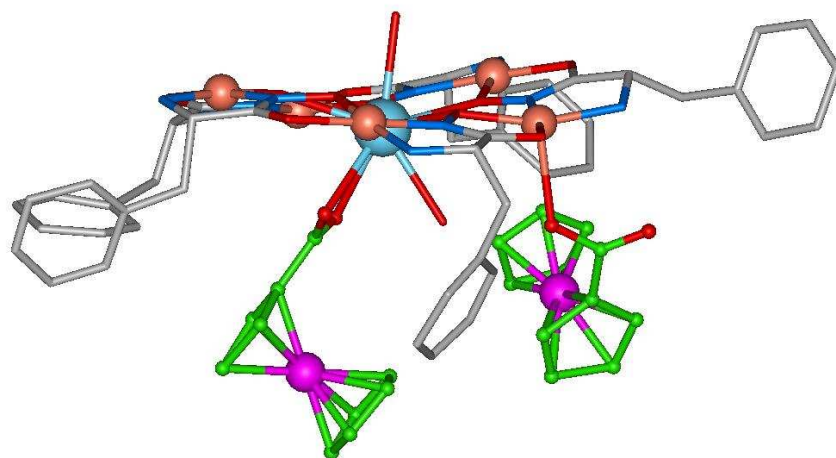


Figure S4. Weblabviewer Pro image of $\text{La}^{\text{III}}(\text{FcC}^-)_2[15\text{-MC}_{\text{Cu}^{\text{II}}, \text{N}, \text{L-phHA}^-5}](\text{NO}_3)$. Two FcC^- are encapsulated in the hydrophobic cavity (Ball and stick representation). One is bound monodentate to a copper ring metal with eclipsed cp rings. The other is bound bidentate to La^{III} with staggered cp rings. The carboxylate of FcC^- is diagonal to the MC plane when bound to the nine-coordinate La^{III} , which extends much of the ferrocene group outside of the hydrophobic cavity. Unbound or Cu-coordinated solvent, nitrate, and hydrogens were removed for clarity. Color scheme: Red, oxygen; blue, nitrogen; grey, carbon; orange, copper; turquoise, lanthanum; green, ferrocene carbon, magenta, iron.

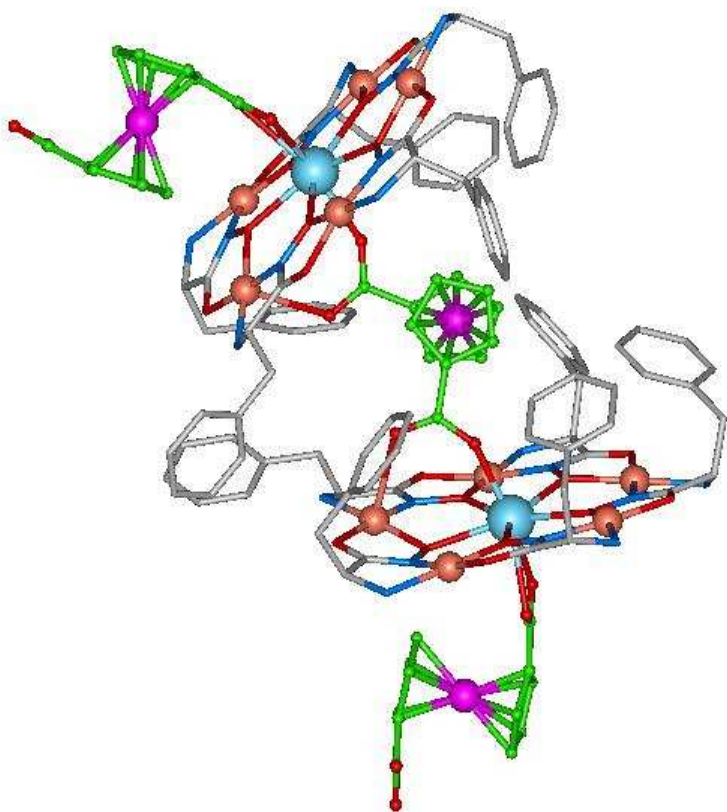


Figure S5. Weblabviewer Pro image of $\text{La}^{\text{III}}(\text{FcDC}^-)[15\text{-MC}_{\text{Cu}^{\text{II}}, \text{N}, \text{L-pheHA-5}}](\text{NO}_3)_{0.5}(\text{OH})_{0.5}$. FcDC^{2-} is bound bidentate to La^{III} and a Cu^{II} ring metal in the hydrophobic compartment. An 11.14 Å distance separates the La^{III} central metals across the hydrophobic faces. The hydrophilic faces are also bridged by FcDC^{2-} , which is bound bidentate to the central La^{III} . Hydrogens, solvent, and unbound anions were removed for clarity. Color scheme: Red, oxygen; blue, nitrogen; grey, carbon; orange, copper, turquoise, lanthanum; green, ferrocene carbon; magenta, iron.

S7

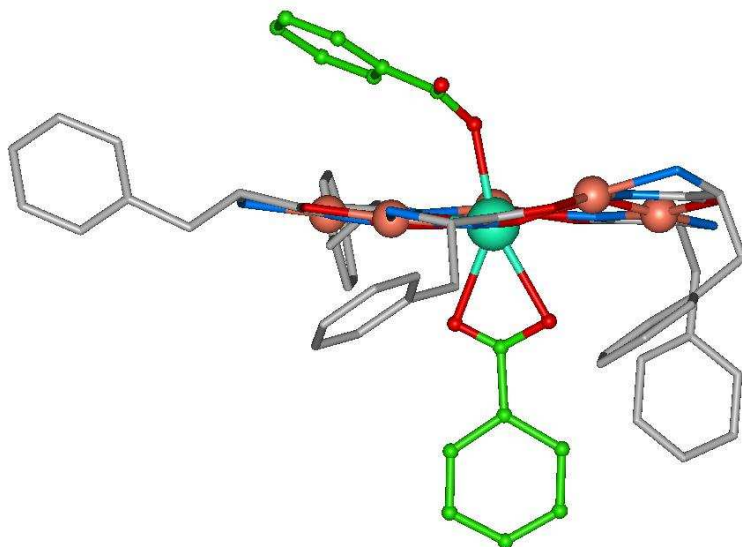


Figure S6. Weblabviewer Pro image of $\text{Dy}^{\text{III}}(\text{benzoate})_2[15\text{-MC}_{\text{Cu}^{\text{II}}, \text{N}, \text{L-pheHA-5}}](\text{benzoate})$. Benzoate is bound bidentate to the 8-coordinate Dy^{III} on the hydrophobic face and monodentate on the hydrophilic face. Benzoate is perpendicular to the metallacrowns plane when coordinated to the eight coordinate metal. Hydrogens, unbound benzoate, and unbound and Cu-coordinated solvent were removed for clarity. Color scheme: Red, oxygen; blue, nitrogen; grey, carbon; orange, copper, sea-green, dysprosium; green, benzoate carbon.

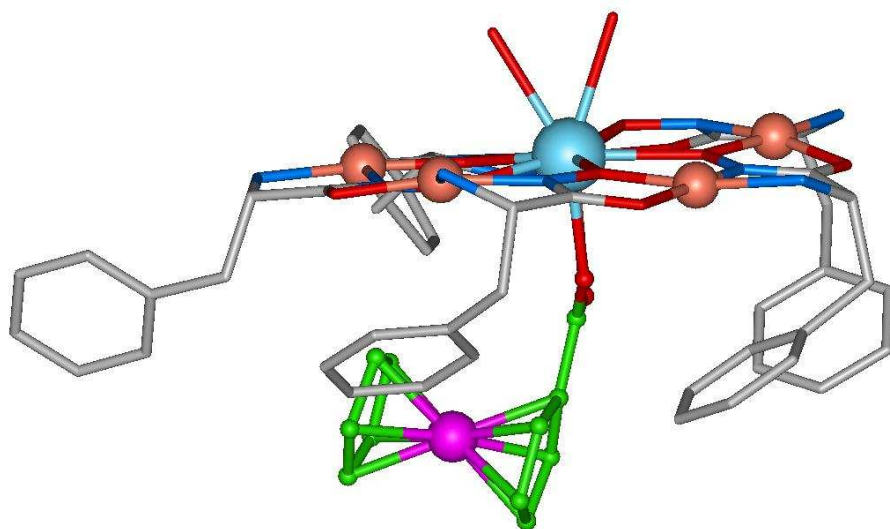


Figure S7. Weblabviewer Pro image of $\text{La}^{\text{III}}(\text{FcDC}^-)[15\text{-MC}_{\text{Cu}^{\text{II}}, \text{N}, \text{L-pheHA}^-5}](\text{NO}_3)_{0.5}(\text{OH})_{0.5}$ that highlights the orientation of the ferrocene group in the hydrophobic cavity. FcDC^- is bound bidentate to La^{III} and a Cu^{II} ring metal. The carboxylate is perpendicular to the MC-plane, which orients the ferrocene group parallel to the plane and within the cavity. The additional carboxylate on FcDC^{2-} , hydrogens, solvent, and other anions were removed for clarity. Color scheme: Red, oxygen; blue, nitrogen; grey, carbon; orange, copper, turquoise, lanthanum; green, ferrocene carbon; magenta, iron.

S9: Crystallographic tables for $\text{La}^{\text{III}}(\text{FcC}^-)_2(\text{NO}_3)[15\text{-MCL}_{\text{-pheHA-5}}]$

Crystal data and structure refinement for $\text{La}^{\text{III}}(\text{FcC}^-)_2(\text{NO}_3)[15\text{-MCL}_{\text{-pheHA-5}}]$.

Identification code	jj130f
Empirical formula	C71 H98 Cu5 Fe2 La N11 O28
Formula weight	2121.91
Temperature	85(2) K
Wavelength	0.71073 Å
Crystal system, space group	ORTHORHOMBIC, P2(1)2(1)2(1)
Unit cell dimensions	a = 16.3243(11) Å alpha = 90 deg. b = 17.5101(11) Å beta = 90 deg. c = 30.507(2) Å gamma = 90 deg.
Volume	8720.1(10) Å ³
Z, Calculated density	4, 1.616 Mg/m ³
Absorption coefficient	2.077 mm ⁻¹
F(000)	4316
Crystal size	0.45 x 0.30 x 0.22 mm
Theta range for data collection	1.71 to 29.61 deg.
Limiting indices	-22<=h<=22, -24<=k<=24, -42<=l<=42
Reflections collected / unique	405792 / 24529 [R(int) = 0.0421]
Completeness to theta = 29.61	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6579 and 0.4550
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	24529 / 840 / 1239
Goodness-of-fit on F ²	1.140

Final R indices [$I > 2\sigma(I)$] R1 = 0.0496, wR2 = 0.1364

R indices (all data) R1 = 0.0549, wR2 = 0.1431

Absolute structure parameter -0.003(15)

Largest diff. peak and hole 3.199 and -1.145 e. \AA^{-3}

Bond lengths [Å] and angles [deg] for $\text{La}^{\text{III}}(\text{FcC}^-)_2(\text{NO}_3)[15\text{-MC}_{\text{L-pheHA-5}}]$.

La(1)-O(4)	2.498(3)
La(1)-O(6)	2.514(4)
La(1)-O(10)	2.517(4)
La(1)-O(8)	2.527(4)
La(1)-O(2)	2.568(3)
La(1)-O(101)	2.5705(12)
La(1)-O(240)	2.5755
La(1)-O(19)	2.6038(10)
La(1)-O(100)	2.6198
La(1)-C(100)	2.9811(11)
Cu(1)-N(10)	1.894(5)
Cu(1)-O(2)	1.933(4)
Cu(1)-O(1)	1.942(4)
Cu(1)-N(9)	2.021(4)
Cu(2)-N(2)	1.918(4)
Cu(2)-O(4)	1.918(4)
Cu(2)-O(3)	1.939(4)
Cu(2)-N(1)	2.024(6)
Cu(2)-O(310)	2.435(6)
Cu(3)-N(4)	1.927(5)
Cu(3)-O(6)	1.932(4)
Cu(3)-O(5)	1.975(5)
Cu(3)-N(3)	2.015(5)
Cu(3)-O(250)	2.3823(12)
Cu(4)-N(6)	1.921(6)
Cu(4)-O(8)	1.920(4)
Cu(4)-O(7)	1.937(5)
Cu(4)-N(5)	2.013(6)
Cu(4)-O(420)	2.31(2)
Cu(5)-N(8)	1.918(4)
Cu(5)-O(10)	1.938(4)
Cu(5)-O(9)	1.961(4)
Cu(5)-N(7)	1.989(5)
Cu(5)-O(150)	2.4215(11)
O(1)-C(1)	1.287(7)
O(2)-N(2)	1.407(6)
O(3)-C(10)	1.290(7)

O(4)-N(4)	1.393(5)
O(5)-C(19)	1.311(8)
O(6)-N(6)	1.381(7)
O(7)-C(28)	1.299(7)
O(8)-N(8)	1.390(6)
O(9)-C(37)	1.319(7)
O(10)-N(10)	1.399(5)
N(1)-C(2)	1.485(8)
N(1)-H(1G)	0.9200
N(1)-H(1H)	0.9200
N(2)-C(1)	1.283(7)
N(3)-C(11)	1.489(9)
N(3)-H(3C)	0.9200
N(3)-H(3D)	0.9200
N(4)-C(10)	1.287(8)
N(5)-C(20)	1.496(11)
N(5)-H(5A)	0.9200
N(5)-H(5B)	0.9200
N(6)-C(19)	1.298(7)
N(7)-C(29)	1.503(8)
N(7)-H(7A)	0.9200
N(7)-H(7B)	0.9200
N(8)-C(28)	1.290(7)
N(9)-C(38)	1.498(7)
N(9)-H(9A)	0.9200
N(9)-H(9B)	0.9200
N(10)-C(37)	1.296(6)
C(1)-C(2)	1.491(9)
C(2)-C(3)	1.593(15)
C(2)-H(2)	1.0000
C(3)-C(4)	1.463(10)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.310(15)
C(4)-C(9)	1.477(15)
C(5)-C(6)	1.410(14)
C(5)-H(5)	0.9500
C(6)-C(7)	1.384(18)
C(6)-H(6)	0.9500
C(7)-C(8)	1.388(17)
C(7)-H(7)	0.9500
C(8)-C(9)	1.333(15)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.525(7)
C(11)-C(12)	1.513(9)
C(11)-H(11)	1.0000
C(12)-C(13)	1.528(15)
C(12)-C(1A)	1.571(15)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(12)-H(12C)	0.9893

C(12)-H(12D)	0.9899
C(13)-C(14)	1.33(2)
C(13)-C(18)	1.37(2)
C(14)-C(15)	1.39(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.41(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.36(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.39(3)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(1A)-C(1B)	1.355(15)
C(1A)-C(1F)	1.461(15)
C(1B)-C(1C)	1.389(16)
C(1B)-H(1B)	0.9500
C(1C)-C(1D)	1.383(18)
C(1C)-H(1C)	0.9500
C(1D)-C(1E)	1.386(17)
C(1D)-H(1D)	0.9500
C(1E)-C(1F)	1.326(16)
C(1E)-H(1E)	0.9500
C(1F)-H(1F)	0.9500
C(19)-C(20)	1.486(9)
C(20)-C(21)	1.548(13)
C(20)-H(20)	1.0000
C(21)-C(22)	1.473(15)
C(21)-C(22A)	1.592(17)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(21)-H(21C)	0.9900
C(21)-H(21D)	0.9901
C(22)-C(23)	1.353(15)
C(22)-C(27)	1.445(15)
C(23)-C(24)	1.374(15)
C(23)-H(23)	0.9500
C(24)-C(25)	1.385(17)
C(24)-H(24)	0.9500
C(25)-C(26)	1.390(17)
C(25)-H(25)	0.9500
C(26)-C(27)	1.362(15)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
Fe(1)-C(108)	1.961(6)
Fe(1)-C(109)	1.994(6)
Fe(1)-C(107)	2.007(6)
Fe(1)-C(104)	2.024(6)
Fe(1)-C(105)	2.019(7)
Fe(1)-C(102)	2.039(11)
Fe(1)-C(103)	2.053(6)
Fe(1)-C(101)	2.046(10)
Fe(1)-C(110)	2.061(7)

Fe(1)-C(106)	2.068(6)
C(101)-C(105)	1.376(11)
C(101)-C(102)	1.429(14)
C(101)-C(100)	1.491(8)
C(102)-C(103)	1.392(10)
C(102)-H(102)	0.968(12)
C(103)-C(104)	1.4199
C(103)-H(103)	0.9500
C(104)-C(105)	1.4202
C(104)-H(104)	0.9500
C(105)-H(105)	0.9500
C(106)-C(107)	1.4198
C(106)-C(110)	1.4202
C(106)-H(106)	0.9500
C(107)-C(108)	1.4205
C(107)-H(107)	0.9500
C(108)-C(109)	1.4201
C(108)-H(108)	0.9500
C(109)-C(110)	1.4202
C(109)-H(109)	0.9500
C(110)-H(110)	0.9500
C(22A)-C(22B)	1.350(18)
C(22A)-C(22F)	1.473(16)
C(22B)-C(22C)	1.399(18)
C(22B)-H(22B)	0.9500
C(22C)-C(22D)	1.379(19)
C(22C)-H(22C)	0.9500
C(22D)-C(22E)	1.388(19)
C(22D)-H(22D)	0.9500
C(22E)-C(22F)	1.348(17)
C(22E)-H(22E)	0.9500
C(22F)-H(22F)	0.9500
Fe(1A)-C(10H)	1.948(13)
Fe(1A)-C(10E)	1.951(13)
Fe(1A)-C(10I)	1.991(13)
Fe(1A)-C(10D)	2.015(13)
Fe(1A)-C(10B)	2.018(14)
Fe(1A)-C(10A)	2.022(12)
Fe(1A)-C(10G)	2.029(14)
Fe(1A)-C(10C)	2.034(12)
Fe(1A)-C(10J)	2.089(13)
Fe(1A)-C(10F)	2.097(13)
C(10A)-C(10E)	1.417(17)
C(10A)-C(10B)	1.443(16)
C(10A)-C(100)	1.627(13)
C(10B)-C(10C)	1.392(17)
C(10B)-H(10B)	0.9500
C(10C)-C(10D)	1.406(17)
C(10C)-H(10C)	0.9500
C(10D)-C(10E)	1.376(16)
C(10D)-H(10D)	0.9500
C(10E)-H(102)	1.095(17)

C(10E)-H(10E)	0.9500
C(10F)-C(10J)	1.394(17)
C(10F)-C(10G)	1.401(17)
C(10F)-H(10F)	0.9500
C(10G)-C(10H)	1.343(17)
C(10G)-H(10G)	0.9500
C(10H)-C(10I)	1.403(17)
C(10H)-H(10H)	0.9500
C(10I)-C(10J)	1.345(17)
C(10I)-H(10I)	0.9500
C(10J)-H(10J)	0.9500
C(28)-C(29)	1.499(8)
C(29)-C(30)	1.537(8)
C(29)-H(29)	1.0000
C(30)-C(31)	1.515(11)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(36)	1.359(17)
C(31)-C(32)	1.365(17)
C(32)-C(33)	1.47(2)
C(32)-H(32)	0.9500
C(33)-C(34)	1.43(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.29(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.380(14)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-C(38)	1.500(6)
C(38)-C(39)	1.509(5)
C(38)-H(38)	1.0000
C(39)-C(40)	1.5417
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(41)	1.3893
C(40)-C(45)	1.3902
C(41)-C(42)	1.3902
C(41)-H(41)	0.9500
C(42)-C(43)	1.3906
C(42)-H(42)	0.9496
C(43)-C(44)	1.3897
C(43)-H(43)	0.9501
C(44)-C(45)	1.3901
C(44)-H(44)	0.9504
C(45)-H(45)	0.9489
O(100)-C(100)	1.2295
O(101)-C(100)	1.2804
O(150)-C(150)	1.3110
O(151)-C(150)	1.2630
C(150)-C(151)	1.4850
Fe(2)-C(158)	1.9358
Fe(2)-C(159)	1.9641

Fe(2)-C(155)	1.9808
Fe(2)-C(157)	1.9929
Fe(2)-C(154)	2.0152
Fe(2)-C(151)	2.0362
Fe(2)-C(160)	2.0372
Fe(2)-C(152)	2.0506
Fe(2)-C(156)	2.0549
Fe(2)-C(153)	2.0577
C(151)-C(155)	1.3522
C(151)-C(152)	1.4944
C(152)-C(153)	1.4194
C(152)-H(152)	0.9505
C(153)-C(154)	1.4203
C(153)-H(153)	0.9500
C(154)-C(155)	1.4187
C(154)-H(154)	0.9500
C(155)-H(155)	0.9500
C(156)-C(157)	1.4201
C(156)-C(160)	1.4203
C(156)-H(156)	0.9500
C(157)-C(158)	1.4195
C(157)-H(157)	0.9500
C(158)-C(159)	1.4197
C(158)-H(158)	0.9500
C(159)-C(160)	1.4193
C(159)-H(159)	0.9500
C(160)-H(160)	0.9500
O(250)-C(250)	1.442(8)
O(250)-H(25F)	0.8500
C(250)-C(251)	1.510(13)
C(250)-H(25A)	0.9900
C(250)-H(25B)	0.9900
C(251)-H(25C)	0.9800
C(251)-H(25D)	0.9800
C(251)-H(25E)	0.9800
O(455)-C(455)	1.572(18)
O(455)-H(455)	0.8400
C(455)-C(456)	1.519(17)
C(455)-H(45A)	0.9900
C(455)-H(45B)	0.9900
C(456)-H(45C)	0.9800
C(456)-H(45D)	0.9800
C(456)-H(45E)	0.9800
N(400)-O(400)	1.216(15)
N(400)-O(402)	1.226(16)
N(400)-O(401)	1.241(15)
N(420)-O(420)	1.183(16)
N(420)-O(421)	1.186(16)
N(420)-O(422)	1.219(16)
O(4)-La(1)-O(6)	69.66(13)
O(4)-La(1)-O(10)	136.90(12)

O(6)-La(1)-O(10)	138.23(13)
O(4)-La(1)-O(8)	132.40(13)
O(6)-La(1)-O(8)	69.14(13)
O(10)-La(1)-O(8)	70.69(12)
O(4)-La(1)-O(2)	71.58(11)
O(6)-La(1)-O(2)	137.15(13)
O(10)-La(1)-O(2)	68.05(11)
O(8)-La(1)-O(2)	131.48(12)
O(4)-La(1)-O(101)	78.12(10)
O(6)-La(1)-O(101)	118.12(10)
O(10)-La(1)-O(101)	101.06(10)
O(8)-La(1)-O(101)	143.86(9)
O(2)-La(1)-O(101)	69.74(10)
O(4)-La(1)-O(240)	140.57(10)
O(6)-La(1)-O(240)	108.32(10)
O(10)-La(1)-O(240)	71.80(10)
O(8)-La(1)-O(240)	75.76(9)
O(2)-La(1)-O(240)	113.09(9)
O(101)-La(1)-O(240)	68.4
O(4)-La(1)-O(19)	79.15(10)
O(6)-La(1)-O(19)	78.57(10)
O(10)-La(1)-O(19)	77.66(10)
O(8)-La(1)-O(19)	70.32(10)
O(2)-La(1)-O(19)	76.88(10)
O(101)-La(1)-O(19)	144.1
O(240)-La(1)-O(19)	140.2
O(4)-La(1)-O(100)	75.28(10)
O(6)-La(1)-O(100)	71.45(10)
O(10)-La(1)-O(100)	136.36(10)
O(8)-La(1)-O(100)	112.19(9)
O(2)-La(1)-O(100)	115.07(9)
O(101)-La(1)-O(100)	49.6
O(240)-La(1)-O(100)	67.4
O(19)-La(1)-O(100)	145.8
O(4)-La(1)-C(100)	74.65(10)
O(6)-La(1)-C(100)	94.14(10)
O(10)-La(1)-C(100)	121.10(10)
O(8)-La(1)-C(100)	130.87(9)
O(2)-La(1)-C(100)	92.67(10)
O(101)-La(1)-C(100)	25.3
O(240)-La(1)-C(100)	66.1
O(19)-La(1)-C(100)	153.7
O(100)-La(1)-C(100)	24.3
N(10)-Cu(1)-O(2)	91.27(17)
N(10)-Cu(1)-O(1)	175.30(17)
O(2)-Cu(1)-O(1)	84.33(16)
N(10)-Cu(1)-N(9)	81.45(19)
O(2)-Cu(1)-N(9)	172.55(18)
O(1)-Cu(1)-N(9)	102.90(19)
N(2)-Cu(2)-O(4)	93.50(17)
N(2)-Cu(2)-O(3)	171.8(2)
O(4)-Cu(2)-O(3)	84.86(16)

N(2)-Cu(2)-N(1)	81.9(2)
O(4)-Cu(2)-N(1)	172.4(2)
O(3)-Cu(2)-N(1)	98.8(2)
N(2)-Cu(2)-O(310)	96.0(2)
O(4)-Cu(2)-O(310)	88.4(2)
O(3)-Cu(2)-O(310)	91.98(19)
N(1)-Cu(2)-O(310)	98.1(3)
N(4)-Cu(3)-O(6)	90.69(17)
N(4)-Cu(3)-O(5)	164.1(2)
O(6)-Cu(3)-O(5)	83.51(18)
N(4)-Cu(3)-N(3)	81.6(2)
O(6)-Cu(3)-N(3)	171.84(18)
O(5)-Cu(3)-N(3)	103.3(2)
N(4)-Cu(3)-O(250)	101.63(16)
O(6)-Cu(3)-O(250)	96.74(13)
O(5)-Cu(3)-O(250)	93.77(17)
N(3)-Cu(3)-O(250)	87.37(15)
N(6)-Cu(4)-O(8)	90.91(19)
N(6)-Cu(4)-O(7)	175.0(2)
O(8)-Cu(4)-O(7)	84.57(17)
N(6)-Cu(4)-N(5)	81.4(3)
O(8)-Cu(4)-N(5)	170.0(3)
O(7)-Cu(4)-N(5)	102.8(3)
N(6)-Cu(4)-O(420)	85.9(5)
O(8)-Cu(4)-O(420)	100.8(6)
O(7)-Cu(4)-O(420)	97.1(4)
N(5)-Cu(4)-O(420)	85.0(6)
N(8)-Cu(5)-O(10)	90.96(17)
N(8)-Cu(5)-O(9)	171.49(18)
O(10)-Cu(5)-O(9)	83.55(15)
N(8)-Cu(5)-N(7)	82.1(2)
O(10)-Cu(5)-N(7)	162.5(2)
O(9)-Cu(5)-N(7)	101.28(18)
N(8)-Cu(5)-O(150)	93.90(14)
O(10)-Cu(5)-O(150)	105.26(14)
O(9)-Cu(5)-O(150)	93.81(12)
N(7)-Cu(5)-O(150)	91.32(15)
C(1)-O(1)-Cu(1)	107.6(4)
N(2)-O(2)-Cu(1)	108.2(3)
N(2)-O(2)-La(1)	118.4(3)
Cu(1)-O(2)-La(1)	120.22(17)
C(10)-O(3)-Cu(2)	106.9(3)
N(4)-O(4)-Cu(2)	108.7(3)
N(4)-O(4)-La(1)	120.2(3)
Cu(2)-O(4)-La(1)	123.59(16)
C(19)-O(5)-Cu(3)	108.4(4)
N(6)-O(6)-Cu(3)	110.0(3)
N(6)-O(6)-La(1)	126.3(3)
Cu(3)-O(6)-La(1)	123.21(19)
C(28)-O(7)-Cu(4)	108.4(4)
N(8)-O(8)-Cu(4)	108.9(3)
N(8)-O(8)-La(1)	123.1(3)

Cu(4)-O(8)-La(1)	127.82(18)
C(37)-O(9)-Cu(5)	108.6(3)
N(10)-O(10)-Cu(5)	110.1(3)
N(10)-O(10)-La(1)	120.8(3)
Cu(5)-O(10)-La(1)	122.33(16)
C(2)-N(1)-Cu(2)	110.2(4)
C(2)-N(1)-H(1G)	109.6
Cu(2)-N(1)-H(1G)	109.6
C(2)-N(1)-H(1H)	109.6
Cu(2)-N(1)-H(1H)	109.6
H(1G)-N(1)-H(1H)	108.1
C(1)-N(2)-O(2)	114.6(4)
C(1)-N(2)-Cu(2)	119.2(4)
O(2)-N(2)-Cu(2)	125.7(3)
C(11)-N(3)-Cu(3)	111.5(3)
C(11)-N(3)-H(3C)	109.3
Cu(3)-N(3)-H(3C)	109.3
C(11)-N(3)-H(3D)	109.3
Cu(3)-N(3)-H(3D)	109.3
H(3C)-N(3)-H(3D)	108.0
C(10)-N(4)-O(4)	114.4(5)
C(10)-N(4)-Cu(3)	120.3(4)
O(4)-N(4)-Cu(3)	124.9(4)
C(20)-N(5)-Cu(4)	112.7(5)
C(20)-N(5)-H(5A)	109.0
Cu(4)-N(5)-H(5A)	109.0
C(20)-N(5)-H(5B)	109.0
Cu(4)-N(5)-H(5B)	109.0
H(5A)-N(5)-H(5B)	107.8
C(19)-N(6)-O(6)	116.1(5)
C(19)-N(6)-Cu(4)	119.2(5)
O(6)-N(6)-Cu(4)	124.5(3)
C(29)-N(7)-Cu(5)	111.8(4)
C(29)-N(7)-H(7A)	109.2
Cu(5)-N(7)-H(7A)	109.2
C(29)-N(7)-H(7B)	109.2
Cu(5)-N(7)-H(7B)	109.2
H(7A)-N(7)-H(7B)	107.9
C(28)-N(8)-O(8)	115.6(4)
C(28)-N(8)-Cu(5)	119.4(4)
O(8)-N(8)-Cu(5)	125.0(3)
C(38)-N(9)-Cu(1)	112.5(3)
C(38)-N(9)-H(9A)	109.1
Cu(1)-N(9)-H(9A)	109.1
C(38)-N(9)-H(9B)	109.1
Cu(1)-N(9)-H(9B)	109.1
H(9A)-N(9)-H(9B)	107.8
C(37)-N(10)-O(10)	114.9(4)
C(37)-N(10)-Cu(1)	120.3(4)
O(10)-N(10)-Cu(1)	124.8(3)
N(2)-C(1)-O(1)	124.1(5)
N(2)-C(1)-C(2)	116.1(5)

O(1)-C(1)-C(2)	119.7(5)
N(1)-C(2)-C(1)	109.9(5)
N(1)-C(2)-C(3)	107.6(7)
C(1)-C(2)-C(3)	105.1(8)
N(1)-C(2)-H(2)	111.3
C(1)-C(2)-H(2)	111.3
C(3)-C(2)-H(2)	111.3
C(4)-C(3)-C(2)	117.1(12)
C(4)-C(3)-H(3A)	108.0
C(2)-C(3)-H(3A)	108.0
C(4)-C(3)-H(3B)	108.0
C(2)-C(3)-H(3B)	108.0
H(3A)-C(3)-H(3B)	107.3
C(5)-C(4)-C(9)	115.0(11)
C(5)-C(4)-C(3)	124.0(15)
C(9)-C(4)-C(3)	119.7(14)
C(4)-C(5)-C(6)	126.7(17)
C(4)-C(5)-H(5)	116.6
C(6)-C(5)-H(5)	116.6
C(7)-C(6)-C(5)	115.2(16)
C(7)-C(6)-H(6)	122.4
C(5)-C(6)-H(6)	122.4
C(6)-C(7)-C(8)	119.1(15)
C(6)-C(7)-H(7)	120.5
C(8)-C(7)-H(7)	120.5
C(9)-C(8)-C(7)	123.1(19)
C(9)-C(8)-H(8)	118.4
C(7)-C(8)-H(8)	118.4
C(8)-C(9)-C(4)	117.0(17)
C(8)-C(9)-H(9)	121.5
C(4)-C(9)-H(9)	121.5
N(4)-C(10)-O(3)	124.5(5)
N(4)-C(10)-C(11)	114.2(5)
O(3)-C(10)-C(11)	121.2(5)
N(3)-C(11)-C(12)	110.0(5)
N(3)-C(11)-C(10)	108.4(5)
C(12)-C(11)-C(10)	111.8(5)
N(3)-C(11)-H(11)	108.9
C(12)-C(11)-H(11)	108.9
C(10)-C(11)-H(11)	108.9
C(11)-C(12)-C(13)	108.5(8)
C(11)-C(12)-C(1A)	116.6(8)
C(13)-C(12)-C(1A)	18.3(6)
C(11)-C(12)-H(12A)	110.0
C(13)-C(12)-H(12A)	110.0
C(1A)-C(12)-H(12A)	91.7
C(11)-C(12)-H(12B)	110.0
C(13)-C(12)-H(12B)	110.0
C(1A)-C(12)-H(12B)	118.1
H(12A)-C(12)-H(12B)	108.4
C(11)-C(12)-H(12C)	108.2
C(13)-C(12)-H(12C)	126.6

C(1A)-C(12)-H(12C)	108.7
H(12A)-C(12)-H(12C)	19.1
H(12B)-C(12)-H(12C)	92.0
C(11)-C(12)-H(12D)	108.2
C(13)-C(12)-H(12D)	96.4
C(1A)-C(12)-H(12D)	107.4
H(12A)-C(12)-H(12D)	122.5
H(12B)-C(12)-H(12D)	16.1
H(12C)-C(12)-H(12D)	107.4
C(14)-C(13)-C(18)	121.8(14)
C(14)-C(13)-C(12)	119.1(15)
C(18)-C(13)-C(12)	118.5(12)
C(13)-C(14)-C(15)	119.2(16)
C(13)-C(14)-H(14)	120.4
C(15)-C(14)-H(14)	120.4
C(14)-C(15)-C(16)	119.3(15)
C(14)-C(15)-H(15)	120.3
C(16)-C(15)-H(15)	120.3
C(17)-C(16)-C(15)	120.5(19)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	119(2)
C(16)-C(17)-H(17)	120.7
C(18)-C(17)-H(17)	120.7
C(13)-C(18)-C(17)	120.2(14)
C(13)-C(18)-H(18)	119.9
C(17)-C(18)-H(18)	119.9
C(1B)-C(1A)-C(1F)	116.7(13)
C(1B)-C(1A)-C(12)	121.9(13)
C(1F)-C(1A)-C(12)	120.7(12)
C(1A)-C(1B)-C(1C)	122.7(15)
C(1A)-C(1B)-H(1B)	118.6
C(1C)-C(1B)-H(1B)	118.6
C(1D)-C(1C)-C(1B)	119.0(18)
C(1D)-C(1C)-H(1C)	120.5
C(1B)-C(1C)-H(1C)	120.5
C(1C)-C(1D)-C(1E)	118.4(17)
C(1C)-C(1D)-H(1D)	120.8
C(1E)-C(1D)-H(1D)	120.8
C(1F)-C(1E)-C(1D)	123.0(16)
C(1F)-C(1E)-H(1E)	118.5
C(1D)-C(1E)-H(1E)	118.5
C(1E)-C(1F)-C(1A)	119.4(15)
C(1E)-C(1F)-H(1F)	120.3
C(1A)-C(1F)-H(1F)	120.3
N(6)-C(19)-O(5)	122.0(6)
N(6)-C(19)-C(20)	116.8(6)
O(5)-C(19)-C(20)	121.1(5)
C(19)-C(20)-N(5)	107.8(5)
C(19)-C(20)-C(21)	109.7(8)
N(5)-C(20)-C(21)	110.9(8)
C(19)-C(20)-H(20)	109.5

N(5)-C(20)-H(20)	109.5
C(21)-C(20)-H(20)	109.5
C(22)-C(21)-C(20)	114.4(10)
C(22)-C(21)-C(22A)	18.2(18)
C(20)-C(21)-C(22A)	104.3(19)
C(22)-C(21)-H(21A)	108.7
C(20)-C(21)-H(21A)	108.7
C(22A)-C(21)-H(21A)	126.9
C(22)-C(21)-H(21B)	108.7
C(20)-C(21)-H(21B)	108.7
C(22A)-C(21)-H(21B)	99.6
H(21A)-C(21)-H(21B)	107.6
C(22)-C(21)-H(21C)	117.1
C(20)-C(21)-H(21C)	111.0
C(22A)-C(21)-H(21C)	110.6
H(21A)-C(21)-H(21C)	95.0
H(21B)-C(21)-H(21C)	13.0
C(22)-C(21)-H(21D)	92.9
C(20)-C(21)-H(21D)	110.9
C(22A)-C(21)-H(21D)	111.1
H(21A)-C(21)-H(21D)	17.2
H(21B)-C(21)-H(21D)	120.7
H(21C)-C(21)-H(21D)	109.0
C(23)-C(22)-C(27)	120.0(13)
C(23)-C(22)-C(21)	119.9(15)
C(27)-C(22)-C(21)	120.0(13)
C(22)-C(23)-C(24)	118.7(14)
C(22)-C(23)-H(23)	120.7
C(24)-C(23)-H(23)	120.7
C(23)-C(24)-C(25)	121.6(14)
C(23)-C(24)-H(24)	119.2
C(25)-C(24)-H(24)	119.2
C(24)-C(25)-C(26)	119.4(13)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(27)-C(26)-C(25)	118.9(16)
C(27)-C(26)-H(26)	120.6
C(25)-C(26)-H(26)	120.6
C(26)-C(27)-C(22)	120.0(15)
C(26)-C(27)-H(27)	120.0
C(22)-C(27)-H(27)	120.0
C(108)-Fe(1)-C(109)	42.07(13)
C(108)-Fe(1)-C(107)	41.93(13)
C(109)-Fe(1)-C(107)	70.09(19)
C(108)-Fe(1)-C(104)	135.3(4)
C(109)-Fe(1)-C(104)	107.7(3)
C(107)-Fe(1)-C(104)	177.2(4)
C(108)-Fe(1)-C(105)	175.1(4)
C(109)-Fe(1)-C(105)	133.3(4)
C(107)-Fe(1)-C(105)	141.6(4)
C(104)-Fe(1)-C(105)	41.13(12)
C(108)-Fe(1)-C(102)	114.1(5)

C(109)-Fe(1)-C(102)	143.2(5)
C(107)-Fe(1)-C(102)	112.5(5)
C(104)-Fe(1)-C(102)	68.1(4)
C(105)-Fe(1)-C(102)	68.7(4)
C(108)-Fe(1)-C(103)	110.6(4)
C(109)-Fe(1)-C(103)	112.6(3)
C(107)-Fe(1)-C(103)	138.1(5)
C(104)-Fe(1)-C(103)	40.76(11)
C(105)-Fe(1)-C(103)	68.70(18)
C(102)-Fe(1)-C(103)	39.8(3)
C(108)-Fe(1)-C(101)	145.1(5)
C(109)-Fe(1)-C(101)	172.8(5)
C(107)-Fe(1)-C(101)	115.1(4)
C(104)-Fe(1)-C(101)	67.2(3)
C(105)-Fe(1)-C(101)	39.6(3)
C(102)-Fe(1)-C(101)	40.9(4)
C(103)-Fe(1)-C(101)	67.2(4)
C(108)-Fe(1)-C(110)	69.65(19)
C(109)-Fe(1)-C(110)	40.96(13)
C(107)-Fe(1)-C(110)	68.78(19)
C(104)-Fe(1)-C(110)	110.8(4)
C(105)-Fe(1)-C(110)	107.7(4)
C(102)-Fe(1)-C(110)	175.8(5)
C(103)-Fe(1)-C(110)	141.8(4)
C(101)-Fe(1)-C(110)	134.8(5)
C(108)-Fe(1)-C(106)	69.48(18)
C(109)-Fe(1)-C(106)	68.9(2)
C(107)-Fe(1)-C(106)	40.74(11)
C(104)-Fe(1)-C(106)	140.5(5)
C(105)-Fe(1)-C(106)	111.4(4)
C(102)-Fe(1)-C(106)	138.3(4)
C(103)-Fe(1)-C(106)	178.0(4)
C(101)-Fe(1)-C(106)	111.5(4)
C(110)-Fe(1)-C(106)	40.24(13)
C(105)-C(101)-C(102)	109.4(7)
C(105)-C(101)-C(100)	129.2(9)
C(102)-C(101)-C(100)	120.7(8)
C(105)-C(101)-Fe(1)	69.1(5)
C(102)-C(101)-Fe(1)	69.2(6)
C(100)-C(101)-Fe(1)	119.8(7)
C(103)-C(102)-C(101)	107.2(9)
C(103)-C(102)-Fe(1)	70.6(5)
C(101)-C(102)-Fe(1)	69.8(6)
C(103)-C(102)-H(102)	127.3(11)
C(101)-C(102)-H(102)	125.3(10)
Fe(1)-C(102)-H(102)	128.4(10)
C(102)-C(103)-C(104)	108.0(5)
C(102)-C(103)-Fe(1)	69.6(5)
C(104)-C(103)-Fe(1)	68.5(2)
C(102)-C(103)-H(103)	126.0
C(104)-C(103)-H(103)	126.0
Fe(1)-C(103)-H(103)	127.4

C(103)-C(104)-C(105)	108.0
C(103)-C(104)-Fe(1)	70.7(2)
C(105)-C(104)-Fe(1)	69.2(2)
C(103)-C(104)-H(104)	126.0
C(105)-C(104)-H(104)	126.0
Fe(1)-C(104)-H(104)	125.6
C(101)-C(105)-C(104)	107.4(5)
C(101)-C(105)-Fe(1)	71.3(5)
C(104)-C(105)-Fe(1)	69.63(18)
C(101)-C(105)-H(105)	126.3
C(104)-C(105)-H(105)	126.3
Fe(1)-C(105)-H(105)	124.4
C(107)-C(106)-C(110)	108.0
C(107)-C(106)-Fe(1)	67.3(2)
C(110)-C(106)-Fe(1)	69.6(2)
C(107)-C(106)-H(106)	126.0
C(110)-C(106)-H(106)	126.0
Fe(1)-C(106)-H(106)	128.6
C(106)-C(107)-C(108)	108.0
C(106)-C(107)-Fe(1)	71.9(2)
C(108)-C(107)-Fe(1)	67.28(19)
C(106)-C(107)-H(107)	126.0
C(108)-C(107)-H(107)	126.0
Fe(1)-C(107)-H(107)	126.3
C(109)-C(108)-C(107)	108.0
C(109)-C(108)-Fe(1)	70.2(2)
C(107)-C(108)-Fe(1)	70.79(19)
C(109)-C(108)-H(108)	126.0
C(107)-C(108)-H(108)	126.0
Fe(1)-C(108)-H(108)	124.6
C(108)-C(109)-C(110)	108.0
C(108)-C(109)-Fe(1)	67.7(2)
C(110)-C(109)-Fe(1)	72.0(2)
C(108)-C(109)-H(109)	126.0
C(110)-C(109)-H(109)	126.0
Fe(1)-C(109)-H(109)	125.8
C(109)-C(110)-C(106)	108.0
C(109)-C(110)-Fe(1)	67.0(2)
C(106)-C(110)-Fe(1)	70.16(18)
C(109)-C(110)-H(110)	126.0
C(106)-C(110)-H(110)	126.0
Fe(1)-C(110)-H(110)	128.4
C(22B)-C(22A)-C(22F)	112.9(17)
C(22B)-C(22A)-C(21)	115(2)
C(22F)-C(22A)-C(21)	132(2)
C(22A)-C(22B)-C(22C)	125(2)
C(22A)-C(22B)-H(22B)	117.6
C(22C)-C(22B)-H(22B)	117.6
C(22D)-C(22C)-C(22B)	121(2)
C(22D)-C(22C)-H(22C)	119.6
C(22B)-C(22C)-H(22C)	119.6
C(22C)-C(22D)-C(22E)	117(2)

C(22C)-C(22D)-H(22D)	121.7
C(22E)-C(22D)-H(22D)	121.7
C(22F)-C(22E)-C(22D)	122(2)
C(22F)-C(22E)-H(22E)	118.8
C(22D)-C(22E)-H(22E)	118.8
C(22E)-C(22F)-C(22A)	122.0(19)
C(22E)-C(22F)-H(22F)	119.0
C(22A)-C(22F)-H(22F)	119.0
C(10H)-Fe(1A)-C(10E)	127.6(8)
C(10H)-Fe(1A)-C(10I)	41.7(6)
C(10E)-Fe(1A)-C(10I)	111.9(9)
C(10H)-Fe(1A)-C(10D)	159.7(9)
C(10E)-Fe(1A)-C(10D)	40.5(5)
C(10I)-Fe(1A)-C(10D)	120.6(9)
C(10H)-Fe(1A)-C(10B)	123.1(9)
C(10E)-Fe(1A)-C(10B)	68.3(7)
C(10I)-Fe(1A)-C(10B)	162.3(8)
C(10D)-Fe(1A)-C(10B)	71.9(7)
C(10H)-Fe(1A)-C(10A)	108.6(8)
C(10E)-Fe(1A)-C(10A)	41.8(5)
C(10I)-Fe(1A)-C(10A)	126.1(7)
C(10D)-Fe(1A)-C(10A)	72.5(7)
C(10B)-Fe(1A)-C(10A)	41.9(5)
C(10H)-Fe(1A)-C(10G)	39.4(5)
C(10E)-Fe(1A)-C(10G)	161.3(9)
C(10I)-Fe(1A)-C(10G)	67.7(8)
C(10D)-Fe(1A)-C(10G)	156.8(9)
C(10B)-Fe(1A)-C(10G)	106.0(8)
C(10A)-Fe(1A)-C(10G)	122.1(9)
C(10H)-Fe(1A)-C(10C)	159.3(9)
C(10E)-Fe(1A)-C(10C)	63.9(7)
C(10I)-Fe(1A)-C(10C)	157.0(9)
C(10D)-Fe(1A)-C(10C)	40.6(5)
C(10B)-Fe(1A)-C(10C)	40.2(5)
C(10A)-Fe(1A)-C(10C)	67.4(7)
C(10G)-Fe(1A)-C(10C)	124.0(9)
C(10H)-Fe(1A)-C(10J)	69.2(8)
C(10E)-Fe(1A)-C(10J)	121.6(9)
C(10I)-Fe(1A)-C(10J)	38.4(5)
C(10D)-Fe(1A)-C(10J)	102.0(9)
C(10B)-Fe(1A)-C(10J)	157.4(8)
C(10A)-Fe(1A)-C(10J)	158.6(9)
C(10G)-Fe(1A)-C(10J)	70.7(8)
C(10C)-Fe(1A)-C(10J)	122.2(9)
C(10H)-Fe(1A)-C(10F)	62.9(8)
C(10E)-Fe(1A)-C(10F)	157.8(9)
C(10I)-Fe(1A)-C(10F)	60.9(8)
C(10D)-Fe(1A)-C(10F)	122.1(9)
C(10B)-Fe(1A)-C(10F)	125.5(8)
C(10A)-Fe(1A)-C(10F)	160.2(9)
C(10G)-Fe(1A)-C(10F)	39.6(5)
C(10C)-Fe(1A)-C(10F)	113.6(9)

C(10J)-Fe(1A)-C(10F)	38.9(5)
C(10E)-C(10A)-C(10B)	102.4(11)
C(10E)-C(10A)-C(100)	135.2(13)
C(10B)-C(10A)-C(100)	122.3(14)
C(10E)-C(10A)-Fe(1A)	66.5(7)
C(10B)-C(10A)-Fe(1A)	68.9(7)
C(100)-C(10A)-Fe(1A)	128.9(8)
C(10C)-C(10B)-C(10A)	105.0(13)
C(10C)-C(10B)-Fe(1A)	70.5(8)
C(10A)-C(10B)-Fe(1A)	69.2(7)
C(10C)-C(10B)-H(10B)	127.5
C(10A)-C(10B)-H(10B)	127.5
Fe(1A)-C(10B)-H(10B)	124.5
C(10B)-C(10C)-C(10D)	115.7(14)
C(10B)-C(10C)-Fe(1A)	69.3(7)
C(10D)-C(10C)-Fe(1A)	69.0(7)
C(10B)-C(10C)-H(10C)	122.2
C(10D)-C(10C)-H(10C)	122.2
Fe(1A)-C(10C)-H(10C)	132.0
C(10E)-C(10D)-C(10C)	98.7(14)
C(10E)-C(10D)-Fe(1A)	67.2(7)
C(10C)-C(10D)-Fe(1A)	70.4(7)
C(10E)-C(10D)-H(10D)	130.7
C(10C)-C(10D)-H(10D)	130.7
Fe(1A)-C(10D)-H(10D)	123.7
C(10D)-C(10E)-C(10A)	117.4(14)
C(10D)-C(10E)-Fe(1A)	72.2(8)
C(10A)-C(10E)-Fe(1A)	71.8(7)
C(10D)-C(10E)-H(102)	116.7(14)
C(10A)-C(10E)-H(102)	89.8(15)
Fe(1A)-C(10E)-H(102)	161.4(16)
C(10D)-C(10E)-H(10E)	121.3
C(10A)-C(10E)-H(10E)	121.3
Fe(1A)-C(10E)-H(10E)	126.5
H(102)-C(10E)-H(10E)	64.6
C(10J)-C(10F)-C(10G)	116.9(15)
C(10J)-C(10F)-Fe(1A)	70.2(7)
C(10G)-C(10F)-Fe(1A)	67.6(7)
C(10J)-C(10F)-H(10F)	121.5
C(10G)-C(10F)-H(10F)	121.5
Fe(1A)-C(10F)-H(10F)	133.5
C(10H)-C(10G)-C(10F)	100.8(16)
C(10H)-C(10G)-Fe(1A)	67.1(8)
C(10F)-C(10G)-Fe(1A)	72.8(8)
C(10H)-C(10G)-H(10G)	129.6
C(10F)-C(10G)-H(10G)	129.6
Fe(1A)-C(10G)-H(10G)	122.5
C(10G)-C(10H)-C(10I)	109.3(16)
C(10G)-C(10H)-Fe(1A)	73.5(8)
C(10I)-C(10H)-Fe(1A)	70.8(8)
C(10G)-C(10H)-H(10H)	125.3
C(10I)-C(10H)-H(10H)	125.3

Fe(1A)-C(10H)-H(10H)	122.0
C(10J)-C(10I)-C(10H)	113.3(16)
C(10J)-C(10I)-Fe(1A)	74.7(8)
C(10H)-C(10I)-Fe(1A)	67.5(7)
C(10J)-C(10I)-H(10I)	123.3
C(10H)-C(10I)-H(10I)	123.3
Fe(1A)-C(10I)-H(10I)	126.0
C(10I)-C(10J)-C(10F)	98.4(16)
C(10I)-C(10J)-Fe(1A)	66.8(7)
C(10F)-C(10J)-Fe(1A)	70.9(7)
C(10I)-C(10J)-H(10J)	130.8
C(10F)-C(10J)-H(10J)	130.8
Fe(1A)-C(10J)-H(10J)	123.5
N(8)-C(28)-O(7)	122.6(5)
N(8)-C(28)-C(29)	115.8(5)
O(7)-C(28)-C(29)	121.6(5)
C(28)-C(29)-N(7)	108.5(5)
C(28)-C(29)-C(30)	112.4(5)
N(7)-C(29)-C(30)	112.1(6)
C(28)-C(29)-H(29)	107.9
N(7)-C(29)-H(29)	107.9
C(30)-C(29)-H(29)	107.9
C(31)-C(30)-C(29)	111.0(6)
C(31)-C(30)-H(30A)	109.4
C(29)-C(30)-H(30A)	109.4
C(31)-C(30)-H(30B)	109.4
C(29)-C(30)-H(30B)	109.4
H(30A)-C(30)-H(30B)	108.0
C(36)-C(31)-C(32)	119.3(11)
C(36)-C(31)-C(30)	121.3(10)
C(32)-C(31)-C(30)	119.4(11)
C(31)-C(32)-C(33)	117.2(17)
C(31)-C(32)-H(32)	121.4
C(33)-C(32)-H(32)	121.4
C(34)-C(33)-C(32)	119.4(16)
C(34)-C(33)-H(33)	120.3
C(32)-C(33)-H(33)	120.3
C(35)-C(34)-C(33)	119.7(15)
C(35)-C(34)-H(34)	120.1
C(33)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	120.5(18)
C(34)-C(35)-H(35)	119.8
C(36)-C(35)-H(35)	119.8
C(31)-C(36)-C(35)	123.7(14)
C(31)-C(36)-H(36)	118.1
C(35)-C(36)-H(36)	118.1
N(10)-C(37)-O(9)	122.5(4)
N(10)-C(37)-C(38)	116.7(5)
O(9)-C(37)-C(38)	120.8(4)
N(9)-C(38)-C(37)	107.7(4)
N(9)-C(38)-C(39)	113.1(4)
C(37)-C(38)-C(39)	111.9(4)

N(9)-C(38)-H(38)	108.0
C(37)-C(38)-H(38)	108.0
C(39)-C(38)-H(38)	108.0
C(38)-C(39)-C(40)	112.0(2)
C(38)-C(39)-H(39A)	109.2
C(40)-C(39)-H(39A)	109.2
C(38)-C(39)-H(39B)	109.2
C(40)-C(39)-H(39B)	109.2
H(39A)-C(39)-H(39B)	107.9
C(41)-C(40)-C(45)	120.0
C(41)-C(40)-C(39)	120.2
C(45)-C(40)-C(39)	119.7
C(40)-C(41)-C(42)	120.0
C(40)-C(41)-H(41)	120.0
C(42)-C(41)-H(41)	120.0
C(41)-C(42)-C(43)	119.9
C(41)-C(42)-H(42)	120.0
C(43)-C(42)-H(42)	120.0
C(44)-C(43)-C(42)	120.0
C(44)-C(43)-H(43)	120.0
C(42)-C(43)-H(43)	120.0
C(43)-C(44)-C(45)	120.0
C(43)-C(44)-H(44)	120.0
C(45)-C(44)-H(44)	120.0
C(44)-C(45)-C(40)	120.0
C(44)-C(45)-H(45)	120.0
C(40)-C(45)-H(45)	120.0
C(100)-O(100)-La(1)	94.6
C(100)-O(101)-La(1)	95.6
O(100)-C(100)-O(101)	120.2
O(100)-C(100)-C(101)	117.8(5)
O(101)-C(100)-C(101)	121.8(5)
O(100)-C(100)-C(10A)	129.2(6)
O(101)-C(100)-C(10A)	109.7(6)
C(101)-C(100)-C(10A)	18.1(7)
O(100)-C(100)-La(1)	61.2
O(101)-C(100)-La(1)	59.1
C(101)-C(100)-La(1)	173.3(4)
C(10A)-C(100)-La(1)	167.1(7)
C(150)-O(150)-Cu(5)	125.2
O(151)-C(150)-O(150)	122.1
O(151)-C(150)-C(151)	120.6
O(150)-C(150)-C(151)	117.2
C(158)-Fe(2)-C(159)	42.7
C(158)-Fe(2)-C(155)	155.7
C(159)-Fe(2)-C(155)	161.6
C(158)-Fe(2)-C(157)	42.3
C(159)-Fe(2)-C(157)	71.0
C(155)-Fe(2)-C(157)	122.6
C(158)-Fe(2)-C(154)	156.2
C(159)-Fe(2)-C(154)	122.3
C(155)-Fe(2)-C(154)	41.6

C(157)-Fe(2)-C(154)	161.4
C(158)-Fe(2)-C(151)	118.4
C(159)-Fe(2)-C(151)	155.8
C(155)-Fe(2)-C(151)	39.3
C(157)-Fe(2)-C(151)	105.1
C(154)-Fe(2)-C(151)	68.3
C(158)-Fe(2)-C(160)	70.6
C(159)-Fe(2)-C(160)	41.5
C(155)-Fe(2)-C(160)	127.3
C(157)-Fe(2)-C(160)	69.5
C(154)-Fe(2)-C(160)	110.7
C(151)-Fe(2)-C(160)	161.0
C(158)-Fe(2)-C(152)	100.0
C(159)-Fe(2)-C(152)	116.9
C(155)-Fe(2)-C(152)	69.4
C(157)-Fe(2)-C(152)	119.0
C(154)-Fe(2)-C(152)	68.8
C(151)-Fe(2)-C(152)	42.9
C(160)-Fe(2)-C(152)	155.9
C(158)-Fe(2)-C(156)	70.2
C(159)-Fe(2)-C(156)	69.7
C(155)-Fe(2)-C(156)	111.3
C(157)-Fe(2)-C(156)	41.0
C(154)-Fe(2)-C(156)	127.1
C(151)-Fe(2)-C(156)	123.7
C(160)-Fe(2)-C(156)	40.6
C(152)-Fe(2)-C(156)	158.2
C(158)-Fe(2)-C(153)	117.5
C(159)-Fe(2)-C(153)	103.8
C(155)-Fe(2)-C(153)	69.3
C(157)-Fe(2)-C(153)	155.1
C(154)-Fe(2)-C(153)	40.8
C(151)-Fe(2)-C(153)	69.3
C(160)-Fe(2)-C(153)	123.3
C(152)-Fe(2)-C(153)	40.4
C(156)-Fe(2)-C(153)	161.3
C(155)-C(151)-C(150)	131.2
C(155)-C(151)-C(152)	107.5
C(150)-C(151)-C(152)	121.2
C(155)-C(151)-Fe(2)	68.1
C(150)-C(151)-Fe(2)	125.7
C(152)-C(151)-Fe(2)	69.1
C(153)-C(152)-C(151)	106.1
C(153)-C(152)-Fe(2)	70.1
C(151)-C(152)-Fe(2)	68.0
C(153)-C(152)-H(152)	126.9
C(151)-C(152)-H(152)	127.0
Fe(2)-C(152)-H(152)	126.5
C(152)-C(153)-C(154)	108.0
C(152)-C(153)-Fe(2)	69.5
C(154)-C(153)-Fe(2)	68.0
C(152)-C(153)-H(153)	126.0

C(154)-C(153)-H(153)	126.0
Fe(2)-C(153)-H(153)	128.1
C(155)-C(154)-C(153)	108.0
C(155)-C(154)-Fe(2)	67.9
C(153)-C(154)-Fe(2)	71.2
C(155)-C(154)-H(154)	126.0
C(153)-C(154)-H(154)	126.0
Fe(2)-C(154)-H(154)	126.4
C(151)-C(155)-C(154)	110.3
C(151)-C(155)-Fe(2)	72.6
C(154)-C(155)-Fe(2)	70.5
C(151)-C(155)-H(155)	124.8
C(154)-C(155)-H(155)	124.8
Fe(2)-C(155)-H(155)	123.7
C(157)-C(156)-C(160)	108.0
C(157)-C(156)-Fe(2)	67.1
C(160)-C(156)-Fe(2)	69.0
C(157)-C(156)-H(156)	126.0
C(160)-C(156)-H(156)	126.0
Fe(2)-C(156)-H(156)	129.4
C(158)-C(157)-C(156)	108.0
C(158)-C(157)-Fe(2)	66.7
C(156)-C(157)-Fe(2)	71.8
C(158)-C(157)-H(157)	126.0
C(156)-C(157)-H(157)	126.0
Fe(2)-C(157)-H(157)	127.0
C(157)-C(158)-C(159)	108.0
C(157)-C(158)-Fe(2)	71.0
C(159)-C(158)-Fe(2)	69.7
C(157)-C(158)-H(158)	126.0
C(159)-C(158)-H(158)	126.0
Fe(2)-C(158)-H(158)	124.9
C(160)-C(159)-C(158)	108.0
C(160)-C(159)-Fe(2)	72.0
C(158)-C(159)-Fe(2)	67.6
C(160)-C(159)-H(159)	126.0
C(158)-C(159)-H(159)	126.0
Fe(2)-C(159)-H(159)	126.0
C(159)-C(160)-C(156)	108.0
C(159)-C(160)-Fe(2)	66.5
C(156)-C(160)-Fe(2)	70.4
C(159)-C(160)-H(160)	126.0
C(156)-C(160)-H(160)	126.0
Fe(2)-C(160)-H(160)	128.7
C(250)-O(250)-Cu(3)	116.2(4)
C(250)-O(250)-H(25F)	122.3
Cu(3)-O(250)-H(25F)	121.5
O(250)-C(250)-C(251)	109.1(8)
O(250)-C(250)-H(25A)	109.9
C(251)-C(250)-H(25A)	109.9
O(250)-C(250)-H(25B)	109.9
C(251)-C(250)-H(25B)	109.9

H(25A)-C(250)-H(25B)	108.3
C(250)-C(251)-H(25C)	109.5
C(250)-C(251)-H(25D)	109.5
H(25C)-C(251)-H(25D)	109.5
C(250)-C(251)-H(25E)	109.5
H(25C)-C(251)-H(25E)	109.5
H(25D)-C(251)-H(25E)	109.5
C(455)-O(455)-H(455)	109.5
C(456)-C(455)-O(455)	108.0(14)
C(456)-C(455)-H(45A)	110.1
O(455)-C(455)-H(45A)	110.1
C(456)-C(455)-H(45B)	110.1
O(455)-C(455)-H(45B)	110.1
H(45A)-C(455)-H(45B)	108.4
C(455)-C(456)-H(45C)	109.5
C(455)-C(456)-H(45D)	109.5
H(45C)-C(456)-H(45D)	109.5
C(455)-C(456)-H(45E)	109.5
H(45C)-C(456)-H(45E)	109.5
H(45D)-C(456)-H(45E)	109.5
O(400)-N(400)-O(402)	117.1(15)
O(400)-N(400)-O(401)	117.3(16)
O(402)-N(400)-O(401)	125(2)
O(420)-N(420)-O(421)	125(2)
O(420)-N(420)-O(422)	103(2)
O(421)-N(420)-O(422)	131(2)
N(420)-O(420)-Cu(4)	126.6(15)

Symmetry transformations used to generate equivalent atoms:

S32: Crystallographic tables for $\text{La}^{\text{III}}(\text{FcDC}^-)[15\text{-MCL}_{\text{-pheHA-5}}](\text{NO}_3)$

Crystal data and structure refinement for $\text{La}^{\text{III}}(\text{FcDC}^-)[15\text{-MCL}_{\text{-pheHA-5}}](\text{NO}_3)$

Empirical formula	C57.50 H83 Cu5 Fe La N11 O29
Formula weight	1904.81
Temperature	85(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, I2(1)2(1)2(1)
Unit cell dimensions	a = 13.8915(9) Å alpha = 90 deg. b = 30.956(2) Å beta = 90 deg. c = 35.708(2) Å gamma = 90 deg.
Volume	15355.6(17) Å ³
Z, Calculated density	8, 1.648 Mg/m ³
Absorption coefficient	2.170 mm ⁻¹
F(000)	7720
Crystal size	0.26 x 0.16 x 0.10 mm
Theta range for data collection	1.57 to 29.66 deg.
Limiting indices	-19<=h<=19, -43<=k<=43, -49<=l<=49
Reflections collected / unique	302773 / 21700 [R(int) = 0.0495]
Completeness to theta = 29.66	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8122 and 0.6022
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	21700 / 322 / 1094
Goodness-of-fit on F ²	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0948

R indices (all data) R1 = 0.0374, wR2 = 0.0982

Absolute structure parameter 0.007(8)

Largest diff. peak and hole 1.515 and -0.862 e.A⁻³

Bond lengths [Å] and angles [deg] for La^{III}(FcDC⁻)[15-MC_{L-pheHA}-5](NO₃).

La(1)-O(100)	2.402(2)
La(1)-O(2)	2.459(2)
La(1)-O(8)	2.464(2)
La(1)-O(10)	2.473(2)
La(1)-O(4)	2.488(2)
La(1)-O(6)	2.503(2)
La(1)-O(201)	2.614(3)
La(1)-O(200)	2.647(3)
La(1)-C(200)	3.008(3)
Cu(1)-O(2)	1.907(2)
Cu(1)-N(10)	1.938(3)
Cu(1)-O(1)	1.943(3)
Cu(1)-N(9)	1.990(3)
Cu(1)-O(52C)	2.524(9)
Cu(2)-N(2)	1.908(3)
Cu(2)-O(4)	1.913(2)
Cu(2)-O(3)	1.956(2)
Cu(2)-N(1)	2.009(3)
Cu(3)-O(6)	1.925(2)
Cu(3)-N(4)	1.934(3)
Cu(3)-O(5)	1.957(2)
Cu(3)-N(3)	2.018(3)
Cu(3)-O(301)	2.412(3)
Cu(4)-O(8)	1.917(2)
Cu(4)-N(6)	1.926(3)
Cu(4)-O(7)	1.958(2)
Cu(4)-N(5)	2.015(4)
Cu(4)-O(302)	2.414(4)
Cu(5)-N(8)	1.912(3)
Cu(5)-O(10)	1.931(2)
Cu(5)-O(9)	1.938(3)
Cu(5)-N(7)	2.022(3)
N(1)-C(2)	1.491(4)
N(2)-C(1)	1.298(4)
N(2)-O(2)	1.383(4)
N(3)-C(11)	1.491(4)
N(4)-C(10)	1.286(4)
N(4)-O(4)	1.386(3)
N(5)-C(20)	1.489(5)
N(6)-C(19)	1.291(4)
N(6)-O(6)	1.389(3)
N(7)-C(29)	1.488(4)

N(8)-C(28)	1.296(4)
N(8)-O(8)	1.388(3)
N(9)-C(38)	1.487(6)
N(10)-C(37)	1.301(4)
N(10)-O(10)	1.381(4)
O(1)-C(1)	1.288(4)
O(3)-C(10)	1.303(4)
O(5)-C(19)	1.297(4)
O(7)-C(28)	1.303(4)
O(9)-C(37)	1.277(5)
C(1)-C(2)	1.510(5)
C(2)-C(3)	1.527(6)
C(3)-C(4)	1.444(13)
C(3)-C(0A)	1.575(15)
C(4)-C(5)	1.421(13)
C(4)-C(9)	1.434(14)
C(5)-C(6)	1.486(13)
C(6)-C(7)	1.305(17)
C(7)-C(8)	1.443(15)
C(8)-C(9)	1.345(11)
C(0A)-C(0F)	1.393(16)
C(0A)-C(0B)	1.452(14)
C(0B)-C(0C)	1.406(13)
C(0C)-C(0D)	1.40(2)
C(0D)-C(0E)	1.56(3)
C(0E)-C(0F)	1.35(2)
C(10)-C(11)	1.505(4)
C(11)-C(12)	1.559(5)
C(12)-C(13)	1.514(5)
C(13)-C(18)	1.389(5)
C(13)-C(14)	1.390(5)
C(14)-C(15)	1.380(5)
C(15)-C(16)	1.394(6)
C(16)-C(17)	1.391(6)
C(17)-C(18)	1.390(6)
C(19)-C(20)	1.526(5)
C(20)-C(21)	1.520(6)
C(21)-C(22)	1.530(5)
C(22)-C(23)	1.336(8)
C(22)-C(27)	1.383(8)
C(23)-C(24)	1.413(8)
C(24)-C(25)	1.336(10)
C(25)-C(26)	1.416(9)
C(26)-C(27)	1.380(6)
C(28)-C(29)	1.514(4)
C(29)-C(30)	1.532(5)
C(30)-C(31)	1.513(5)
C(31)-C(32)	1.384(6)
C(31)-C(36)	1.396(6)
C(32)-C(33)	1.403(7)
C(33)-C(34)	1.381(9)
C(34)-C(35)	1.374(9)

C(35)-C(36)	1.380(6)
C(37)-C(38)	1.528(5)
C(38)-C(39)	1.520(7)
C(39)-C(40)	1.495(7)
C(40)-C(45)	1.390(6)
C(40)-C(41)	1.410(6)
C(41)-C(42)	1.409(7)
C(42)-C(43)	1.379(6)
C(43)-C(44)	1.394(7)
C(44)-C(45)	1.391(7)
Fe(1)-C(105)	2.034(3)
Fe(1)-C(105)#1	2.034(3)
Fe(1)-C(101)#1	2.034(3)
Fe(1)-C(101)	2.034(3)
Fe(1)-C(103)#1	2.037(4)
Fe(1)-C(103)	2.037(4)
Fe(1)-C(102)	2.048(4)
Fe(1)-C(102)#1	2.048(4)
Fe(1)-C(104)#1	2.053(4)
Fe(1)-C(104)	2.053(4)
O(101)-C(100)	1.250(4)
O(100)-C(100)	1.267(4)
C(100)-C(101)	1.494(5)
C(101)-C(102)	1.429(5)
C(101)-C(105)#1	1.430(5)
C(102)-C(104)#1	1.404(5)
C(103)-C(105)	1.430(5)
C(103)-C(104)	1.443(6)
C(104)-C(102)#1	1.404(5)
C(105)-C(101)#1	1.430(5)
Fe(2)-C(201)	2.010(3)
Fe(2)-C(201)#2	2.010(3)
Fe(2)-C(202)	2.023(4)
Fe(2)-C(202)#2	2.023(4)
Fe(2)-C(205)#2	2.042(3)
Fe(2)-C(205)	2.042(3)
Fe(2)-C(203)	2.060(3)
Fe(2)-C(203)#2	2.060(3)
Fe(2)-C(204)#2	2.075(4)
Fe(2)-C(204)	2.075(4)
O(200)-C(200)	1.258(4)
O(201)-C(200)	1.273(4)
C(200)-C(201)	1.470(5)
C(201)-C(205)	1.417(5)
C(201)-C(202)	1.434(5)
C(202)-C(203)	1.406(5)
C(203)-C(204)	1.424(6)
C(204)-C(205)	1.422(5)
O(52C)-C(52C)	1.589(14)
O(53A)-O(53A)#3	1.39(7)
O(400)-N(400)	1.215(8)
N(400)-O(400)#4	1.215(8)

N(400)-O(401)	1.215(9)
N(40A)-O(40C)	1.175(9)
N(40A)-O(40A)#4	1.21(2)
N(40A)-N(40A)#4	1.21(2)
N(40A)-O(40B)	1.253(8)
N(40A)-O(40B)#4	1.846(12)
O(40B)-O(40B)#4	1.52(2)
O(40B)-N(40A)#4	1.846(12)
O(100)-La(1)-O(2)	85.89(8)
O(100)-La(1)-O(8)	79.15(9)
O(2)-La(1)-O(8)	145.40(8)
O(100)-La(1)-O(10)	81.46(8)
O(2)-La(1)-O(10)	73.60(7)
O(8)-La(1)-O(10)	73.43(8)
O(100)-La(1)-O(4)	100.48(9)
O(2)-La(1)-O(4)	70.54(7)
O(8)-La(1)-O(4)	142.69(8)
O(10)-La(1)-O(4)	143.81(7)
O(100)-La(1)-O(6)	92.61(8)
O(2)-La(1)-O(6)	141.60(7)
O(8)-La(1)-O(6)	70.70(7)
O(10)-La(1)-O(6)	144.12(7)
O(4)-La(1)-O(6)	72.06(7)
O(100)-La(1)-O(201)	151.65(8)
O(2)-La(1)-O(201)	120.75(8)
O(8)-La(1)-O(201)	73.16(9)
O(10)-La(1)-O(201)	96.15(8)
O(4)-La(1)-O(201)	97.89(8)
O(6)-La(1)-O(201)	72.77(7)
O(100)-La(1)-O(200)	154.22(8)
O(2)-La(1)-O(200)	71.45(9)
O(8)-La(1)-O(200)	112.75(9)
O(10)-La(1)-O(200)	80.48(8)
O(4)-La(1)-O(200)	83.76(8)
O(6)-La(1)-O(200)	112.73(8)
O(201)-La(1)-O(200)	49.35(8)
O(100)-La(1)-C(200)	165.92(8)
O(2)-La(1)-C(200)	96.07(9)
O(8)-La(1)-C(200)	91.68(9)
O(10)-La(1)-C(200)	85.71(8)
O(4)-La(1)-C(200)	93.29(8)
O(6)-La(1)-C(200)	94.42(8)
O(201)-La(1)-C(200)	24.93(9)
O(200)-La(1)-C(200)	24.66(9)
O(2)-Cu(1)-N(10)	92.83(11)
O(2)-Cu(1)-O(1)	84.29(10)
N(10)-Cu(1)-O(1)	171.42(12)
O(2)-Cu(1)-N(9)	173.82(13)
N(10)-Cu(1)-N(9)	81.04(14)
O(1)-Cu(1)-N(9)	101.89(13)
O(2)-Cu(1)-O(52C)	85.5(2)

N(10)-Cu(1)-O(52C)	89.9(3)
O(1)-Cu(1)-O(52C)	97.9(3)
N(9)-Cu(1)-O(52C)	93.7(3)
N(2)-Cu(2)-O(4)	90.80(11)
N(2)-Cu(2)-O(3)	174.18(11)
O(4)-Cu(2)-O(3)	84.05(10)
N(2)-Cu(2)-N(1)	81.22(12)
O(4)-Cu(2)-N(1)	168.86(12)
O(3)-Cu(2)-N(1)	104.24(11)
O(6)-Cu(3)-N(4)	91.77(10)
O(6)-Cu(3)-O(5)	84.31(10)
N(4)-Cu(3)-O(5)	171.22(12)
O(6)-Cu(3)-N(3)	172.34(11)
N(4)-Cu(3)-N(3)	80.67(11)
O(5)-Cu(3)-N(3)	103.02(11)
O(6)-Cu(3)-O(301)	85.98(9)
N(4)-Cu(3)-O(301)	96.96(11)
O(5)-Cu(3)-O(301)	90.62(10)
N(3)-Cu(3)-O(301)	96.03(10)
O(8)-Cu(4)-N(6)	90.68(11)
O(8)-Cu(4)-O(7)	84.31(10)
N(6)-Cu(4)-O(7)	167.94(13)
O(8)-Cu(4)-N(5)	172.44(13)
N(6)-Cu(4)-N(5)	82.23(14)
O(7)-Cu(4)-N(5)	102.13(14)
O(8)-Cu(4)-O(302)	89.16(13)
N(6)-Cu(4)-O(302)	99.43(13)
O(7)-Cu(4)-O(302)	91.49(13)
N(5)-Cu(4)-O(302)	94.6(2)
N(8)-Cu(5)-O(10)	93.14(11)
N(8)-Cu(5)-O(9)	175.83(12)
O(10)-Cu(5)-O(9)	84.23(10)
N(8)-Cu(5)-N(7)	80.77(12)
O(10)-Cu(5)-N(7)	169.61(11)
O(9)-Cu(5)-N(7)	101.34(11)
C(2)-N(1)-Cu(2)	109.7(2)
C(1)-N(2)-O(2)	114.5(3)
C(1)-N(2)-Cu(2)	119.6(2)
O(2)-N(2)-Cu(2)	125.9(2)
C(11)-N(3)-Cu(3)	109.04(19)
C(10)-N(4)-O(4)	115.2(3)
C(10)-N(4)-Cu(3)	118.3(2)
O(4)-N(4)-Cu(3)	126.10(19)
C(20)-N(5)-Cu(4)	112.8(2)
C(19)-N(6)-O(6)	114.7(3)
C(19)-N(6)-Cu(4)	119.0(2)
O(6)-N(6)-Cu(4)	125.8(2)
C(29)-N(7)-Cu(5)	111.69(19)
C(28)-N(8)-O(8)	115.0(3)
C(28)-N(8)-Cu(5)	120.6(2)
O(8)-N(8)-Cu(5)	124.4(2)
C(38)-N(9)-Cu(1)	111.2(2)

C(37)-N(10)-O(10)	114.0(3)
C(37)-N(10)-Cu(1)	116.7(3)
O(10)-N(10)-Cu(1)	126.1(2)
C(1)-O(1)-Cu(1)	107.8(2)
N(2)-O(2)-Cu(1)	109.66(19)
N(2)-O(2)-La(1)	125.26(18)
Cu(1)-O(2)-La(1)	125.06(11)
C(10)-O(3)-Cu(2)	107.81(19)
N(4)-O(4)-Cu(2)	109.85(17)
N(4)-O(4)-La(1)	122.88(17)
Cu(2)-O(4)-La(1)	127.19(11)
C(19)-O(5)-Cu(3)	106.8(2)
N(6)-O(6)-Cu(3)	108.89(17)
N(6)-O(6)-La(1)	123.62(17)
Cu(3)-O(6)-La(1)	123.61(10)
C(28)-O(7)-Cu(4)	107.7(2)
N(8)-O(8)-Cu(4)	109.85(18)
N(8)-O(8)-La(1)	122.45(18)
Cu(4)-O(8)-La(1)	127.63(11)
C(37)-O(9)-Cu(5)	107.4(2)
N(10)-O(10)-Cu(5)	108.89(18)
N(10)-O(10)-La(1)	122.25(18)
Cu(5)-O(10)-La(1)	120.10(10)
O(1)-C(1)-N(2)	123.2(3)
O(1)-C(1)-C(2)	122.4(3)
N(2)-C(1)-C(2)	114.2(3)
N(1)-C(2)-C(1)	107.3(3)
N(1)-C(2)-C(3)	110.6(3)
C(1)-C(2)-C(3)	111.4(3)
C(4)-C(3)-C(2)	110.5(6)
C(4)-C(3)-C(0A)	15.8(6)
C(2)-C(3)-C(0A)	116.1(7)
C(5)-C(4)-C(9)	118.8(10)
C(5)-C(4)-C(3)	119.1(9)
C(9)-C(4)-C(3)	122.1(8)
C(4)-C(5)-C(6)	117.8(10)
C(7)-C(6)-C(5)	118.6(9)
C(6)-C(7)-C(8)	124.9(9)
C(9)-C(8)-C(7)	117.2(9)
C(8)-C(9)-C(4)	122.5(9)
C(0F)-C(0A)-C(0B)	123.4(13)
C(0F)-C(0A)-C(3)	118.7(11)
C(0B)-C(0A)-C(3)	117.6(10)
C(0C)-C(0B)-C(0A)	116.0(11)
C(0D)-C(0C)-C(0B)	125.1(13)
C(0C)-C(0D)-C(0E)	114.7(12)
C(0F)-C(0E)-C(0D)	120.6(14)
C(0E)-C(0F)-C(0A)	120.0(15)
N(4)-C(10)-O(3)	122.9(3)
N(4)-C(10)-C(11)	115.5(3)
O(3)-C(10)-C(11)	121.5(3)
N(3)-C(11)-C(10)	107.9(2)

N(3)-C(11)-C(12)	110.5(3)
C(10)-C(11)-C(12)	110.6(3)
C(13)-C(12)-C(11)	113.3(3)
C(18)-C(13)-C(14)	118.5(3)
C(18)-C(13)-C(12)	121.6(3)
C(14)-C(13)-C(12)	119.9(3)
C(15)-C(14)-C(13)	120.9(3)
C(14)-C(15)-C(16)	120.8(4)
C(17)-C(16)-C(15)	118.3(4)
C(18)-C(17)-C(16)	120.7(4)
C(13)-C(18)-C(17)	120.7(4)
N(6)-C(19)-O(5)	124.1(3)
N(6)-C(19)-C(20)	116.0(3)
O(5)-C(19)-C(20)	119.7(3)
N(5)-C(20)-C(21)	111.5(4)
N(5)-C(20)-C(19)	108.4(3)
C(21)-C(20)-C(19)	107.3(3)
C(20)-C(21)-C(22)	114.2(4)
C(23)-C(22)-C(27)	118.6(4)
C(23)-C(22)-C(21)	121.7(5)
C(27)-C(22)-C(21)	119.6(4)
C(22)-C(23)-C(24)	121.4(6)
C(25)-C(24)-C(23)	121.0(6)
C(24)-C(25)-C(26)	118.1(5)
C(27)-C(26)-C(25)	119.8(6)
C(26)-C(27)-C(22)	121.0(5)
N(8)-C(28)-O(7)	123.2(3)
N(8)-C(28)-C(29)	114.9(3)
O(7)-C(28)-C(29)	121.9(3)
N(7)-C(29)-C(28)	107.6(3)
N(7)-C(29)-C(30)	113.7(3)
C(28)-C(29)-C(30)	111.2(3)
C(31)-C(30)-C(29)	111.2(3)
C(32)-C(31)-C(36)	119.0(4)
C(32)-C(31)-C(30)	121.6(4)
C(36)-C(31)-C(30)	119.4(4)
C(31)-C(32)-C(33)	120.0(5)
C(34)-C(33)-C(32)	119.5(5)
C(35)-C(34)-C(33)	121.1(4)
C(34)-C(35)-C(36)	119.2(5)
C(35)-C(36)-C(31)	121.2(5)
O(9)-C(37)-N(10)	124.5(3)
O(9)-C(37)-C(38)	120.5(3)
N(10)-C(37)-C(38)	114.9(3)
N(9)-C(38)-C(39)	111.3(4)
N(9)-C(38)-C(37)	108.2(3)
C(39)-C(38)-C(37)	112.4(4)
C(40)-C(39)-C(38)	114.1(3)
C(45)-C(40)-C(41)	118.3(4)
C(45)-C(40)-C(39)	121.0(4)
C(41)-C(40)-C(39)	120.6(4)
C(42)-C(41)-C(40)	120.5(4)

C(43)-C(42)-C(41)	119.7(4)
C(42)-C(43)-C(44)	120.3(5)
C(45)-C(44)-C(43)	119.9(4)
C(40)-C(45)-C(44)	121.2(4)
C(105)-Fe(1)-C(105)#1	112.4(2)
C(105)-Fe(1)-C(101)#1	41.16(13)
C(105)#1-Fe(1)-C(101)#1	107.79(14)
C(105)-Fe(1)-C(101)	107.79(14)
C(105)#1-Fe(1)-C(101)	41.16(13)
C(101)#1-Fe(1)-C(101)	132.6(2)
C(105)-Fe(1)-C(103)#1	143.97(15)
C(105)#1-Fe(1)-C(103)#1	41.14(14)
C(101)#1-Fe(1)-C(103)#1	113.39(15)
C(101)-Fe(1)-C(103)#1	69.10(14)
C(105)-Fe(1)-C(103)	41.14(14)
C(105)#1-Fe(1)-C(103)	143.97(15)
C(101)#1-Fe(1)-C(103)	69.10(14)
C(101)-Fe(1)-C(103)	113.39(15)
C(103)#1-Fe(1)-C(103)	174.3(2)
C(105)-Fe(1)-C(102)	133.61(15)
C(105)#1-Fe(1)-C(102)	68.86(14)
C(101)#1-Fe(1)-C(102)	173.05(15)
C(101)-Fe(1)-C(102)	40.98(14)
C(103)#1-Fe(1)-C(102)	68.45(16)
C(103)-Fe(1)-C(102)	109.75(16)
C(105)-Fe(1)-C(102)#1	68.86(14)
C(105)#1-Fe(1)-C(102)#1	133.61(15)
C(101)#1-Fe(1)-C(102)#1	40.98(14)
C(101)-Fe(1)-C(102)#1	173.05(15)
C(103)#1-Fe(1)-C(102)#1	109.75(16)
C(103)-Fe(1)-C(102)#1	68.45(16)
C(102)-Fe(1)-C(102)#1	145.6(2)
C(105)-Fe(1)-C(104)#1	173.15(15)
C(105)#1-Fe(1)-C(104)#1	69.30(15)
C(101)#1-Fe(1)-C(104)#1	145.44(14)
C(101)-Fe(1)-C(104)#1	68.78(14)
C(103)#1-Fe(1)-C(104)#1	41.31(16)
C(103)-Fe(1)-C(104)#1	133.93(16)
C(102)-Fe(1)-C(104)#1	40.06(15)
C(102)#1-Fe(1)-C(104)#1	115.20(15)
C(105)-Fe(1)-C(104)	69.30(15)
C(105)#1-Fe(1)-C(104)	173.15(15)
C(101)#1-Fe(1)-C(104)	68.78(14)
C(101)-Fe(1)-C(104)	145.44(14)
C(103)#1-Fe(1)-C(104)	133.93(16)
C(103)-Fe(1)-C(104)	41.31(16)
C(102)-Fe(1)-C(104)	115.20(15)
C(102)#1-Fe(1)-C(104)	40.06(15)
C(104)#1-Fe(1)-C(104)	109.9(2)
C(100)-O(100)-La(1)	142.6(2)
O(101)-C(100)-O(100)	125.1(3)
O(101)-C(100)-C(101)	119.7(3)

O(100)-C(100)-C(101)	115.1(3)
C(102)-C(101)-C(105)#1	107.7(3)
C(102)-C(101)-C(100)	123.7(3)
C(105)#1-C(101)-C(100)	128.5(3)
C(102)-C(101)-Fe(1)	70.0(2)
C(105)#1-C(101)-Fe(1)	69.40(19)
C(100)-C(101)-Fe(1)	122.6(2)
C(104)#1-C(102)-C(101)	109.1(3)
C(104)#1-C(102)-Fe(1)	70.2(2)
C(101)-C(102)-Fe(1)	69.0(2)
C(105)-C(103)-C(104)	108.0(3)
C(105)-C(103)-Fe(1)	69.3(2)
C(104)-C(103)-Fe(1)	69.9(2)
C(102)#1-C(104)-C(103)	107.6(3)
C(102)#1-C(104)-Fe(1)	69.8(2)
C(103)-C(104)-Fe(1)	68.7(2)
C(101)#1-C(105)-C(103)	107.7(3)
C(101)#1-C(105)-Fe(1)	69.44(19)
C(103)-C(105)-Fe(1)	69.5(2)
C(201)-Fe(2)-C(201)#2	146.4(2)
C(201)-Fe(2)-C(202)	41.64(13)
C(201)#2-Fe(2)-C(202)	113.44(14)
C(201)-Fe(2)-C(202)#2	113.44(14)
C(201)#2-Fe(2)-C(202)#2	41.64(13)
C(202)-Fe(2)-C(202)#2	105.6(2)
C(201)-Fe(2)-C(205)#2	170.73(15)
C(201)#2-Fe(2)-C(205)#2	40.93(15)
C(202)-Fe(2)-C(205)#2	147.42(14)
C(202)#2-Fe(2)-C(205)#2	69.01(16)
C(201)-Fe(2)-C(205)	40.93(15)
C(201)#2-Fe(2)-C(205)	170.73(15)
C(202)-Fe(2)-C(205)	69.01(16)
C(202)#2-Fe(2)-C(205)	147.42(14)
C(205)#2-Fe(2)-C(205)	132.8(2)
C(201)-Fe(2)-C(203)	68.72(13)
C(201)#2-Fe(2)-C(203)	107.46(14)
C(202)-Fe(2)-C(203)	40.28(15)
C(202)#2-Fe(2)-C(203)	129.14(16)
C(205)#2-Fe(2)-C(203)	117.27(15)
C(205)-Fe(2)-C(203)	68.22(15)
C(201)-Fe(2)-C(203)#2	107.46(14)
C(201)#2-Fe(2)-C(203)#2	68.72(13)
C(202)-Fe(2)-C(203)#2	129.14(16)
C(202)#2-Fe(2)-C(203)#2	40.28(15)
C(205)#2-Fe(2)-C(203)#2	68.22(15)
C(205)-Fe(2)-C(203)#2	117.27(15)
C(203)-Fe(2)-C(203)#2	167.5(2)
C(201)-Fe(2)-C(204)#2	131.18(14)
C(201)#2-Fe(2)-C(204)#2	68.41(15)
C(202)-Fe(2)-C(204)#2	168.88(16)
C(202)#2-Fe(2)-C(204)#2	68.09(16)
C(205)#2-Fe(2)-C(204)#2	40.40(15)

C(205)-Fe(2)-C(204)#2	111.03(17)
C(203)-Fe(2)-C(204)#2	150.73(17)
C(203)#2-Fe(2)-C(204)#2	40.28(17)
C(201)-Fe(2)-C(204)	68.41(15)
C(201)#2-Fe(2)-C(204)	131.18(14)
C(202)-Fe(2)-C(204)	68.09(16)
C(202)#2-Fe(2)-C(204)	168.88(16)
C(205)#2-Fe(2)-C(204)	111.03(17)
C(205)-Fe(2)-C(204)	40.40(15)
C(203)-Fe(2)-C(204)	40.28(17)
C(203)#2-Fe(2)-C(204)	150.73(17)
C(204)#2-Fe(2)-C(204)	119.6(3)
C(200)-O(200)-La(1)	93.9(2)
C(200)-O(201)-La(1)	95.1(2)
O(200)-C(200)-O(201)	120.4(3)
O(200)-C(200)-C(201)	120.2(3)
O(201)-C(200)-C(201)	119.3(3)
O(200)-C(200)-La(1)	61.41(18)
O(201)-C(200)-La(1)	59.95(18)
C(201)-C(200)-La(1)	168.9(2)
C(205)-C(201)-C(202)	107.8(3)
C(205)-C(201)-C(200)	125.0(3)
C(202)-C(201)-C(200)	126.2(3)
C(205)-C(201)-Fe(2)	70.7(2)
C(202)-C(201)-Fe(2)	69.67(18)
C(200)-C(201)-Fe(2)	116.0(2)
C(203)-C(202)-C(201)	108.0(3)
C(203)-C(202)-Fe(2)	71.2(2)
C(201)-C(202)-Fe(2)	68.69(19)
C(202)-C(203)-C(204)	108.4(3)
C(202)-C(203)-Fe(2)	68.5(2)
C(204)-C(203)-Fe(2)	70.4(2)
C(205)-C(204)-C(203)	107.9(4)
C(205)-C(204)-Fe(2)	68.6(2)
C(203)-C(204)-Fe(2)	69.3(2)
C(201)-C(205)-C(204)	108.0(3)
C(201)-C(205)-Fe(2)	68.33(19)
C(204)-C(205)-Fe(2)	71.0(2)
C(52C)-O(52C)-Cu(1)	127.8(7)
O(400)#4-N(400)-O(400)	116.0(12)
O(400)#4-N(400)-O(401)	122.0(6)
O(400)-N(400)-O(401)	122.0(6)
O(40C)-N(40A)-O(40A)#4	135.3(11)
O(40C)-N(40A)-N(40A)#4	135.3(11)
O(40A)#4-N(40A)-N(40A)#4	0.0(9)
O(40C)-N(40A)-O(40B)	127.2(15)
O(40A)#4-N(40A)-O(40B)	97.1(7)
N(40A)#4-N(40A)-O(40B)	97.1(7)
O(40C)-N(40A)-O(40B)#4	170.8(16)
O(40A)#4-N(40A)-O(40B)#4	42.3(4)
N(40A)#4-N(40A)-O(40B)#4	42.3(4)
O(40B)-N(40A)-O(40B)#4	54.9(8)

N(40A)-O(40B)-O(40B)#4 82.8(7)
N(40A)-O(40B)-N(40A)#4 40.6(8)
O(40B)#4-O(40B)-N(40A)#4 42.3(4)

Symmetry transformations used to generate equivalent atoms:

#1 $x+0, -y+0, -z+1/2$ #2 $-x-1/2, y+0, -z+1$

#3 $-x+0, -y-1/2, z+0$ #4 $-x+1/2, y+0, -z+1$

S43: Crystallographic tables for Dy^{III}(benzoate)₂[15-MC_L-pHeHA-5](benzoate)_{0.75}Cl_{0.25}

Crystal data and structure refinement for Dy^{III}(benzoate)₂[15-MC_L-pHeHA-5](benzoate)_{0.75}Cl_{0.25}

Empirical formula C132.25 H174.75 Cl0.25 Cu10 Dy2 N20 O52.50

Formula weight 3853.93

Temperature 85(2) K

Wavelength 0.71073 Å

Crystal system, space group Monoclinic, P2(1)

Unit cell dimensions a = 15.5327(7) Å alpha = 90 deg.
b = 25.4741(12) Å beta = 98.379(1) deg.
c = 19.7410(9) Å gamma = 90 deg.

Volume 7727.8(6) Å³

Z, Calculated density 2, 1.656 Mg/m³

Absorption coefficient 2.394 mm⁻¹

F(000) 3909

Crystal size 0.44 x 0.34 x 0.12 mm

Theta range for data collection 1.31 to 29.58 deg.

Limiting indices -21 ≤ h ≤ 21, -35 ≤ k ≤ 35, -27 ≤ l ≤ 27

Reflections collected / unique 299821 / 43365 [R(int) = 0.0309]

Completeness to theta = 29.58 99.9 %

Absorption correction Semi-empirical from equivalents

Max. and min. transmission 0.6299 and 0.5109

Refinement method Full-matrix least-squares on F²

Data / restraints / parameters 43365 / 555 / 2171

Goodness-of-fit on F² 1.153

Final R indices [$I > 2\sigma(I)$] R1 = 0.0353, wR2 = 0.0909

R indices (all data) R1 = 0.0384, wR2 = 0.0931

Absolute structure parameter -0.018(5)

Largest diff. peak and hole 1.287 and -0.872 e. \AA^{-3}

Bond lengths [\AA] and angles [deg] for Dy^{III}(benzoate)₂[15-MC_L-pheHA-5](benzoate)_{0.75}Cl_{0.25}

Dy(1)-O(300)	2.263(3)
Dy(1)-O(2)	2.396(3)
Dy(1)-O(10)	2.396(3)
Dy(1)-O(6)	2.398(3)
Dy(1)-O(8)	2.401(3)
Dy(1)-O(100)	2.414(4)
Dy(1)-O(4)	2.425(3)
Dy(1)-O(101)	2.496(4)
Dy(1)-C(100)	2.822(14)
Dy(1)-C(10G)	2.852(12)
Dy(2)-O(250)	2.260(3)
Dy(2)-O(18)	2.345(3)
Dy(2)-O(111)	2.372(9)
Dy(2)-O(12)	2.392(3)
Dy(2)-O(20)	2.404(3)
Dy(2)-O(16)	2.420(3)
Dy(2)-O(14)	2.427(3)
Dy(2)-O(11A)	2.476(11)
Dy(2)-O(110)	2.514(3)
Dy(2)-C(110)	2.824(16)
Dy(2)-C(11A)	2.851(16)
Cu(1)-N(10)	1.907(3)
Cu(1)-O(2)	1.948(3)
Cu(1)-O(1)	1.959(3)
Cu(1)-N(9)	2.037(4)
Cu(1)-O(401)	2.311(4)
Cu(2)-N(2)	1.902(3)
Cu(2)-O(3)	1.929(3)
Cu(2)-O(4)	1.946(3)
Cu(2)-N(1)	2.010(4)
Cu(2)-O(404)	2.344(4)
Cu(3)-N(4)	1.900(3)
Cu(3)-O(5)	1.945(3)
Cu(3)-O(6)	1.948(3)
Cu(3)-N(3)	2.040(4)
Cu(3)-O(400)	2.386(4)
Cu(4)-N(6)	1.883(4)
Cu(4)-O(7)	1.916(3)
Cu(4)-O(8)	1.919(3)
Cu(4)-N(5)	2.011(3)
Cu(5)-N(8)	1.885(3)

Cu(5)-O(9)	1.923(3)
Cu(5)-O(10)	1.936(3)
Cu(5)-N(7)	2.031(3)
Cu(6)-N(20)	1.904(4)
Cu(6)-O(12)	1.917(3)
Cu(6)-O(11)	1.944(3)
Cu(6)-N(19)	1.980(3)
Cu(7)-N(12)	1.880(3)
Cu(7)-O(13)	1.914(3)
Cu(7)-O(14)	1.923(3)
Cu(7)-N(11)	2.004(3)
Cu(8)-N(14)	1.907(3)
Cu(8)-O(16)	1.925(3)
Cu(8)-O(15)	1.933(3)
Cu(8)-N(13)	2.024(3)
Cu(9)-N(16)	1.903(4)
Cu(9)-O(18)	1.938(3)
Cu(9)-O(17)	1.961(3)
Cu(9)-N(15)	2.018(4)
Cu(9)-O(402)	2.285(4)
Cu(10)-N(18)	1.914(4)
Cu(10)-O(19)	1.945(3)
Cu(10)-O(20)	1.947(3)
Cu(10)-N(17)	2.010(4)
Cu(10)-O(403)	2.352(5)
N(1)-C(2)	1.491(6)
N(2)-C(1)	1.307(5)
N(2)-O(2)	1.387(4)
N(3)-C(11)	1.485(6)
N(4)-C(10)	1.286(5)
N(4)-O(4)	1.405(4)
N(5)-C(20)	1.489(5)
N(6)-C(19)	1.299(5)
N(6)-O(6)	1.404(4)
N(7)-C(29)	1.495(5)
N(8)-C(28)	1.296(5)
N(8)-O(8)	1.402(4)
N(9)-C(38)	1.478(6)
N(10)-C(37)	1.281(6)
N(10)-O(10)	1.386(4)
N(11)-C(47)	1.486(5)
N(12)-C(46)	1.321(5)
N(12)-O(12)	1.395(4)
N(13)-C(56)	1.491(5)
N(14)-C(55)	1.288(5)
N(14)-O(14)	1.377(4)
N(15)-C(65)	1.502(6)
N(16)-C(64)	1.290(5)
N(16)-O(16)	1.393(4)
N(17)-C(74)	1.494(6)
N(18)-C(73)	1.289(5)
N(18)-O(18)	1.383(4)

N(19)-C(83)	1.479(6)
N(20)-C(82)	1.295(5)
N(20)-O(20)	1.387(4)
O(1)-C(1)	1.300(5)
O(3)-C(10)	1.289(5)
O(5)-C(19)	1.289(5)
O(7)-C(28)	1.296(4)
O(9)-C(37)	1.306(5)
O(11)-C(46)	1.279(5)
O(13)-C(55)	1.298(5)
O(15)-C(64)	1.303(5)
O(17)-C(73)	1.293(5)
O(19)-C(82)	1.283(5)
C(1)-C(2)	1.514(6)
C(2)-C(3)	1.538(6)
C(3)-C(4)	1.519(9)
C(4)-C(9)	1.355(9)
C(4)-C(5)	1.414(10)
C(5)-C(6)	1.368(14)
C(6)-C(7)	1.404(16)
C(7)-C(8)	1.376(13)
C(8)-C(9)	1.394(9)
C(10)-C(11)	1.502(6)
C(11)-C(12)	1.557(7)
C(12)-C(13)	1.500(6)
C(13)-C(18)	1.386(7)
C(13)-C(14)	1.397(6)
C(14)-C(15)	1.387(7)
C(15)-C(16)	1.350(9)
C(16)-C(17)	1.398(8)
C(17)-C(18)	1.379(8)
C(19)-C(20)	1.507(6)
C(20)-C(21)	1.536(7)
C(21)-C(22)	1.518(6)
C(22)-C(23)	1.385(7)
C(22)-C(27)	1.407(7)
C(23)-C(24)	1.393(8)
C(24)-C(25)	1.381(10)
C(25)-C(26)	1.368(10)
C(26)-C(27)	1.385(8)
C(28)-C(29)	1.505(5)
C(29)-C(30)	1.532(5)
C(30)-C(31)	1.510(5)
C(31)-C(36)	1.378(6)
C(31)-C(32)	1.393(6)
C(32)-C(33)	1.399(7)
C(33)-C(34)	1.363(8)
C(34)-C(35)	1.380(8)
C(35)-C(36)	1.405(6)
C(37)-C(38)	1.522(6)
C(38)-C(39)	1.547(6)
C(39)-C(40)	1.520(6)

C(40)-C(45)	1.375(7)
C(40)-C(41)	1.398(8)
C(41)-C(42)	1.387(7)
C(42)-C(43)	1.405(9)
C(43)-C(44)	1.366(9)
C(44)-C(45)	1.406(7)
C(46)-C(47)	1.524(5)
C(47)-C(48)	1.536(6)
C(48)-C(49)	1.508(6)
C(49)-C(54)	1.389(6)
C(49)-C(50)	1.393(6)
C(50)-C(51)	1.402(7)
C(51)-C(52)	1.382(8)
C(52)-C(53)	1.381(8)
C(53)-C(54)	1.393(7)
C(55)-C(56)	1.523(5)
C(56)-C(57)	1.536(6)
C(57)-C(58)	1.509(5)
C(58)-C(59)	1.369(6)
C(58)-C(63)	1.387(7)
C(59)-C(60)	1.388(7)
C(60)-C(61)	1.350(9)
C(61)-C(62)	1.392(9)
C(62)-C(63)	1.390(7)
C(64)-C(65)	1.527(6)
C(65)-C(66)	1.527(6)
C(66)-C(67)	1.519(6)
C(67)-C(68)	1.367(8)
C(67)-C(72)	1.383(7)
C(68)-C(69)	1.430(10)
C(69)-C(70)	1.359(13)
C(70)-C(71)	1.346(12)
C(71)-C(72)	1.368(8)
C(73)-C(74)	1.513(6)
C(74)-C(75)	1.506(9)
C(75)-C(76)	1.556(8)
C(76)-C(77)	1.3900
C(76)-C(81)	1.3900
C(77)-C(78)	1.3900
C(78)-C(79)	1.3900
C(79)-C(80)	1.3900
C(80)-C(81)	1.3900
C(82)-C(83)	1.522(6)
C(83)-C(84)	1.551(7)
C(84)-C(85)	1.510(7)
C(85)-C(86)	1.393(7)
C(85)-C(90)	1.403(8)
C(86)-C(87)	1.364(8)
C(87)-C(88)	1.405(10)
C(88)-C(89)	1.384(10)
C(89)-C(90)	1.385(9)
O(100)-C(100)	1.19(2)

O(100)-C(10G)	1.32(2)
O(101)-C(10G)	1.20(2)
O(101)-C(100)	1.30(2)
O(110)-C(110)	1.15(2)
O(110)-C(11A)	1.384(19)
C(100)-C(101)	1.504(13)
C(101)-C(102)	1.367(12)
C(101)-C(106)	1.401(12)
C(102)-C(103)	1.389(13)
C(103)-C(104)	1.397(15)
C(104)-C(105)	1.411(14)
C(105)-C(106)	1.378(13)
O(111)-C(110)	1.27(2)
C(110)-C(111)	1.512(19)
C(111)-C(112)	1.35(3)
C(111)-C(116)	1.375(19)
C(112)-C(113)	1.40(2)
C(113)-C(114)	1.36(6)
C(114)-C(115)	1.34(3)
C(115)-C(116)	1.369(14)
O(120)-C(120)	1.30(2)
O(121)-C(120)	1.29(3)
C(120)-C(121)	1.515(14)
C(121)-C(126)	1.366(13)
C(121)-C(122)	1.370(14)
C(122)-C(123)	1.405(14)
C(123)-C(124)	1.408(15)
C(124)-C(125)	1.439(15)
C(125)-C(126)	1.375(14)
C(10G)-C(10A)	1.508(11)
C(10A)-C(10B)	1.371(14)
C(10A)-C(10F)	1.392(14)
C(10B)-C(10C)	1.392(14)
C(10C)-C(10D)	1.402(17)
C(10D)-C(10E)	1.395(15)
C(10E)-C(10F)	1.383(13)
O(11A)-C(11A)	1.26(2)
C(11A)-C(11B)	1.503(14)
C(11B)-C(11C)	1.364(15)
C(11B)-C(11G)	1.409(13)
C(11C)-C(11D)	1.393(16)
C(11D)-C(11E)	1.400(17)
C(11E)-C(11F)	1.412(14)
C(11F)-C(11G)	1.379(13)
O(150)-C(150)	1.240(11)
O(151)-C(150)	1.273(12)
C(150)-C(151)	1.518(11)
C(151)-C(156)	1.376(9)
C(151)-C(152)	1.396(9)
C(152)-C(153)	1.362(10)
C(153)-C(154)	1.377(11)
C(154)-C(155)	1.372(14)

C(155)-C(156)	1.398(12)
O(250)-C(250)	1.271(6)
O(251)-C(250)	1.252(6)
C(250)-C(251)	1.498(6)
C(251)-C(252)	1.382(7)
C(251)-C(256)	1.395(6)
C(252)-C(253)	1.387(7)
C(253)-C(254)	1.393(7)
C(254)-C(255)	1.385(8)
C(255)-C(256)	1.382(8)
O(300)-C(300)	1.276(6)
O(301)-C(300)	1.242(7)
C(300)-C(301)	1.522(8)
C(301)-C(306)	1.366(10)
C(301)-C(302)	1.371(11)
C(302)-C(303)	1.387(11)
C(303)-C(304)	1.388(16)
C(304)-C(305)	1.333(16)
C(305)-C(306)	1.371(11)
O(404)-C(404)	1.401(8)
O(506)-C(506)	1.423(7)

O(300)-Dy(1)-O(2)	94.45(11)
O(300)-Dy(1)-O(10)	81.90(12)
O(2)-Dy(1)-O(10)	71.53(9)
O(300)-Dy(1)-O(6)	85.37(12)
O(2)-Dy(1)-O(6)	143.17(9)
O(10)-Dy(1)-O(6)	144.10(9)
O(300)-Dy(1)-O(8)	78.47(11)
O(2)-Dy(1)-O(8)	144.22(9)
O(10)-Dy(1)-O(8)	72.76(9)
O(6)-Dy(1)-O(8)	71.86(9)
O(300)-Dy(1)-O(100)	148.51(12)
O(2)-Dy(1)-O(100)	93.17(17)
O(10)-Dy(1)-O(100)	71.69(15)
O(6)-Dy(1)-O(100)	106.03(17)
O(8)-Dy(1)-O(100)	77.56(15)
O(300)-Dy(1)-O(4)	86.66(10)
O(2)-Dy(1)-O(4)	70.62(9)
O(10)-Dy(1)-O(4)	139.31(10)
O(6)-Dy(1)-O(4)	72.61(10)
O(8)-Dy(1)-O(4)	142.34(9)
O(100)-Dy(1)-O(4)	124.60(13)
O(300)-Dy(1)-O(101)	159.15(11)
O(2)-Dy(1)-O(101)	85.46(12)
O(10)-Dy(1)-O(101)	117.50(12)
O(6)-Dy(1)-O(101)	82.39(12)
O(8)-Dy(1)-O(101)	113.23(12)
O(100)-Dy(1)-O(101)	52.02(13)
O(4)-Dy(1)-O(101)	73.61(12)
O(300)-Dy(1)-C(100)	173.0(5)
O(2)-Dy(1)-C(100)	88.3(5)

O(10)-Dy(1)-C(100)	92.9(5)
O(6)-Dy(1)-C(100)	96.3(5)
O(8)-Dy(1)-C(100)	95.6(4)
O(100)-Dy(1)-C(100)	24.6(5)
O(4)-Dy(1)-C(100)	100.3(5)
O(101)-Dy(1)-C(100)	27.5(5)
O(300)-Dy(1)-C(10G)	175.6(5)
O(2)-Dy(1)-C(10G)	87.8(6)
O(10)-Dy(1)-C(10G)	95.3(5)
O(6)-Dy(1)-C(10G)	95.0(5)
O(8)-Dy(1)-C(10G)	97.5(5)
O(100)-Dy(1)-C(10G)	27.4(5)
O(4)-Dy(1)-C(10G)	97.6(5)
O(101)-Dy(1)-C(10G)	24.7(5)
C(100)-Dy(1)-C(10G)	2.7(9)
O(250)-Dy(2)-O(18)	89.34(11)
O(250)-Dy(2)-O(111)	152.3(2)
O(18)-Dy(2)-O(111)	90.35(19)
O(250)-Dy(2)-O(12)	90.15(11)
O(18)-Dy(2)-O(12)	144.80(9)
O(111)-Dy(2)-O(12)	105.60(19)
O(250)-Dy(2)-O(20)	81.73(11)
O(18)-Dy(2)-O(20)	72.18(10)
O(111)-Dy(2)-O(20)	124.3(2)
O(12)-Dy(2)-O(20)	72.92(10)
O(250)-Dy(2)-O(16)	76.46(10)
O(18)-Dy(2)-O(16)	73.35(9)
O(111)-Dy(2)-O(16)	76.9(2)
O(12)-Dy(2)-O(16)	140.22(10)
O(20)-Dy(2)-O(16)	139.07(10)
O(250)-Dy(2)-O(14)	90.03(11)
O(18)-Dy(2)-O(14)	143.69(9)
O(111)-Dy(2)-O(14)	74.2(2)
O(12)-Dy(2)-O(14)	71.51(9)
O(20)-Dy(2)-O(14)	143.41(10)
O(16)-Dy(2)-O(14)	71.23(9)
O(250)-Dy(2)-O(11A)	144.4(3)
O(18)-Dy(2)-O(11A)	79.1(3)
O(111)-Dy(2)-O(11A)	12.9(2)
O(12)-Dy(2)-O(11A)	118.4(2)
O(20)-Dy(2)-O(11A)	124.9(3)
O(16)-Dy(2)-O(11A)	68.0(3)
O(14)-Dy(2)-O(11A)	80.6(3)
O(250)-Dy(2)-O(110)	156.08(12)
O(18)-Dy(2)-O(110)	81.06(11)
O(111)-Dy(2)-O(110)	50.4(2)
O(12)-Dy(2)-O(110)	85.41(11)
O(20)-Dy(2)-O(110)	74.49(12)
O(16)-Dy(2)-O(110)	120.72(11)
O(14)-Dy(2)-O(110)	110.64(11)
O(11A)-Dy(2)-O(110)	55.0(3)
O(250)-Dy(2)-C(110)	172.3(3)

O(18)-Dy(2)-C(110)	83.2(3)
O(111)-Dy(2)-C(110)	26.6(5)
O(12)-Dy(2)-C(110)	97.1(3)
O(20)-Dy(2)-C(110)	97.8(5)
O(16)-Dy(2)-C(110)	99.3(4)
O(14)-Dy(2)-C(110)	94.8(4)
O(11A)-Dy(2)-C(110)	31.7(4)
O(110)-Dy(2)-C(110)	23.9(4)
O(250)-Dy(2)-C(11A)	164.5(3)
O(18)-Dy(2)-C(11A)	77.0(4)
O(111)-Dy(2)-C(11A)	24.2(5)
O(12)-Dy(2)-C(11A)	105.2(3)
O(20)-Dy(2)-C(11A)	100.6(5)
O(16)-Dy(2)-C(11A)	92.5(4)
O(14)-Dy(2)-C(11A)	96.7(5)
O(11A)-Dy(2)-C(11A)	26.1(5)
O(110)-Dy(2)-C(11A)	29.0(4)
C(110)-Dy(2)-C(11A)	8.1(4)
N(10)-Cu(1)-O(2)	89.67(13)
N(10)-Cu(1)-O(1)	167.66(17)
O(2)-Cu(1)-O(1)	85.26(12)
N(10)-Cu(1)-N(9)	81.84(15)
O(2)-Cu(1)-N(9)	166.83(16)
O(1)-Cu(1)-N(9)	101.01(14)
N(10)-Cu(1)-O(401)	98.86(16)
O(2)-Cu(1)-O(401)	98.48(13)
O(1)-Cu(1)-O(401)	93.02(14)
N(9)-Cu(1)-O(401)	92.79(18)
N(2)-Cu(2)-O(3)	171.77(15)
N(2)-Cu(2)-O(4)	88.92(13)
O(3)-Cu(2)-O(4)	85.63(12)
N(2)-Cu(2)-N(1)	83.54(15)
O(3)-Cu(2)-N(1)	101.53(14)
O(4)-Cu(2)-N(1)	171.86(15)
N(2)-Cu(2)-O(404)	97.54(16)
O(3)-Cu(2)-O(404)	88.99(16)
O(4)-Cu(2)-O(404)	94.00(14)
N(1)-Cu(2)-O(404)	90.01(17)
N(4)-Cu(3)-O(5)	171.74(16)
N(4)-Cu(3)-O(6)	90.72(13)
O(5)-Cu(3)-O(6)	85.34(12)
N(4)-Cu(3)-N(3)	80.68(15)
O(5)-Cu(3)-N(3)	102.97(15)
O(6)-Cu(3)-N(3)	171.24(14)
N(4)-Cu(3)-O(400)	95.53(17)
O(5)-Cu(3)-O(400)	91.73(16)
O(6)-Cu(3)-O(400)	89.97(17)
N(3)-Cu(3)-O(400)	92.53(18)
N(6)-Cu(4)-O(7)	175.50(16)
N(6)-Cu(4)-O(8)	91.06(14)
O(7)-Cu(4)-O(8)	86.16(12)
N(6)-Cu(4)-N(5)	83.49(15)

O(7)-Cu(4)-N(5)	99.20(14)
O(8)-Cu(4)-N(5)	174.39(14)
N(8)-Cu(5)-O(9)	175.64(14)
N(8)-Cu(5)-O(10)	90.98(12)
O(9)-Cu(5)-O(10)	85.77(12)
N(8)-Cu(5)-N(7)	82.68(13)
O(9)-Cu(5)-N(7)	100.24(13)
O(10)-Cu(5)-N(7)	171.32(13)
N(20)-Cu(6)-O(12)	90.79(13)
N(20)-Cu(6)-O(11)	176.72(14)
O(12)-Cu(6)-O(11)	86.21(12)
N(20)-Cu(6)-N(19)	81.89(15)
O(12)-Cu(6)-N(19)	172.49(14)
O(11)-Cu(6)-N(19)	101.14(14)
N(12)-Cu(7)-O(13)	176.19(13)
N(12)-Cu(7)-O(14)	90.32(13)
O(13)-Cu(7)-O(14)	86.03(12)
N(12)-Cu(7)-N(11)	83.39(14)
O(13)-Cu(7)-N(11)	100.21(14)
O(14)-Cu(7)-N(11)	173.12(13)
N(14)-Cu(8)-O(16)	90.15(13)
N(14)-Cu(8)-O(15)	174.19(13)
O(16)-Cu(8)-O(15)	84.91(12)
N(14)-Cu(8)-N(13)	83.26(14)
O(16)-Cu(8)-N(13)	172.88(13)
O(15)-Cu(8)-N(13)	101.52(13)
N(16)-Cu(9)-O(18)	90.69(13)
N(16)-Cu(9)-O(17)	167.19(15)
O(18)-Cu(9)-O(17)	84.07(12)
N(16)-Cu(9)-N(15)	82.46(15)
O(18)-Cu(9)-N(15)	168.48(14)
O(17)-Cu(9)-N(15)	100.67(14)
N(16)-Cu(9)-O(402)	98.04(15)
O(18)-Cu(9)-O(402)	90.94(14)
O(17)-Cu(9)-O(402)	93.74(14)
N(15)-Cu(9)-O(402)	99.16(16)
N(18)-Cu(10)-O(19)	171.25(16)
N(18)-Cu(10)-O(20)	89.10(14)
O(19)-Cu(10)-O(20)	84.65(13)
N(18)-Cu(10)-N(17)	83.73(16)
O(19)-Cu(10)-N(17)	100.85(15)
O(20)-Cu(10)-N(17)	164.70(16)
N(18)-Cu(10)-O(403)	92.23(16)
O(19)-Cu(10)-O(403)	95.06(16)
O(20)-Cu(10)-O(403)	102.08(15)
N(17)-Cu(10)-O(403)	91.72(19)
C(2)-N(1)-Cu(2)	111.4(3)
C(1)-N(2)-O(2)	116.5(3)
C(1)-N(2)-Cu(2)	118.4(3)
O(2)-N(2)-Cu(2)	125.1(2)
C(11)-N(3)-Cu(3)	107.7(2)
C(10)-N(4)-O(4)	115.7(3)

C(10)-N(4)-Cu(3)	119.3(3)
O(4)-N(4)-Cu(3)	124.7(2)
C(20)-N(5)-Cu(4)	110.1(3)
C(19)-N(6)-O(6)	115.8(3)
C(19)-N(6)-Cu(4)	118.5(3)
O(6)-N(6)-Cu(4)	123.8(3)
C(29)-N(7)-Cu(5)	110.9(2)
C(28)-N(8)-O(8)	114.9(3)
C(28)-N(8)-Cu(5)	119.6(3)
O(8)-N(8)-Cu(5)	125.3(2)
C(38)-N(9)-Cu(1)	109.8(2)
C(37)-N(10)-O(10)	116.0(3)
C(37)-N(10)-Cu(1)	119.1(3)
O(10)-N(10)-Cu(1)	124.4(2)
C(47)-N(11)-Cu(7)	110.3(3)
C(46)-N(12)-O(12)	114.4(3)
C(46)-N(12)-Cu(7)	118.7(3)
O(12)-N(12)-Cu(7)	125.3(2)
C(56)-N(13)-Cu(8)	110.9(2)
C(55)-N(14)-O(14)	115.8(3)
C(55)-N(14)-Cu(8)	118.7(3)
O(14)-N(14)-Cu(8)	125.2(2)
C(65)-N(15)-Cu(9)	112.1(3)
C(64)-N(16)-O(16)	114.5(3)
C(64)-N(16)-Cu(9)	120.4(3)
O(16)-N(16)-Cu(9)	125.1(3)
C(74)-N(17)-Cu(10)	110.8(3)
C(73)-N(18)-O(18)	116.0(3)
C(73)-N(18)-Cu(10)	118.0(3)
O(18)-N(18)-Cu(10)	124.8(3)
C(83)-N(19)-Cu(6)	109.8(3)
C(82)-N(20)-O(20)	115.3(4)
C(82)-N(20)-Cu(6)	117.3(3)
O(20)-N(20)-Cu(6)	125.6(3)
C(1)-O(1)-Cu(1)	107.0(2)
N(2)-O(2)-Cu(1)	107.4(2)
N(2)-O(2)-Dy(1)	124.7(2)
Cu(1)-O(2)-Dy(1)	127.75(12)
C(10)-O(3)-Cu(2)	106.9(2)
N(4)-O(4)-Cu(2)	106.4(2)
N(4)-O(4)-Dy(1)	124.1(2)
Cu(2)-O(4)-Dy(1)	124.85(13)
C(19)-O(5)-Cu(3)	106.9(3)
N(6)-O(6)-Cu(3)	106.6(2)
N(6)-O(6)-Dy(1)	125.3(2)
Cu(3)-O(6)-Dy(1)	126.39(14)
C(28)-O(7)-Cu(4)	107.2(2)
N(8)-O(8)-Cu(4)	107.6(2)
N(8)-O(8)-Dy(1)	124.1(2)
Cu(4)-O(8)-Dy(1)	126.95(13)
C(37)-O(9)-Cu(5)	106.7(3)
N(10)-O(10)-Cu(5)	107.3(2)

N(10)-O(10)-Dy(1)	126.2(2)
Cu(5)-O(10)-Dy(1)	126.43(12)
C(46)-O(11)-Cu(6)	106.4(2)
N(12)-O(12)-Cu(6)	108.1(2)
N(12)-O(12)-Dy(2)	125.0(2)
Cu(6)-O(12)-Dy(2)	126.82(13)
C(55)-O(13)-Cu(7)	106.5(2)
N(14)-O(14)-Cu(7)	107.3(2)
N(14)-O(14)-Dy(2)	125.4(2)
Cu(7)-O(14)-Dy(2)	126.89(13)
C(64)-O(15)-Cu(8)	107.3(3)
N(16)-O(16)-Cu(8)	108.8(2)
N(16)-O(16)-Dy(2)	123.0(2)
Cu(8)-O(16)-Dy(2)	127.73(13)
C(73)-O(17)-Cu(9)	106.9(3)
N(18)-O(18)-Cu(9)	107.9(2)
N(18)-O(18)-Dy(2)	124.4(2)
Cu(9)-O(18)-Dy(2)	126.83(14)
C(82)-O(19)-Cu(10)	106.9(3)
N(20)-O(20)-Cu(10)	107.5(2)
N(20)-O(20)-Dy(2)	123.8(2)
Cu(10)-O(20)-Dy(2)	123.24(14)
O(1)-C(1)-N(2)	123.4(4)
O(1)-C(1)-C(2)	120.1(4)
N(2)-C(1)-C(2)	116.6(4)
N(1)-C(2)-C(1)	109.3(3)
N(1)-C(2)-C(3)	112.7(4)
C(1)-C(2)-C(3)	113.0(4)
C(4)-C(3)-C(2)	117.3(4)
C(9)-C(4)-C(5)	118.2(7)
C(9)-C(4)-C(3)	125.1(5)
C(5)-C(4)-C(3)	116.6(6)
C(6)-C(5)-C(4)	120.6(9)
C(5)-C(6)-C(7)	119.5(9)
C(8)-C(7)-C(6)	120.5(8)
C(7)-C(8)-C(9)	118.4(8)
C(4)-C(9)-C(8)	122.7(7)
N(4)-C(10)-O(3)	124.5(4)
N(4)-C(10)-C(11)	114.9(4)
O(3)-C(10)-C(11)	120.6(3)
N(3)-C(11)-C(10)	108.2(3)
N(3)-C(11)-C(12)	110.4(4)
C(10)-C(11)-C(12)	111.0(3)
C(13)-C(12)-C(11)	113.6(4)
C(18)-C(13)-C(14)	118.5(4)
C(18)-C(13)-C(12)	120.2(4)
C(14)-C(13)-C(12)	121.2(4)
C(15)-C(14)-C(13)	119.9(5)
C(16)-C(15)-C(14)	121.2(5)
C(15)-C(16)-C(17)	119.9(5)
C(18)-C(17)-C(16)	119.4(5)
C(17)-C(18)-C(13)	121.1(5)

O(5)-C(19)-N(6)	124.1(4)
O(5)-C(19)-C(20)	121.0(4)
N(6)-C(19)-C(20)	114.9(4)
N(5)-C(20)-C(19)	108.8(3)
N(5)-C(20)-C(21)	111.3(4)
C(19)-C(20)-C(21)	108.6(4)
C(22)-C(21)-C(20)	113.4(4)
C(23)-C(22)-C(27)	118.2(5)
C(23)-C(22)-C(21)	121.3(5)
C(27)-C(22)-C(21)	120.5(5)
C(22)-C(23)-C(24)	120.1(6)
C(25)-C(24)-C(23)	121.0(6)
C(26)-C(25)-C(24)	119.3(5)
C(25)-C(26)-C(27)	120.6(5)
C(26)-C(27)-C(22)	120.7(5)
N(8)-C(28)-O(7)	124.0(3)
N(8)-C(28)-C(29)	116.7(3)
O(7)-C(28)-C(29)	119.2(3)
N(7)-C(29)-C(28)	108.7(3)
N(7)-C(29)-C(30)	113.5(3)
C(28)-C(29)-C(30)	111.8(3)
C(31)-C(30)-C(29)	115.4(3)
C(36)-C(31)-C(32)	118.9(4)
C(36)-C(31)-C(30)	119.3(4)
C(32)-C(31)-C(30)	121.7(4)
C(31)-C(32)-C(33)	120.2(4)
C(34)-C(33)-C(32)	120.7(4)
C(33)-C(34)-C(35)	119.6(4)
C(34)-C(35)-C(36)	120.3(4)
C(31)-C(36)-C(35)	120.3(4)
N(10)-C(37)-O(9)	124.2(4)
N(10)-C(37)-C(38)	116.0(4)
O(9)-C(37)-C(38)	119.7(4)
N(9)-C(38)-C(37)	108.7(4)
N(9)-C(38)-C(39)	113.1(4)
C(37)-C(38)-C(39)	110.1(4)
C(40)-C(39)-C(38)	111.5(4)
C(45)-C(40)-C(41)	119.1(4)
C(45)-C(40)-C(39)	121.6(5)
C(41)-C(40)-C(39)	119.3(5)
C(42)-C(41)-C(40)	121.0(5)
C(41)-C(42)-C(43)	119.1(6)
C(44)-C(43)-C(42)	120.0(5)
C(43)-C(44)-C(45)	120.4(5)
C(40)-C(45)-C(44)	120.3(5)
O(11)-C(46)-N(12)	124.9(4)
O(11)-C(46)-C(47)	121.8(3)
N(12)-C(46)-C(47)	113.1(3)
N(11)-C(47)-C(46)	107.9(3)
N(11)-C(47)-C(48)	111.0(3)
C(46)-C(47)-C(48)	108.3(3)
C(49)-C(48)-C(47)	114.3(4)

C(54)-C(49)-C(50)	118.8(4)
C(54)-C(49)-C(48)	121.0(4)
C(50)-C(49)-C(48)	120.3(4)
C(49)-C(50)-C(51)	120.5(4)
C(52)-C(51)-C(50)	119.9(5)
C(53)-C(52)-C(51)	120.0(5)
C(52)-C(53)-C(54)	120.2(5)
C(49)-C(54)-C(53)	120.7(5)
N(14)-C(55)-O(13)	123.9(4)
N(14)-C(55)-C(56)	116.9(3)
O(13)-C(55)-C(56)	119.1(3)
N(13)-C(56)-C(55)	109.1(3)
N(13)-C(56)-C(57)	113.9(3)
C(55)-C(56)-C(57)	110.4(3)
C(58)-C(57)-C(56)	116.1(4)
C(59)-C(58)-C(63)	117.6(4)
C(59)-C(58)-C(57)	121.4(4)
C(63)-C(58)-C(57)	120.8(4)
C(58)-C(59)-C(60)	121.0(5)
C(61)-C(60)-C(59)	121.8(5)
C(60)-C(61)-C(62)	118.5(5)
C(63)-C(62)-C(61)	119.7(5)
C(58)-C(63)-C(62)	121.4(5)
N(16)-C(64)-O(15)	124.1(4)
N(16)-C(64)-C(65)	116.0(4)
O(15)-C(64)-C(65)	119.9(4)
N(15)-C(65)-C(64)	108.4(3)
N(15)-C(65)-C(66)	112.8(4)
C(64)-C(65)-C(66)	111.1(3)
C(67)-C(66)-C(65)	112.8(4)
C(68)-C(67)-C(72)	118.8(5)
C(68)-C(67)-C(66)	120.6(5)
C(72)-C(67)-C(66)	120.6(5)
C(67)-C(68)-C(69)	117.9(6)
C(70)-C(69)-C(68)	121.0(7)
C(71)-C(70)-C(69)	120.6(6)
C(70)-C(71)-C(72)	119.0(7)
C(71)-C(72)-C(67)	122.7(6)
N(18)-C(73)-O(17)	123.3(4)
N(18)-C(73)-C(74)	116.5(4)
O(17)-C(73)-C(74)	120.2(4)
N(17)-C(74)-C(75)	113.0(5)
N(17)-C(74)-C(73)	109.8(4)
C(75)-C(74)-C(73)	110.1(5)
C(74)-C(75)-C(76)	112.0(6)
C(77)-C(76)-C(81)	120.0
C(77)-C(76)-C(75)	117.2(5)
C(81)-C(76)-C(75)	122.7(5)
C(78)-C(77)-C(76)	120.0
C(77)-C(78)-C(79)	120.0
C(80)-C(79)-C(78)	120.0
C(79)-C(80)-C(81)	120.0

C(80)-C(81)-C(76)	120.0
O(19)-C(82)-N(20)	124.5(4)
O(19)-C(82)-C(83)	120.4(4)
N(20)-C(82)-C(83)	115.0(4)
N(19)-C(83)-C(82)	107.8(3)
N(19)-C(83)-C(84)	111.0(4)
C(82)-C(83)-C(84)	111.9(4)
C(85)-C(84)-C(83)	111.6(4)
C(86)-C(85)-C(90)	118.0(5)
C(86)-C(85)-C(84)	121.4(5)
C(90)-C(85)-C(84)	120.6(5)
C(87)-C(86)-C(85)	121.9(6)
C(86)-C(87)-C(88)	119.5(6)
C(89)-C(88)-C(87)	119.9(6)
C(88)-C(89)-C(90)	119.8(7)
C(89)-C(90)-C(85)	120.9(6)
C(100)-O(100)-C(10G)	2.2(13)
C(100)-O(100)-Dy(1)	97.4(8)
C(10G)-O(100)-Dy(1)	95.2(7)
C(10G)-O(101)-C(100)	4.2(13)
C(10G)-O(101)-Dy(1)	94.5(8)
C(100)-O(101)-Dy(1)	90.4(8)
C(110)-O(110)-C(11A)	14.7(13)
C(110)-O(110)-Dy(2)	93.4(8)
C(11A)-O(110)-Dy(2)	89.1(7)
O(100)-C(100)-O(101)	120.0(11)
O(100)-C(100)-C(101)	121.6(15)
O(101)-C(100)-C(101)	117.6(15)
O(100)-C(100)-Dy(1)	58.0(6)
O(101)-C(100)-Dy(1)	62.2(6)
C(101)-C(100)-Dy(1)	175.4(15)
C(102)-C(101)-C(106)	117.5(10)
C(102)-C(101)-C(100)	122.8(12)
C(106)-C(101)-C(100)	119.7(11)
C(101)-C(102)-C(103)	122.8(11)
C(102)-C(103)-C(104)	116.3(13)
C(103)-C(104)-C(105)	123.1(11)
C(106)-C(105)-C(104)	116.1(11)
C(105)-C(106)-C(101)	122.9(11)
C(110)-O(111)-Dy(2)	97.0(10)
O(110)-C(110)-O(111)	118.7(14)
O(110)-C(110)-C(111)	124.3(15)
O(111)-C(110)-C(111)	116.9(16)
O(110)-C(110)-Dy(2)	62.7(7)
O(111)-C(110)-Dy(2)	56.5(8)
C(111)-C(110)-Dy(2)	171.5(10)
C(112)-C(111)-C(116)	118.6(14)
C(112)-C(111)-C(110)	120.4(17)
C(116)-C(111)-C(110)	120.9(13)
C(111)-C(112)-C(113)	123(3)
C(114)-C(113)-C(112)	115(3)
C(115)-C(114)-C(113)	123.2(15)

C(114)-C(115)-C(116)	119.7(16)
C(115)-C(116)-C(111)	119.8(14)
O(121)-C(120)-O(120)	119(3)
O(121)-C(120)-C(121)	118(3)
O(120)-C(120)-C(121)	121.4(14)
C(126)-C(121)-C(122)	117.9(12)
C(126)-C(121)-C(120)	123.7(12)
C(122)-C(121)-C(120)	118.4(12)
C(121)-C(122)-C(123)	121.0(13)
C(122)-C(123)-C(124)	116.9(12)
C(123)-C(124)-C(125)	124.5(12)
C(126)-C(125)-C(124)	110.9(12)
C(121)-C(126)-C(125)	128.3(13)
O(101)-C(10G)-O(100)	118.0(9)
O(101)-C(10G)-C(10A)	120.3(16)
O(100)-C(10G)-C(10A)	120.1(16)
O(101)-C(10G)-Dy(1)	60.8(5)
O(100)-C(10G)-Dy(1)	57.4(5)
C(10A)-C(10G)-Dy(1)	163.4(16)
C(10B)-C(10A)-C(10F)	117.9(12)
C(10B)-C(10A)-C(10G)	119.9(15)
C(10F)-C(10A)-C(10G)	122.1(13)
C(10A)-C(10B)-C(10C)	122.5(16)
C(10B)-C(10C)-C(10D)	116.3(16)
C(10E)-C(10D)-C(10C)	123.2(13)
C(10F)-C(10E)-C(10D)	116.1(14)
C(10E)-C(10F)-C(10A)	123.1(13)
C(11A)-O(11A)-Dy(2)	93.9(9)
O(11A)-C(11A)-O(110)	121.6(13)
O(11A)-C(11A)-C(11B)	120.9(14)
O(110)-C(11A)-C(11B)	117.3(15)
O(11A)-C(11A)-Dy(2)	60.0(8)
O(110)-C(11A)-Dy(2)	61.9(6)
C(11B)-C(11A)-Dy(2)	169.6(14)
C(11C)-C(11B)-C(11G)	116.7(12)
C(11C)-C(11B)-C(11A)	122.8(13)
C(11G)-C(11B)-C(11A)	120.4(11)
C(11B)-C(11C)-C(11D)	122.4(18)
C(11C)-C(11D)-C(11E)	119.0(18)
C(11D)-C(11E)-C(11F)	120.7(13)
C(11G)-C(11F)-C(11E)	116.8(11)
C(11F)-C(11G)-C(11B)	124.1(11)
O(150)-C(150)-O(151)	124.9(9)
O(150)-C(150)-C(151)	118.8(8)
O(151)-C(150)-C(151)	116.3(8)
C(156)-C(151)-C(152)	119.2(6)
C(156)-C(151)-C(150)	120.9(7)
C(152)-C(151)-C(150)	119.8(6)
C(153)-C(152)-C(151)	120.5(7)
C(152)-C(153)-C(154)	120.3(8)
C(155)-C(154)-C(153)	120.3(7)
C(154)-C(155)-C(156)	119.7(7)

C(151)-C(156)-C(155)	120.0(8)
C(250)-O(250)-Dy(2)	132.4(3)
O(251)-C(250)-O(250)	123.2(5)
O(251)-C(250)-C(251)	119.8(4)
O(250)-C(250)-C(251)	117.0(4)
C(252)-C(251)-C(256)	119.3(5)
C(252)-C(251)-C(250)	119.6(4)
C(256)-C(251)-C(250)	121.1(4)
C(251)-C(252)-C(253)	120.1(4)
C(252)-C(253)-C(254)	120.3(5)
C(255)-C(254)-C(253)	119.6(5)
C(256)-C(255)-C(254)	119.8(4)
C(255)-C(256)-C(251)	120.8(5)
C(300)-O(300)-Dy(1)	134.0(4)
O(301)-C(300)-O(300)	125.7(5)
O(301)-C(300)-C(301)	117.0(5)
O(300)-C(300)-C(301)	117.2(5)
C(306)-C(301)-C(302)	118.9(7)
C(306)-C(301)-C(300)	120.7(7)
C(302)-C(301)-C(300)	120.4(6)
C(301)-C(302)-C(303)	118.6(9)
C(302)-C(303)-C(304)	120.0(10)
C(305)-C(304)-C(303)	121.7(8)
C(304)-C(305)-C(306)	117.5(10)
C(301)-C(306)-C(305)	123.4(11)
C(404)-O(404)-Cu(2)	135.3(4)
