Inorganic Chemistry
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Table S1-1. Crystallographic and Experimental Data for **2**

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formula	$C_{44}H_{60}N_2O_{14}ZnCo$
formula weight	965.29
color	pink
size, mm	0.38 x 0.26 x 0.15
cryst. system	monoclinic
space group	$P2_1/c$ (No. 14)
no. refs used for cell determination	20 ($20 < 2\theta < 30°$)
lattice const.	a = 17.725(7) Å
	b = 12.354(4) Å
	c = 21.815(6) Å
	β = 90.45(3)°
	V = 4777(2) Å^3
Z	4
D_{calc}, g cm^{-3}	1.343
μ (Mo $K\alpha$), cm^{-1}	9.16 (trans. 0.93 ~ 1.00)
	An absorption correction by ψ-scan method was applied.
radiation	Mo $K\alpha$ (λ = 0.71069 Å)
monochromator	graphite
temp,°C	-85
2θ range, deg	$3 < 2\theta < 45$
h, k, l range	+h, +k, ±l
scan method	ω - 2θ
scan speed, deg min^{-1}	variable (2 ~ 8)
scan width	1.00 + 0.35 tanθ
std. reflections	3 every ~200 (3600 sec)

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(Table S1-1, contd.)

solution	direct methods (SHELXS86)
refinement	full-matrix least-squares
	All non-hydrogen atoms were refined with aniotropic temperature factors.
function minimized	$\Sigma w(\|F_o\| - \|F_c\|)^2$
weighting scheme	$1/\sigma^2(F_o)$
anomalous dispersion	all non-hydrogen atoms
hydrogen atoms	All hydrogen atoms were determined by difference Fourier syntheses, and were not refined.
no. reflections measured	6688
no. unique reflections	3884 ($I > 3\sigma(I)$)
p-factor	0.03
no. variables	560
data / param ratio	6.94
R [a]	0.049
R_w [b]	0.051
GOF[c]	1.59
max shift/error in final cycle	0.001
ρ_{max}, eÅ^3	0.47 around Zn(1)

[a] $R = \Sigma|\,|F_o| - |F_c|\,|/\Sigma|F_o|$.

[b] $Rw = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$ ($w = 1/\sigma^2(F_o)$).

[c] GOF = $[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_p)]^{1/2}$ (N_o = no. data, N_p = no. variables)

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Table S1-2. Final Positional Parameters and B_{eq} for $2^{a,b,c}$

atom	x	y	z	B_{eq}
Zn(1)	0.28423(5)	0.19348(7)	0.92904(4)	2.94(4)
Co(1)	0.29092(5)	0.21191(7)	0.77182(4)	2.64(4)
O(1)	0.2740(3)	0.0673(3)	0.7313(2)	3.3(2)
O(2)	0.3724(2)	0.2425(4)	0.7095(2)	3.3(2)
O(3)	0.3437(2)	0.1302(3)	0.8522(2)	3.1(2)
O(4)	0.3352(3)	0.0901(4)	0.9838(2)	4.1(3)
O(5)	0.2127(2)	0.3003(4)	0.7119(2)	3.3(2)
O(6)	0.2410(3)	0.2813(4)	1.0038(2)	3.8(2)
O(101)	0.1883(3)	0.1178(4)	0.9135(2)	3.5(2)
O(102)	0.1931(2)	0.1911(4)	0.8207(2)	2.9(2)
O(103)	0.0202(2)	0.2358(4)	0.9615(2)	3.4(2)
O(104)	0.0654(2)	0.3367(4)	0.7656(2)	3.2(2)
O(201)	0.3364(2)	0.3310(3)	0.9136(2)	2.7(2)
O(202)	0.3184(2)	0.3560(3)	0.8130(2)	2.8(2)
O(203)	0.2639(2)	0.5064(4)	0.9964(2)	2.9(2)
O(204)	0.2168(3)	0.6015(4)	0.7993(2)	3.6(3)
N(101)	0.0388(3)	0.2882(4)	0.8634(2)	2.5(3)
N(201)	0.2412(3)	0.5522(4)	0.8978(2)	2.1(3)
C(1)	0.2656(4)	-0.0686(6)	0.6547(3)	3.6(4)
C(2)	0.2931(4)	0.0411(6)	0.6773(3)	3.0(4)
C(3)	0.3369(4)	0.1050(6)	0.6383(3)	3.1(4)
C(4)	0.3727(4)	0.2003(6)	0.6562(3)	3.2(4)
C(5)	0.4166(4)	0.2631(6)	0.6089(3)	4.3(4)
C(6)	0.4365(4)	0.0305(7)	0.8005(4)	5.2(5)
C(7)	0.3937(4)	0.0564(6)	0.8561(4)	3.7(4)
C(8)	0.4087(5)	-0.0017(6)	0.9093(4)	4.9(5)
C(9)	0.3798(5)	0.0160(6)	0.9684(4)	4.5(5)
C(10)	0.4036(6)	-0.0573(6)	1.0198(4)	8.1(6)
C(21)	0.2315(4)	0.4052(6)	0.6876(4)	5.0(5)
C(22)	0.1802(5)	0.2521(8)	1.0428(4)	6.0(5)
C(101)	0.1658(4)	0.1245(5)	0.8581(3)	2.9(4)
C(102)	0.0152(4)	0.2122(6)	0.9078(3)	2.9(4)
C(103)	0.0404(3)	0.2683(6)	0.8000(3)	2.8(4)
C(104)	0.1561(4)	-0.0631(5)	0.8273(4)	4.2(4)
C(105)	-0.0789(4)	0.0708(6)	0.9305(3)	4.5(4)
C(106)	-0.0233(4)	0.1746(6)	0.7129(3)	4.3(4)
C(107)	0.1085(4)	0.0410(5)	0.8363(3)	3.0(4)
C(108)	0.0468(4)	0.0212(5)	0.8832(3)	3.5(4)
C(109)	-0.0169(4)	0.1048(6)	0.8857(3)	3.4(4)
C(110)	-0.0510(4)	0.1201(6)	0.8214(3)	3.4(4)
C(111)	0.0100(4)	0.1582(5)	0.7775(3)	3.2(4)
C(112)	0.0735(4)	0.0726(5)	0.7743(3)	3.0(3)
C(201)	0.3492(4)	0.3779(5)	0.8629(3)	2.6(3)

(Table S1-2, contd.)

C(202)	0.2881(4)	0.5479(5)	0.9495(3)	2.4(3)
C(203)	0.2630(4)	0.5987(5)	0.8406(3)	2.7(3)
C(204)	0.4829(4)	0.3980(6)	0.8448(3)	3.8(4)
C(205)	0.3872(4)	0.6409(6)	1.0097(3)	3.6(4)
C(206)	0.3422(4)	0.7336(6)	0.7870(3)	4.2(4)
C(207)	0.4115(4)	0.4629(5)	0.8632(3)	2.8(3)
C(208)	0.4235(4)	0.5116(5)	0.9274(3)	3.3(4)
C(209)	0.3655(4)	0.5975(5)	0.9458(3)	2.9(3)
C(210)	0.3653(4)	0.6883(5)	0.8988(3)	3.1(3)
C(211)	0.3420(4)	0.6433(5)	0.8360(3)	2.9(3)
C(212)	0.3982(4)	0.5535(5)	0.8157(3)	3.1(4)
C(301)	0.1397(3)	0.4198(5)	0.8822(3)	2.3(3)
C(302)	0.0640(3)	0.3932(5)	0.8854(3)	2.1(3)
C(303)	0.0112(4)	0.4650(5)	0.9072(3)	2.6(3)
C(304)	0.0371(4)	0.5639(5)	0.9307(3)	2.7(3)
C(305)	0.1120(4)	0.5928(5)	0.9284(3)	2.2(3)
C(306)	0.1626(3)	0.5193(5)	0.9037(3)	2.1(3)
C(307)	-0.0719(4)	0.4450(6)	0.9048(3)	3.6(4)
C(308)	0.1366(4)	0.7057(5)	0.9499(3)	3.4(4)
H(1)	-0.055	0.054	0.968	4.4
H(2)	-0.128	0.127	0.921	4.4
H(3)	-0.082	-0.011	0.927	4.4
H(4)	-0.101	0.178	0.817	4.4
H(5)	-0.074	0.047	0.807	4.4
H(6)	-0.069	0.227	0.709	4.4
H(7)	-0.043	0.119	0.701	4.4
H(8)	0.020	0.203	0.685	4.4
H(9)	0.054	-0.017	0.762	4.4
H(10)	0.118	0.107	0.746	4.4
H(11)	0.126	-0.127	0.816	4.4
H(12)	0.193	-0.032	0.795	4.4
H(13)	0.184	-0.098	0.865	4.4
H(14)	0.076	-0.011	0.920	4.4
H(15)	0.020	-0.045	0.875	4.4
H(16)	0.179	0.359	0.863	4.4
H(17)	-0.001	0.624	0.954	4.4
H(18)	-0.077	0.379	0.933	4.4
H(19)	-0.113	0.479	0.930	4.4
H(20)	0.080	0.750	0.960	4.4
H(21)	0.168	0.680	0.972	4.4
H(22)	0.169	0.747	0.918	4.4
H(23)	0.406	0.577	1.039	4.4
H(24)	0.353	0.692	1.029	4.4
H(25)	0.444	0.676	1.001	4.4
H(26)	0.323	0.749	0.901	4.4
H(27)	0.418	0.722	0.892	4.4

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(Table S1-2, contd.)

H(28)	0.310	0.793	0.806	4.4
H(29)	0.392	0.764	0.777	4.4
H(30)	0.332	0.685	0.750	4.4
H(31)	0.446	0.604	0.800	4.4
H(32)	0.375	0.492	0.778	4.4
H(33)	0.527	0.446	0.837	4.4
H(34)	0.482	0.394	0.796	4.4
H(35)	0.429	0.447	0.958	4.4
H(36)	0.475	0.550	0.930	4.4
H(37)	0.258	-0.056	0.604	4.4
H(38)	0.216	-0.095	0.682	4.4
H(39)	0.345	0.079	0.589	4.4
H(40)	0.390	0.320	0.597	4.4
H(41)	0.464	0.301	0.614	4.4
H(42)	0.430	0.218	0.574	4.4
H(43)	0.446	0.092	0.765	4.4
H(44)	0.484	-0.016	0.804	4.4
H(45)	0.190	0.283	1.091	4.4
H(46)	0.198	0.220	1.042	4.4
H(47)	0.133	0.273	1.038	4.4
H(48)	0.429	-0.121	1.017	4.4
H(49)	0.447	-0.072	0.914	4.4
H(50)	0.484	0.333	0.863	4.4
H(51)	0.188	0.419	0.650	4.4
H(52)	0.237	0.487	0.693	4.4
H(53)	0.150	0.301	0.730	4.4
H(54)	0.314	-0.133	0.654	4.4
H(55)	0.404	0.027	0.755	4.4
H(56)	-0.094	0.381	0.882	4.4
H(57)	0.299	0.415	0.697	4.4
H(58)	0.389	0.015	1.057	4.4
H(59)	0.370	-0.105	1.052	4.4
H(60)	0.243	0.370	1.003	4.4

[a]Estimated standard deviations are given in parentheses. [b]All non-hydrogen atoms were assigned anisotropic thermal parameters given as the isotropic equivalent displacement parameter defined as $B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a^*_i \cdot a^*_j \, a_i \cdot a_j$. [c]All hydrogen atoms were determined by difference Fourier syntheses and were not refined with the appropriate B_{iso}.

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Table S1-3. Final Anisotropic Thermal Parameters for **2**[a,b]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	0.0461(5)	0.0338(5)	0.0317(5)	-0.0004(4)	-0.0031(4)	0.0034(4)
Co(1)	0.0406(6)	0.0337(6)	0.0262(6)	-0.0001(5)	0.0032(4)	-0.0029(5)
O(1)	0.056(3)	0.036(3)	0.034(3)	-0.006(2)	0.011(2)	-0.007(2)
O(2)	0.041(3)	0.042(3)	0.041(3)	-0.003(2)	0.005(2)	-0.002(3)
O(3)	0.040(3)	0.038(3)	0.041(3)	0.015(2)	-0.002(2)	-0.005(2)
O(4)	0.073(4)	0.044(3)	0.041(3)	0.007(3)	-0.018(3)	0.006(3)
O(5)	0.040(3)	0.055(3)	0.032(3)	0.004(3)	0.000(2)	0.007(3)
O(6)	0.066(3)	0.038(3)	0.039(3)	-0.010(3)	0.022(3)	-0.003(2)
O(101)	0.051(3)	0.047(3)	0.033(3)	-0.006(3)	-0.005(2)	0.004(3)
O(102)	0.041(3)	0.034(3)	0.035(3)	-0.003(2)	0.005(2)	0.006(3)
O(103)	0.050(3)	0.050(3)	0.029(3)	-0.005(2)	0.003(2)	-0.004(3)
O(104)	0.052(3)	0.040(3)	0.028(3)	-0.002(3)	-0.002(2)	0.001(2)
O(201)	0.046(3)	0.034(3)	0.023(3)	-0.007(2)	0.004(2)	0.003(2)
O(202)	0.047(3)	0.031(3)	0.029(3)	-0.001(2)	-0.007(2)	-0.003(2)
O(203)	0.046(3)	0.037(3)	0.028(3)	-0.008(2)	0.000(2)	0.000(2)
O(204)	0.047(3)	0.056(3)	0.033(3)	0.002(3)	-0.006(3)	0.014(3)
N(101)	0.036(3)	0.033(3)	0.025(3)	-0.004(3)	0.001(3)	-0.007(3)
N(201)	0.027(3)	0.028(3)	0.026(3)	-0.003(3)	-0.003(3)	-0.005(3)
C(1)	0.058(5)	0.049(5)	0.029(4)	-0.002(4)	-0.004(4)	-0.011(4)
C(2)	0.039(5)	0.043(5)	0.034(5)	0.016(4)	-0.009(4)	-0.010(4)
C(3)	0.047(5)	0.045(5)	0.025(4)	0.003(4)	0.002(3)	-0.001(4)
C(4)	0.035(4)	0.050(5)	0.036(5)	0.013(4)	0.004(3)	0.007(4)
C(5)	0.054(5)	0.050(5)	0.058(6)	0.002(4)	0.029(4)	0.012(4)
C(6)	0.063(6)	0.083(6)	0.051(6)	0.047(5)	0.011(4)	-0.000(5)
C(7)	0.039(5)	0.043(5)	0.057(6)	0.002(4)	-0.008(4)	-0.015(4)
C(8)	0.084(7)	0.041(5)	0.060(6)	0.031(5)	-0.021(5)	-0.003(5)
C(9)	0.074(6)	0.033(5)	0.065(7)	-0.002(5)	-0.027(5)	-0.003(5)
C(10)	0.22(1)	0.032(5)	0.061(7)	0.045(7)	-0.027(7)	0.018(5)
C(21)	0.067(6)	0.056(6)	0.065(6)	-0.003(5)	-0.021(5)	0.026(5)
C(22)	0.067(6)	0.116(8)	0.045(6)	-0.000(6)	0.014(5)	-0.013(6)
C(101)	0.034(4)	0.030(4)	0.044(5)	0.007(4)	0.003(4)	-0.006(4)
C(102)	0.031(4)	0.041(5)	0.037(5)	-0.004(4)	0.005(3)	-0.003(4)
C(103)	0.026(4)	0.044(5)	0.036(5)	0.000(3)	-0.003(3)	-0.006(4)
C(104)	0.065(5)	0.024(4)	0.073(6)	-0.006(4)	-0.000(4)	0.003(4)
C(105)	0.061(5)	0.056(5)	0.053(6)	-0.018(4)	0.007(4)	0.005(4)
C(106)	0.059(5)	0.070(6)	0.034(5)	-0.002(4)	-0.017(4)	-0.010(4)
C(107)	0.048(5)	0.027(4)	0.040(5)	-0.011(4)	0.001(4)	-0.004(3)
C(108)	0.054(5)	0.035(4)	0.043(5)	-0.011(4)	-0.000(4)	0.004(4)
C(109)	0.041(5)	0.046(5)	0.042(5)	-0.020(4)	0.004(4)	-0.004(4)
C(110)	0.040(4)	0.050(5)	0.038(5)	-0.021(4)	-0.005(4)	-0.003(4)
C(111)	0.048(5)	0.046(5)	0.026(4)	-0.007(4)	-0.011(4)	-0.010(4)
C(112)	0.047(5)	0.033(4)	0.033(5)	-0.008(4)	0.003(4)	-0.012(3)

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(Table S1-3, contd.)

C(201)	0.033(4)	0.030(4)	0.035(5)	0.010(3)	0.001(4)	-0.007(4)
C(202)	0.034(4)	0.020(4)	0.036(5)	0.003(3)	-0.001(4)	-0.006(3)
C(203)	0.043(5)	0.028(4)	0.032(5)	0.005(3)	0.006(4)	0.005(3)
C(204)	0.038(4)	0.052(5)	0.053(5)	-0.000(4)	0.012(4)	0.008(4)
C(205)	0.053(5)	0.044(5)	0.039(5)	-0.008(4)	-0.012(4)	-0.010(4)
C(206)	0.061(5)	0.044(5)	0.055(5)	-0.005(4)	0.018(4)	0.013(4)
C(207)	0.032(4)	0.038(4)	0.037(5)	0.001(3)	-0.003(3)	-0.001(4)
C(208)	0.038(4)	0.041(4)	0.045(5)	-0.010(4)	-0.009(4)	0.002(4)
C(209)	0.041(4)	0.033(4)	0.038(5)	-0.006(4)	-0.006(3)	-0.005(4)
C(210)	0.041(4)	0.031(4)	0.047(5)	-0.010(4)	0.004(3)	0.004(4)
C(211)	0.033(4)	0.042(4)	0.033(5)	-0.000(4)	0.005(3)	0.005(4)
C(212)	0.035(4)	0.038(4)	0.045(5)	-0.009(4)	0.008(4)	0.013(4)
C(301)	0.036(4)	0.026(4)	0.025(4)	0.001(3)	0.002(3)	-0.002(3)
C(302)	0.030(4)	0.030(4)	0.020(4)	0.001(3)	-0.001(3)	-0.004(3)
C(303)	0.032(4)	0.040(4)	0.025(4)	-0.002(4)	-0.001(3)	0.009(3)
C(304)	0.038(5)	0.035(4)	0.028(4)	0.002(4)	0.005(3)	-0.003(3)
C(305)	0.043(4)	0.027(4)	0.015(4)	-0.001(3)	0.005(3)	0.003(3)
C(306)	0.033(4)	0.031(4)	0.016(4)	-0.002(3)	0.002(3)	-0.000(3)
C(307)	0.035(5)	0.052(5)	0.049(5)	-0.008(4)	0.009(4)	-0.006(4)
C(308)	0.048(4)	0.029(4)	0.053(5)	0.003(4)	0.009(4)	0.002(4)

[a]Estmated standard deviations are given in parentheses. [b]Parameters have the form $\exp(-2\pi^2(U_{11}h^2a^{*2} + \cdots + 2U_{12}hka^*b^*\cos\gamma + \cdots))$

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Table S1-4. Bond Lengths for Non-hydrogen Atoms of **2**[a]

atom	atom	distance	atom	atom	distance
Zn(1)	O(3)	2.135(4)	N(101)	C(103)	1.404(8)
Zn(1)	O(4)	1.964(5)	N(101)	C(302)	1.452(7)
Zn(1)	O(6)	2.107(4)	N(201)	C(202)	1.397(7)
Zn(1)	O(101)	1.967(5)	N(201)	C(203)	1.430(8)
Zn(1)	O(201)	1.964(4)	N(201)	C(306)	1.459(7)
Co(1)	O(1)	2.014(4)	C(1)	C(2)	1.521(9)
Co(1)	O(2)	2.027(5)	C(2)	C(3)	1.400(9)
Co(1)	O(3)	2.224(5)	C(3)	C(4)	1.392(9)
Co(1)	O(5)	2.190(4)	C(4)	C(5)	1.512(9)
Co(1)	O(102)	2.059(4)	C(6)	C(7)	1.47(1)
Co(1)	O(202)	2.051(4)	C(7)	C(8)	1.39(1)
O(1)	C(2)	1.270(7)	C(8)	C(9)	1.41(1)
O(2)	C(4)	1.273(8)	C(9)	C(10)	1.50(1)
O(3)	C(7)	1.274(8)	C(101)	C(107)	1.522(9)
O(4)	C(9)	1.256(9)	C(102)	C(109)	1.521(9)
O(5)	C(21)	1.440(8)	C(103)	C(111)	1.543(9)
O(6)	C(22)	1.424(8)	C(104)	C(107)	1.551(9)
O(101)	C(101)	1.272(7)	C(105)	C(109)	1.535(9)
O(102)	C(101)	1.258(7)	C(106)	C(111)	1.538(8)
O(103)	C(102)	1.210(7)	C(107)	C(108)	1.523(9)
O(104)	C(103)	1.216(7)	C(107)	C(112)	1.535(9)
O(201)	C(201)	1.270(7)	C(108)	C(109)	1.531(9)
O(202)	C(201)	1.245(7)	C(109)	C(110)	1.535(9)
O(203)	C(202)	1.226(7)	C(110)	C(111)	1.525(9)
O(204)	C(203)	1.214(7)	C(111)	C(112)	1.546(9)
N(101)	C(102)	1.415(8)	C(201)	C(207)	1.524(9)

(Table S1-4, contd.)

C(202)	C(209)	1.504(8)
C(203)	C(211)	1.509(9)
C(204)	C(207)	1.554(9)
C(205)	C(209)	1.539(9)
C(206)	C(211)	1.544(9)
C(207)	C(208)	1.539(9)
C(207)	C(212)	1.542(9)
C(208)	C(209)	1.533(9)
C(209)	C(210)	1.521(9)
C(210)	C(211)	1.531(9)
C(211)	C(212)	1.558(9)
C(301)	C(302)	1.384(8)
C(301)	C(306)	1.376(8)
C(302)	C(303)	1.378(8)
C(303)	C(304)	1.401(9)
C(303)	C(307)	1.493(8)
C(304)	C(305)	1.375(8)
C(305)	C(306)	1.387(8)
C(305)	C(308)	1.534(9)

[a]Estimated standard deviations are given in parentheses.

Table S1-5. Bond Angles for Non-hydrogen Atoms of **2**[a]

atom	atom	atom	angle	atom	atom	atom	angle
O(3)	Zn(1)	O(4)	90.6(2)	Co(1)	O(2)	C(4)	123.0(4)
O(3)	Zn(1)	O(6)	168.7(2)	Zn(1)	O(3)	Co(1)	104.2(2)
O(3)	Zn(1)	O(101)	97.0(2)	Zn(1)	O(3)	C(7)	123.9(5)
O(3)	Zn(1)	O(201)	86.9(2)	Co(1)	O(3)	C(7)	131.7(5)
O(4)	Zn(1)	O(6)	91.9(2)	Zn(1)	O(4)	C(9)	126.8(5)
O(4)	Zn(1)	O(101)	100.9(2)	Co(1)	O(5)	C(21)	121.4(4)
O(4)	Zn(1)	O(201)	116.9(2)	Zn(1)	O(6)	C(22)	127.8(5)
O(6)	Zn(1)	O(101)	93.4(2)	Zn(1)	O(101)	C(101)	113.4(4)
O(6)	Zn(1)	O(201)	82.1(2)	Co(1)	O(102)	C(101)	138.3(4)
O(101)	Zn(1)	O(201)	142.0(2)	Zn(1)	O(201)	C(201)	129.2(4)
O(1)	Co(1)	O(2)	88.6(2)	Co(1)	O(202)	C(201)	132.3(4)
O(1)	Co(1)	O(3)	90.2(2)	C(102)	N(101)	C(103)	124.5(6)
O(1)	Co(1)	O(5)	95.1(2)	C(102)	N(101)	C(302)	117.3(5)
O(1)	Co(1)	O(102)	89.6(2)	C(103)	N(101)	C(302)	118.2(5)
O(1)	Co(1)	O(202)	174.9(2)	C(202)	N(201)	C(203)	123.8(5)
O(2)	Co(1)	O(3)	108.5(2)	C(202)	N(201)	C(306)	118.7(5)
O(2)	Co(1)	O(5)	87.6(2)	C(203)	N(201)	C(306)	117.1(5)
O(2)	Co(1)	O(102)	168.0(2)	O(1)	C(2)	C(1)	116.2(6)
O(2)	Co(1)	O(202)	88.0(2)	O(1)	C(2)	C(3)	124.9(6)
O(3)	Co(1)	O(5)	163.2(2)	C(1)	C(2)	C(3)	118.9(6)
O(3)	Co(1)	O(102)	83.5(2)	C(2)	C(3)	C(4)	124.1(6)
O(3)	Co(1)	O(202)	87.2(2)	O(2)	C(4)	C(3)	126.6(7)
O(5)	Co(1)	O(102)	80.7(2)	O(2)	C(4)	C(5)	114.8(7)
O(5)	Co(1)	O(202)	88.6(2)	C(3)	C(4)	C(5)	118.6(7)
O(102)	Co(1)	O(202)	94.5(2)	O(3)	C(7)	C(6)	117.6(7)
Co(1)	O(1)	C(2)	126.4(4)	O(3)	C(7)	C(8)	123.7(7)

(Table S1-5, contd.)

C(6)	C(7)	C(8)	118.7(7)	C(108)	C(109)	C(110)	109.6(6)
C(7)	C(8)	C(9)	128.0(7)	C(109)	C(110)	C(111)	109.7(5)
O(4)	C(9)	C(8)	126.3(7)	C(103)	C(111)	C(106)	107.8(6)
O(4)	C(9)	C(10)	114.4(8)	C(103)	C(111)	C(110)	108.6(6)
C(8)	C(9)	C(10)	119.3(8)	C(103)	C(111)	C(112)	111.5(5)
O(101)	C(101)	O(102)	122.6(6)	C(106)	C(111)	C(110)	110.4(6)
O(101)	C(101)	C(107)	117.2(6)	C(106)	C(111)	C(112)	108.9(6)
O(102)	C(101)	C(107)	120.0(6)	C(110)	C(111)	C(112)	109.7(6)
O(103)	C(102)	N(101)	118.9(6)	C(107)	C(112)	C(111)	115.1(5)
O(103)	C(102)	C(109)	122.8(6)	O(201)	C(201)	O(202)	125.6(6)
N(101)	C(102)	C(109)	118.3(6)	O(201)	C(201)	C(207)	116.5(6)
O(104)	C(103)	N(101)	119.8(6)	O(202)	C(201)	C(207)	117.8(6)
O(104)	C(103)	C(111)	122.9(6)	O(203)	C(202)	N(201)	118.6(6)
N(101)	C(103)	C(111)	117.3(6)	O(203)	C(202)	C(209)	122.7(6)
C(101)	C(107)	C(104)	103.8(5)	N(201)	C(202)	C(209)	118.6(6)
C(101)	C(107)	C(108)	112.3(6)	O(204)	C(203)	N(201)	118.2(6)
C(101)	C(107)	C(112)	111.6(6)	O(204)	C(203)	C(211)	124.2(6)
C(104)	C(107)	C(108)	110.2(6)	N(201)	C(203)	C(211)	117.5(6)
C(104)	C(107)	C(112)	108.5(6)	C(201)	C(207)	C(204)	103.6(5)
C(108)	C(107)	C(112)	110.2(6)	C(201)	C(207)	C(208)	111.5(6)
C(107)	C(108)	C(109)	116.7(6)	C(201)	C(207)	C(212)	113.0(5)
C(102)	C(109)	C(105)	107.8(6)	C(204)	C(207)	C(208)	109.2(5)
C(102)	C(109)	C(108)	109.1(5)	C(204)	C(207)	C(212)	108.8(5)
C(102)	C(109)	C(110)	109.0(6)	C(208)	C(207)	C(212)	110.4(6)
C(105)	C(109)	C(108)	111.8(6)	C(207)	C(208)	C(209)	114.9(5)
C(105)	C(109)	C(110)	109.6(6)	C(202)	C(209)	C(205)	108.4(6)

(Table S1-5, contd.)

C(202)	C(209)	C(208)	110.2(5)	C(301)	C(306)	C(305)	121.9(6)
C(202)	C(209)	C(210)	109.8(5)				
C(205)	C(209)	C(208)	108.3(5)				
C(205)	C(209)	C(210)	110.7(5)				
C(208)	C(209)	C(210)	109.4(6)				
C(209)	C(210)	C(211)	109.6(5)				
C(203)	C(211)	C(206)	108.5(6)				
C(203)	C(211)	C(210)	108.5(5)				
C(203)	C(211)	C(212)	110.7(5)				
C(206)	C(211)	C(210)	110.8(6)				
C(206)	C(211)	C(212)	108.2(5)				
C(210)	C(211)	C(212)	110.2(5)				
C(207)	C(212)	C(211)	114.9(5)				
C(302)	C(301)	C(306)	118.6(6)				
N(101)	C(302)	C(301)	119.5(5)				
N(101)	C(302)	C(303)	118.8(6)				
C(301)	C(302)	C(303)	121.7(6)				
C(302)	C(303)	C(304)	117.8(6)				
C(302)	C(303)	C(307)	123.6(6)				
C(304)	C(303)	C(307)	118.6(6)				
C(303)	C(304)	C(305)	121.8(6)				
C(304)	C(305)	C(306)	118.1(6)				
C(304)	C(305)	C(308)	119.8(6)				
C(306)	C(305)	C(308)	122.0(6)				
N(201)	C(306)	C(301)	119.8(5)				
N(201)	C(306)	C(305)	118.3(5)				

[a]Estimated deviations are given in parentheses.

Table S2-1. Crystallographic and Experimental Data for **3**

formula	$C_{44}H_{60}N_2O_{14}ZnMn$
formula weight	961.28
color	pale yellow
size, mm	0.40 x 0.37 x 0.21
cryst. system	monoclinic
space group	$P2_1/c$ (No. 14)
no. refs used for cell determination	22 ($20 < 2\theta < 30°$)
lattice const.	a = 17.292(2) Å
	b = 12.450(1) Å
	c = 21.717(2) Å
	β = 91.464(7)°
	V = 4673.9(7) Å^3
Z	4
D_{calc}, g cm^{-3}	1.366
μ (Mo $K\alpha$), cm^{-1}	8.49 (trans. 0.94 ~ 1.00)
	An absorption correction by ψ-scan method was applied.
radiation	Mo $K\alpha$ (λ = 0.71069 Å)
monochromator	graphite
temp,°C	-110
2θ range, deg	$3 < 2\theta < 46$
h, k, l range	+h, +k, ±l
scan method	ω - 2θ
scan speed,° min^{-1}	variable (2 ~ 8)
scan width	0.80 + 0.35 tanθ
std. reflections	3 every ~200 (3600 sec)
solution	direct methods (SHELXS86)

(Table S2-1, contd.)

refinement	full-matrix least-squares All non-hydrogen atoms were refined with aniotropic temperature factors.
function minimized	$\Sigma w(\|F_o\| - \|F_c\|)^2$
weighting scheme	$1/\sigma^2(F_o)$
anomalous dispersion	all non-hydrogen atoms
hydrogen atoms	All hydrogen atoms were determined by difference Fourier syntheses, and were not refined.
no. reflections measured	6976
no. unique reflections	3876 ($I > 3\sigma(I)$)
p-factor	0.03
no. variables	560
data / param ratio	6.92
R [a]	0.046
R_w [b]	0.051
GOF [c]	1.44
max shift/error in final cycle	0.001
ρ_{max}, eÅ^3	0.32 around Zn(1)

[a] $R = \Sigma|\,|F_o| - |F_c|\,|/\Sigma|F_o|$.

[b] $Rw = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$ ($w = 1/\sigma^2(F_o)$).

[c] GOF = $[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_p)]^{1/2}$ (N_o = no. data, N_p = no. variables)

Table S2-2. Final Positional Parameters and B_{eq} for $3^{a,b,c}$

atom	x	y	z	B_{eq}
Zn(1)	0.22300(4)	0.18518(6)	0.93382(3)	3.11(3)
Mn(1)	0.20287(6)	0.18385(8)	0.77228(4)	3.33(5)
O(1)	0.1194(2)	0.2101(3)	0.7010(2)	3.8(2)
O(2)	0.2154(2)	0.0307(3)	0.7322(2)	4.0(2)
O(3)	0.1594(2)	0.1048(3)	0.8624(2)	3.5(2)
O(4)	0.1810(2)	0.0853(3)	0.9954(2)	3.9(2)
O(5)	0.2832(2)	0.2792(3)	0.7119(2)	4.2(2)
O(6)	0.2685(2)	0.2846(3)	1.0043(2)	3.5(2)
O(101)	0.1600(2)	0.3159(3)	0.9162(2)	3.1(2)
O(102)	0.1716(2)	0.3297(3)	0.8143(2)	3.8(2)
O(103)	0.2347(2)	0.5044(3)	0.9913(2)	2.7(2)
O(104)	0.2748(2)	0.5727(3)	0.7897(2)	3.8(2)
O(201)	0.3242(2)	0.1170(3)	0.9184(2)	3.7(2)
O(202)	0.3099(2)	0.1742(3)	0.8221(2)	3.5(2)
O(203)	0.4926(2)	0.2387(3)	0.9635(2)	3.8(2)
O(204)	0.4360(2)	0.3238(3)	0.7642(2)	3.3(2)
N(101)	0.2537(2)	0.5362(3)	0.8899(2)	2.3(2)
N(201)	0.4677(3)	0.2833(4)	0.8638(2)	2.8(2)
C(1)	0.0945(4)	0.2399(5)	0.5942(3)	4.1(3)
C(2)	0.1285(3)	0.1730(5)	0.6470(3)	3.5(3)
C(3)	0.1665(3)	0.0783(5)	0.6329(3)	3.3(3)
C(4)	0.2039(3)	0.0103(5)	0.6752(3)	3.1(3)
C(5)	0.2327(3)	-0.0969(5)	0.6539(3)	3.6(3)
C(6)	0.0635(4)	-0.0068(6)	0.8177(3)	5.8(4)
C(7)	0.1110(4)	0.0312(5)	0.8721(3)	3.9(3)
C(8)	0.0998(4)	-0.0182(5)	0.9293(3)	4.5(4)
C(9)	0.1340(4)	0.0098(5)	0.9857(3)	4.1(4)
C(10)	0.1137(5)	-0.0542(6)	1.0423(3)	5.9(4)
C(21)	0.2609(4)	0.3800(6)	0.6841(3)	5.2(4)
C(22)	0.3346(4)	0.2653(5)	1.0428(3)	4.4(3)
C(101)	0.1424(3)	0.3569(5)	0.8641(3)	3.0(3)
C(102)	0.2081(3)	0.5386(4)	0.9427(3)	2.2(3)
C(103)	0.2285(3)	0.5726(4)	0.8304(3)	2.7(3)
C(104)	0.0056(4)	0.3735(5)	0.8467(3)	4.6(4)
C(105)	0.1108(3)	0.6440(5)	0.9979(3)	3.4(3)
C(106)	0.1429(4)	0.6949(6)	0.7702(3)	4.7(4)
C(107)	0.0777(3)	0.4406(5)	0.8615(3)	3.2(3)
C(108)	0.0686(3)	0.4981(5)	0.9233(3)	3.0(3)
C(109)	0.1278(3)	0.5877(5)	0.9364(3)	2.9(3)
C(110)	0.1252(3)	0.6698(4)	0.8837(3)	2.9(3)
C(111)	0.1475(3)	0.6141(5)	0.8240(3)	3.1(3)
C(112)	0.0886(3)	0.5231(5)	0.8094(3)	3.5(3)
C(201)	0.3425(4)	0.1157(5)	0.8625(3)	3.7(3)

(Table S2-2, contd.)

C(202)	0.4971(3)	0.2127(5)	0.9098(3)	3.2(3)
C(203)	0.4642(3)	0.2588(5)	0.8001(3)	2.9(3)
C(204)	0.3554(4)	-0.0702(5)	0.8368(3)	5.6(4)
C(205)	0.5995(4)	0.0805(5)	0.9356(3)	5.2(4)
C(206)	0.5290(4)	0.1628(5)	0.7153(3)	5.0(4)
C(207)	0.4028(4)	0.0351(5)	0.8421(3)	3.6(3)
C(208)	0.4699(4)	0.0222(5)	0.8908(3)	4.5(4)
C(209)	0.5332(4)	0.1077(5)	0.8900(3)	3.9(3)
C(210)	0.5636(4)	0.1205(5)	0.8255(3)	4.1(3)
C(211)	0.4984(4)	0.1510(5)	0.7805(3)	3.5(3)
C(212)	0.4359(4)	0.0626(5)	0.7790(3)	3.8(3)
C(301)	0.3611(3)	0.4086(4)	0.8789(2)	2.4(3)
C(302)	0.3351(3)	0.5075(4)	0.8981(2)	2.2(3)
C(303)	0.3839(3)	0.5837(4)	0.9232(2)	2.5(3)
C(304)	0.4620(3)	0.5587(4)	0.9278(2)	2.6(3)
C(305)	0.4921(3)	0.4625(5)	0.9070(2)	2.8(3)
C(306)	0.4393(3)	0.3875(4)	0.8837(2)	2.6(3)
C(307)	0.3562(3)	0.6931(5)	0.9431(3)	3.4(3)
C(308)	0.5768(3)	0.4436(5)	0.9069(3)	3.6(3)
H(1)	0.075	0.182	0.559	4.9
H(2)	0.135	0.283	0.574	4.9
H(3)	0.041	0.282	0.611	4.9
H(4)	0.152	0.066	0.584	4.9
H(5)	0.253	-0.088	0.612	4.9
H(6)	0.278	-0.121	0.681	4.9
H(7)	0.187	-0.155	0.656	4.9
H(9)	0.057	-0.083	0.928	4.9
H(13)	0.328	-0.084	0.884	4.9
H(14)	0.314	-0.075	0.806	4.9
H(15)	0.394	-0.122	0.831	4.9
H(16)	-0.002	0.305	0.883	4.9
H(17)	0.002	0.326	0.814	4.9
H(18)	-0.050	0.404	0.843	4.9
H(19)	0.225	0.381	0.656	4.9
H(20)	0.309	0.398	0.648	4.9
H(21)	0.288	0.447	0.705	4.9
H(22)	0.336	0.298	0.735	4.9
H(23)	0.393	0.744	0.958	4.9
H(24)	0.329	0.730	0.914	4.9
H(25)	0.317	0.693	0.976	4.9
H(26)	0.501	0.613	0.946	4.9
H(27)	0.319	0.353	0.859	4.9
H(28)	0.162	0.700	1.002	4.9
H(29)	0.098	0.592	1.033	4.9
H(30)	0.060	0.681	0.998	4.9
H(31)	0.011	0.539	0.925	4.9

(Table S2-2, contd.)

H(32)	0.066	0.433	0.961	4.9
H(33)	0.065	0.700	0.877	4.9
H(34)	0.168	0.736	0.890	4.9
H(35)	0.613	0.501	0.884	4.9
H(36)	0.612	0.481	0.939	4.9
H(37)	0.334	0.189	1.051	4.9
H(38)	0.382	0.326	1.032	4.9
H(39)	0.317	0.300	1.085	4.9
H(40)	0.254	0.346	1.025	4.9
H(41)	0.446	-0.015	0.932	4.9
H(42)	0.488	-0.044	0.875	4.9
H(43)	0.164	0.651	0.729	4.9
H(44)	0.084	0.728	0.762	4.9
H(45)	0.181	0.738	0.772	4.9
H(46)	0.589	0.042	0.810	4.9
H(47)	0.607	0.181	0.818	4.9
H(48)	0.615	0.002	0.917	4.9
H(49)	0.643	0.164	0.944	4.9
H(50)	0.563	0.240	0.707	4.9
H(51)	0.491	0.198	0.688	4.9
H(52)	0.554	0.101	0.701	4.9
H(53)	0.392	0.095	0.746	4.9
H(55)	0.108	0.481	0.770	4.9
H(56)	0.033	0.574	0.798	4.9
H(58)	0.581	0.055	0.980	4.9
H(61)	0.463	-0.015	0.753	4.9
H(62)	0.612	0.365	0.903	4.9
H(66)	0.036	0.055	0.798	4.9
H(67)	0.098	-0.031	0.785	4.9
H(68)	0.029	-0.059	0.826	4.9
H(69)	0.092	-0.010	1.074	4.9
H(70)	0.078	-0.111	1.033	4.9
H(71)	0.160	-0.087	1.061	4.9

[a]Estimated standard deviations are given in parentheses. [b]All non-hydrogen atoms were assigned anisotropic thermal parameters given as the isotropic equivalent displacement parameter defined as $B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a^*_i \cdot a^*_j \, a_i \cdot a_j$. [c]All hydrogen atoms were determined by difference Fourier syntheses and were not refined with the appropriate B_{iso}.

Table S2-3. Final Anisotropic Thermal Parameters for 3[a,b]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	0.0558(5)	0.0356(4)	0.0272(4)	-0.0054(4)	0.0089(3)	-0.0015(4)
Mn(1)	0.0628(7)	0.0385(6)	0.0256(5)	-0.0031(5)	0.0071(4)	-0.0069(5)
O(1)	0.060(3)	0.051(3)	0.034(3)	0.000(2)	0.007(2)	-0.008(2)
O(2)	0.076(3)	0.043(3)	0.032(3)	-0.001(2)	0.005(2)	-0.006(2)
O(3)	0.059(3)	0.038(3)	0.036(3)	-0.017(2)	0.008(2)	-0.008(2)
O(4)	0.076(3)	0.042(3)	0.030(3)	-0.014(3)	0.016(2)	0.001(2)
O(5)	0.067(3)	0.058(3)	0.033(2)	-0.013(2)	-0.000(2)	0.005(2)
O(6)	0.059(3)	0.038(3)	0.035(2)	0.003(2)	-0.006(2)	-0.006(2)
O(101)	0.049(3)	0.043(2)	0.027(2)	0.005(2)	0.002(2)	-0.006(2)
O(102)	0.071(3)	0.042(3)	0.034(2)	0.004(2)	0.019(2)	-0.007(2)
O(103)	0.044(2)	0.037(2)	0.020(2)	0.006(2)	0.001(2)	0.002(2)
O(104)	0.049(3)	0.070(3)	0.025(2)	0.005(2)	0.004(2)	0.010(2)
O(201)	0.067(3)	0.050(3)	0.024(2)	0.007(2)	0.014(2)	0.004(2)
O(202)	0.061(3)	0.032(2)	0.038(2)	0.001(2)	0.006(2)	0.005(2)
O(203)	0.065(3)	0.053(3)	0.026(2)	0.015(2)	0.008(2)	0.003(2)
O(204)	0.062(3)	0.042(3)	0.023(2)	0.009(2)	0.009(2)	0.007(2)
N(101)	0.037(3)	0.032(3)	0.017(3)	0.005(2)	0.002(2)	0.001(2)
N(201)	0.047(3)	0.039(3)	0.021(3)	0.014(2)	0.006(2)	-0.002(2)
C(1)	0.056(4)	0.064(5)	0.035(4)	-0.005(4)	0.000(3)	0.003(4)
C(2)	0.043(4)	0.052(4)	0.038(4)	-0.018(4)	0.005(3)	-0.003(4)
C(3)	0.058(4)	0.045(4)	0.023(3)	-0.005(3)	0.006(3)	-0.006(3)
C(4)	0.038(4)	0.043(4)	0.036(4)	-0.013(3)	0.014(3)	-0.011(3)
C(5)	0.048(4)	0.048(4)	0.043(4)	-0.004(3)	0.010(3)	-0.011(3)
C(6)	0.077(5)	0.079(6)	0.064(5)	-0.036(5)	-0.005(4)	-0.005(4)
C(7)	0.056(5)	0.043(4)	0.049(5)	-0.004(4)	0.006(4)	-0.015(4)
C(8)	0.074(5)	0.046(4)	0.051(5)	-0.024(4)	0.010(4)	-0.009(4)
C(9)	0.071(5)	0.041(4)	0.046(5)	-0.002(4)	0.018(4)	-0.000(4)
C(10)	0.123(7)	0.047(4)	0.056(5)	-0.023(5)	0.026(5)	0.007(4)
C(21)	0.089(6)	0.058(5)	0.048(5)	-0.027(4)	-0.014(4)	0.013(4)
C(22)	0.069(5)	0.057(4)	0.039(4)	0.002(4)	-0.009(4)	-0.006(4)
C(101)	0.045(4)	0.037(4)	0.033(4)	-0.011(3)	0.005(3)	-0.004(3)
C(102)	0.031(3)	0.024(3)	0.029(4)	-0.000(3)	0.004(3)	-0.006(3)
C(103)	0.039(4)	0.035(4)	0.030(4)	0.001(3)	0.003(3)	0.008(3)
C(104)	0.048(4)	0.065(5)	0.064(5)	-0.011(4)	-0.001(4)	-0.018(4)
C(105)	0.046(4)	0.045(4)	0.040(4)	0.007(3)	0.015(3)	-0.007(3)
C(106)	0.058(5)	0.073(5)	0.048(4)	0.009(4)	-0.008(3)	0.028(4)
C(107)	0.033(4)	0.047(4)	0.043(4)	0.007(3)	0.001(3)	-0.009(3)
C(108)	0.038(4)	0.041(4)	0.034(4)	-0.001(3)	0.008(3)	-0.005(3)
C(109)	0.039(4)	0.037(4)	0.034(4)	0.008(3)	0.010(3)	-0.004(3)
C(110)	0.037(3)	0.035(4)	0.040(4)	0.009(3)	0.002(3)	0.008(3)
C(111)	0.038(4)	0.045(4)	0.034(4)	0.006(3)	0.002(3)	0.010(3)
C(112)	0.043(4)	0.059(4)	0.031(4)	0.010(3)	-0.001(3)	0.002(3)

(Table S2-3, contd.)

C(201)	0.062(5)	0.030(4)	0.050(5)	-0.006(3)	0.014(4)	-0.004(3)
C(202)	0.042(4)	0.049(4)	0.032(4)	0.006(3)	0.008(3)	0.009(3)
C(203)	0.042(4)	0.042(4)	0.026(4)	-0.004(3)	0.013(3)	-0.005(3)
C(204)	0.107(6)	0.033(4)	0.074(6)	-0.005(4)	0.020(5)	-0.005(4)
C(205)	0.092(6)	0.060(5)	0.045(4)	0.036(4)	0.002(4)	0.007(4)
C(206)	0.102(6)	0.054(5)	0.035(4)	0.022(4)	0.034(4)	-0.003(3)
C(207)	0.069(5)	0.033(4)	0.037(4)	0.014(3)	0.013(3)	0.004(3)
C(208)	0.091(6)	0.037(4)	0.045(4)	0.027(4)	0.025(4)	0.013(3)
C(209)	0.067(5)	0.041(4)	0.040(4)	0.023(4)	0.013(3)	0.005(3)
C(210)	0.064(5)	0.056(4)	0.035(4)	0.023(4)	0.023(3)	0.003(3)
C(211)	0.064(5)	0.041(4)	0.029(4)	0.014(3)	0.021(3)	-0.000(3)
C(212)	0.077(5)	0.036(4)	0.033(4)	0.007(4)	0.018(3)	-0.001(3)
C(301)	0.039(4)	0.034(3)	0.019(3)	-0.002(3)	0.008(3)	0.002(3)
C(302)	0.024(3)	0.037(4)	0.022(3)	0.002(3)	0.005(3)	0.003(3)
C(303)	0.045(4)	0.032(4)	0.017(3)	0.004(3)	0.005(3)	0.006(3)
C(304)	0.036(4)	0.039(4)	0.023(3)	-0.003(3)	0.003(3)	0.007(3)
C(305)	0.037(4)	0.044(4)	0.025(3)	0.005(3)	0.005(3)	0.009(3)
C(306)	0.043(4)	0.035(4)	0.020(3)	0.009(3)	0.012(3)	0.005(3)
C(307)	0.054(4)	0.032(4)	0.043(4)	0.010(3)	-0.005(3)	-0.004(3)
C(308)	0.030(4)	0.054(4)	0.053(4)	-0.003(3)	0.005(3)	0.000(3)

[a]Estmated standard deviations are given in parentheses. [b]Parameters have the form $\exp(-2\pi^2(U_{11}h^2a^{*2} + \cdots + 2U_{12}hka^*b^*\cos\gamma + \cdots))$

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Table S2-4. Bond Lengths for Non-hydrogen Atoms of 3[a]

atom	atom	distance	atom	atom	distance
Zn(1)	O(3)	2.129(4)	N(101)	C(103)	1.426(6)
Zn(1)	O(4)	1.977(4)	N(101)	C(302)	1.459(6)
Zn(1)	O(6)	2.105(4)	N(201)	C(202)	1.416(7)
Zn(1)	O(101)	1.990(4)	N(201)	C(203)	1.415(7)
Zn(1)	O(201)	1.981(4)	N(201)	C(306)	1.458(7)
Mn(1)	O(1)	2.115(4)	C(1)	C(2)	1.524(8)
Mn(1)	O(2)	2.110(4)	C(2)	C(3)	1.387(8)
Mn(1)	O(3)	2.332(4)	C(3)	C(4)	1.396(8)
Mn(1)	O(5)	2.269(4)	C(4)	C(5)	1.501(8)
Mn(1)	O(102)	2.109(4)	C(6)	C(7)	1.498(8)
Mn(1)	O(202)	2.123(4)	C(7)	C(8)	1.403(9)
O(1)	C(2)	1.274(6)	C(8)	C(9)	1.392(9)
O(2)	C(4)	1.275(6)	C(9)	C(10)	1.513(8)
O(3)	C(7)	1.263(7)	C(101)	C(107)	1.529(8)
O(4)	C(9)	1.256(7)	C(102)	C(109)	1.519(7)
O(5)	C(21)	1.442(8)	C(103)	C(111)	1.495(7)
O(6)	C(22)	1.421(7)	C(104)	C(107)	1.528(8)
O(101)	C(101)	1.271(6)	C(105)	C(109)	1.544(7)
O(102)	C(101)	1.252(6)	C(106)	C(111)	1.543(8)
O(103)	C(102)	1.217(6)	C(107)	C(108)	1.533(7)
O(104)	C(103)	1.210(6)	C(107)	C(112)	1.544(8)
O(201)	C(201)	1.262(7)	C(108)	C(109)	1.535(7)
O(202)	C(201)	1.261(7)	C(109)	C(110)	1.534(7)
O(203)	C(202)	1.215(6)	C(110)	C(111)	1.528(8)
O(204)	C(203)	1.217(6)	C(111)	C(112)	1.551(8)
N(101)	C(102)	1.410(6)	C(201)	C(207)	1.522(8)

(Table S2-4, contd.)

C(202)	C(209)	1.516(8)
C(203)	C(211)	1.532(8)
C(204)	C(207)	1.549(9)
C(205)	C(209)	1.535(9)
C(206)	C(211)	1.532(7)
C(207)	C(208)	1.557(9)
C(207)	C(212)	1.538(8)
C(208)	C(209)	1.527(9)
C(209)	C(210)	1.515(8)
C(210)	C(211)	1.521(8)
C(211)	C(212)	1.543(8)
C(301)	C(302)	1.380(7)
C(301)	C(306)	1.379(7)
C(302)	C(303)	1.373(7)
C(303)	C(304)	1.387(7)
C(303)	C(307)	1.512(7)
C(304)	C(305)	1.387(7)
C(305)	C(306)	1.392(8)
C(305)	C(308)	1.483(8)

[a]Estimated standard deviations are given in parentheses.

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Table S2-5. Bond Angles for Non-hydrogen Atoms of **3**[a]

atom	atom	atom	angle	atom	atom	atom	angle
O(3)	Zn(1)	O(4)	90.3(2)	Mn(1)	O(2)	C(4)	124.5(4)
O(3)	Zn(1)	O(6)	169.4(2)	Zn(1)	O(3)	Mn(1)	104.0(2)
O(3)	Zn(1)	O(101)	88.5(2)	Zn(1)	O(3)	C(7)	123.5(4)
O(3)	Zn(1)	O(201)	96.7(2)	Mn(1)	O(3)	C(7)	132.5(4)
O(4)	Zn(1)	O(6)	90.9(2)	Zn(1)	O(4)	C(9)	127.2(4)
O(4)	Zn(1)	O(101)	115.9(2)	Mn(1)	O(5)	C(21)	122.4(4)
O(4)	Zn(1)	O(201)	100.7(2)	Zn(1)	O(6)	C(22)	127.5(4)
O(6)	Zn(1)	O(101)	81.5(1)	Zn(1)	O(101)	C(101)	128.2(4)
O(6)	Zn(1)	O(201)	93.4(2)	Mn(1)	O(102)	C(101)	136.1(4)
O(101)	Zn(1)	O(201)	143.1(2)	Zn(1)	O(201)	C(201)	114.3(4)
O(1)	Mn(1)	O(2)	85.0(2)	Mn(1)	O(202)	C(201)	139.1(4)
O(1)	Mn(1)	O(3)	116.8(2)	C(102)	N(101)	C(103)	124.5(5)
O(1)	Mn(1)	O(5)	85.0(2)	C(102)	N(101)	C(302)	117.6(4)
O(1)	Mn(1)	O(102)	90.3(2)	C(103)	N(101)	C(302)	117.5(4)
O(1)	Mn(1)	O(202)	162.1(2)	C(202)	N(201)	C(203)	124.2(5)
O(2)	Mn(1)	O(3)	90.2(1)	C(202)	N(201)	C(306)	117.4(4)
O(2)	Mn(1)	O(5)	99.4(2)	C(203)	N(201)	C(306)	118.4(4)
O(2)	Mn(1)	O(102)	170.7(2)	O(1)	C(2)	C(1)	116.1(6)
O(2)	Mn(1)	O(202)	93.5(2)	O(1)	C(2)	C(3)	125.6(6)
O(3)	Mn(1)	O(5)	157.0(1)	C(1)	C(2)	C(3)	118.3(5)
O(3)	Mn(1)	O(102)	84.8(1)	C(2)	C(3)	C(4)	125.8(5)
O(3)	Mn(1)	O(202)	81.0(1)	O(2)	C(4)	C(3)	125.2(5)
O(5)	Mn(1)	O(102)	88.1(1)	O(2)	C(4)	C(5)	115.6(6)
O(5)	Mn(1)	O(202)	77.6(1)	C(3)	C(4)	C(5)	119.3(5)
O(102)	Mn(1)	O(202)	93.3(2)	O(3)	C(7)	C(6)	116.7(6)
Mn(1)	O(1)	C(2)	121.3(4)	O(3)	C(7)	C(8)	124.9(6)

(Table S2-5, contd.)

C(6)	C(7)	C(8)	118.3(6)	C(108)	C(109)	C(110)	109.9(5)
C(7)	C(8)	C(9)	127.2(6)	C(109)	C(110)	C(111)	109.1(5)
O(4)	C(9)	C(8)	126.4(6)	C(103)	C(111)	C(106)	109.0(5)
O(4)	C(9)	C(10)	114.9(6)	C(103)	C(111)	C(110)	109.5(5)
C(8)	C(9)	C(10)	118.7(6)	C(103)	C(111)	C(112)	112.0(5)
O(101)	C(101)	O(102)	124.6(6)	C(106)	C(111)	C(110)	109.7(5)
O(101)	C(101)	C(107)	117.7(5)	C(106)	C(111)	C(112)	107.4(5)
O(102)	C(101)	C(107)	117.6(5)	C(110)	C(111)	C(112)	109.1(5)
O(103)	C(102)	N(101)	119.4(5)	C(107)	C(112)	C(111)	115.3(5)
O(103)	C(102)	C(109)	123.0(5)	O(201)	C(201)	O(202)	122.9(6)
N(101)	C(102)	C(109)	117.6(5)	O(201)	C(201)	C(207)	118.6(6)
O(104)	C(103)	N(101)	118.0(5)	O(202)	C(201)	C(207)	118.4(6)
O(104)	C(103)	C(111)	124.6(5)	O(203)	C(202)	N(201)	118.8(5)
N(101)	C(103)	C(111)	117.2(5)	O(203)	C(202)	C(209)	122.7(5)
C(101)	C(107)	C(104)	103.1(5)	N(201)	C(202)	C(209)	118.5(5)
C(101)	C(107)	C(108)	112.2(5)	O(204)	C(203)	N(201)	119.3(5)
C(101)	C(107)	C(112)	112.2(5)	O(204)	C(203)	C(211)	123.8(5)
C(104)	C(107)	C(108)	109.8(5)	N(201)	C(203)	C(211)	116.9(5)
C(104)	C(107)	C(112)	108.8(5)	C(201)	C(207)	C(204)	102.4(5)
C(108)	C(107)	C(112)	110.4(5)	C(201)	C(207)	C(208)	112.1(5)
C(107)	C(108)	C(109)	114.7(4)	C(201)	C(207)	C(212)	112.7(5)
C(102)	C(109)	C(105)	107.4(5)	C(204)	C(207)	C(208)	110.3(5)
C(102)	C(109)	C(108)	109.1(4)	C(204)	C(207)	C(212)	109.2(5)
C(102)	C(109)	C(110)	110.2(4)	C(208)	C(207)	C(212)	109.9(5)
C(105)	C(109)	C(108)	110.4(4)	C(207)	C(208)	C(209)	116.2(5)
C(105)	C(109)	C(110)	109.9(5)	C(202)	C(209)	C(205)	108.2(5)

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(Table S2-5, contd.)

C(202)	C(209)	C(208)	107.3(5)	C(301)	C(306)	C(305)	122.2(5)
C(202)	C(209)	C(210)	109.1(5)				
C(205)	C(209)	C(208)	111.2(5)				
C(205)	C(209)	C(210)	110.4(5)				
C(208)	C(209)	C(210)	110.4(5)				
C(209)	C(210)	C(211)	110.6(5)				
C(203)	C(211)	C(206)	108.5(5)				
C(203)	C(211)	C(210)	108.9(5)				
C(203)	C(211)	C(212)	110.9(5)				
C(206)	C(211)	C(210)	110.6(5)				
C(206)	C(211)	C(212)	107.9(5)				
C(210)	C(211)	C(212)	110.1(5)				
C(207)	C(212)	C(211)	114.6(5)				
C(302)	C(301)	C(306)	118.3(5)				
N(101)	C(302)	C(301)	120.1(5)				
N(101)	C(302)	C(303)	117.5(5)				
C(301)	C(302)	C(303)	122.3(5)				
C(302)	C(303)	C(304)	117.5(5)				
C(302)	C(303)	C(307)	122.6(5)				
C(304)	C(303)	C(307)	119.9(5)				
C(303)	C(304)	C(305)	122.9(5)				
C(304)	C(305)	C(306)	116.7(5)				
C(304)	C(305)	C(308)	121.1(6)				
C(306)	C(305)	C(308)	122.2(5)				
N(201)	C(306)	C(301)	119.0(5)				
N(201)	C(306)	C(305)	118.8(5)				

[a]Estimated deviations are given in parentheses.

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Table S3-1. Crystallographic and Experimental Data for **4**

formula	$C_{44}H_{60}N_2O_{14}ZnFe$
formula weight	962.19
color	yellow
size, mm	0.38 x 0.39 x 0.30
cryst. system	monoclinic
space group	$P2_1/c$ (No. 14)
no. refs used for cell determination	22 ($23 < 2\theta < 25°$)
lattice const.	a = 17.630(1) Å
	b = 12.374(2) Å
	c = 21.771(2) Å
	β = 90.306(8)°
	V = 4749.4(7) Å^3
Z	4
D_{calc}, g cm^{-3}	1.346
μ (Mo $K\alpha$), cm^{-1}	8.75 (trans. 0.97 ~ 1.00)
	An absorption correction by DIFABS was applied.[a]
radiation	Mo $K\alpha$ (λ = 0.71069 Å)
monochromator	graphite
temp,°C	-75
2θ range, deg	$3 < 2\theta < 40$
h, k, l range	+h, +k, ±l
scan method	ω - 2θ
scan speed,° min^{-1}	variable (2 ~ 8)
scan width	0.80 + 0.35 tanθ
std. reflections	3 every ~200 (3600 sec)
solution	direct methods (SIR92)

(Table S3-1, contd.)

refinement	full-matrix least-squares All non-hydrogen atoms were refined with aniotropic temperature factors.
function minimized	$\Sigma w(\|F_o\| - \|F_c\|)^2$
weighting scheme	$1/\sigma^2(F_o)$
anomalous dispersion	all non-hydrogen atoms
hydrogen atoms	All carbon-bound hydrogen atoms were calculated with C-H = 0.95 Å and those of methanol molecules were determined by difference Fourier syntheses. All hydrogen atoms were not refined
no. reflections measured	4683
no. unique reflections	3248 ($I > 3\sigma(I)$)
p-factor	0.03
no. variables	560
data / param ratio	5.80
R [b]	0.041
R_w [c]	0.049
GOF [d]	1.77
max shift/error in final cycle	0.001
ρ_{max}, eÅ^3	0.38 around C(308)

[a] Walker, N.; Stuart, D. *Acta Crystallogr.* **1983**, *A39*, 158.

[b] $R = \Sigma| |F_o| - |F_c| |/\Sigma|F_o|$.

[c] $R_w = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$ ($w = 1/\sigma^2(F_o)$).

[d] GOF = $[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_p)]^{1/2}$ (N_o = no. data, N_p = no. variables)

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Table S3-2. Final Positional Parameters and B_{eq} for $4^{a,b,c}$

atom	x	y	z	B_{eq}
Zn(1)	0.71706(4)	0.19404(6)	0.07024(3)	2.82(4)
Fe(1)	0.70866(5)	0.20795(8)	0.23028(4)	2.75(5)
O(1)	0.7254(2)	0.0627(3)	0.2717(2)	3.3(2)
O(2)	0.6281(2)	0.2368(4)	0.2951(2)	3.4(2)
O(3)	0.6579(2)	0.1276(4)	0.1466(2)	3.2(2)
O(4)	0.6678(3)	0.0911(4)	0.0148(2)	4.2(3)
O(5)	0.7876(2)	0.3007(4)	0.2883(2)	3.4(2)
O(6)	0.7604(3)	0.2834(3)	-0.0043(2)	3.7(2)
O(101)	0.8146(2)	0.1201(4)	0.0857(2)	3.3(2)
O(102)	0.8078(2)	0.1900(3)	0.1790(2)	2.8(2)
O(103)	0.9810(2)	0.2368(4)	0.0384(2)	3.3(2)
O(104)	0.9360(2)	0.3359(4)	0.2350(2)	3.1(2)
O(201)	0.6629(2)	0.3300(3)	0.0862(2)	2.8(2)
O(202)	0.6814(2)	0.3524(3)	0.1874(2)	2.8(2)
O(203)	0.7351(2)	0.5076(3)	0.0046(2)	2.5(2)
O(204)	0.7831(3)	0.5983(4)	0.2025(2)	3.4(2)
N(101)	0.9622(3)	0.2883(4)	0.1368(2)	2.4(3)
N(201)	0.7577(3)	0.5514(4)	0.1040(2)	2.0(3)
C(1)	0.7330(4)	-0.0742(6)	0.3465(3)	3.9(4)
C(2)	0.7058(4)	0.0348(5)	0.3257(3)	2.6(4)
C(3)	0.6617(4)	0.0976(6)	0.3643(3)	3.1(4)
C(4)	0.6276(3)	0.1949(6)	0.3482(3)	2.9(4)
C(5)	0.5863(4)	0.2582(6)	0.3971(3)	4.0(4)
C(6)	0.5645(4)	0.0256(7)	0.1981(4)	5.8(5)
C(7)	0.6085(4)	0.0521(6)	0.1416(3)	3.6(4)
C(8)	0.5937(4)	-0.0027(6)	0.0874(4)	4.8(5)
C(9)	0.6233(5)	0.0162(6)	0.0290(4)	4.3(5)
C(10)	0.5995(6)	-0.0569(7)	-0.0227(4)	7.6(6)
C(21)	0.7689(4)	0.4034(7)	0.3129(3)	4.9(5)
C(22)	0.8208(4)	0.2554(6)	-0.0435(3)	4.6(4)
C(101)	0.8354(4)	0.1237(5)	0.1409(3)	2.7(4)
C(102)	0.9862(4)	0.2136(5)	0.0917(3)	2.8(4)
C(103)	0.9606(4)	0.2664(6)	0.2005(3)	2.7(4)
C(104)	0.8447(4)	-0.0613(5)	0.1717(3)	4.5(4)
C(105)	1.0792(4)	0.0712(6)	0.0685(3)	4.5(4)
C(106)	1.0249(4)	0.1742(6)	0.2863(3)	4.4(4)
C(107)	0.8926(4)	0.0410(5)	0.1639(3)	2.8(3)
C(108)	0.9551(4)	0.0215(5)	0.1161(3)	3.5(4)
C(109)	1.0185(4)	0.1064(6)	0.1145(3)	3.4(4)
C(110)	1.0528(4)	0.1213(6)	0.1777(3)	3.8(4)
C(111)	0.9918(4)	0.1584(5)	0.2226(3)	2.9(4)
C(112)	0.9287(4)	0.0731(5)	0.2246(3)	3.3(4)
C(201)	0.6499(4)	0.3756(5)	0.1374(3)	2.6(4)

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(Table S3-2, contd.)

C(202)	0.7113(4)	0.5473(5)	0.0518(3)	2.4(4)
C(203)	0.7367(4)	0.5948(5)	0.1621(3)	2.4(4)
C(204)	0.5155(4)	0.3944(6)	0.1565(3)	3.6(4)
C(205)	0.6114(4)	0.6427(5)	-0.0064(3)	3.7(4)
C(206)	0.6566(4)	0.7261(6)	0.2162(3)	4.5(4)
C(207)	0.5866(3)	0.4592(5)	0.1379(3)	2.7(3)
C(208)	0.5746(3)	0.5102(5)	0.0738(3)	2.8(3)
C(209)	0.6322(4)	0.5970(5)	0.0566(3)	2.7(3)
C(210)	0.6337(3)	0.6855(5)	0.1049(3)	3.1(4)
C(211)	0.6564(4)	0.6382(5)	0.1668(3)	2.9(4)
C(212)	0.6008(3)	0.5489(6)	0.1855(3)	3.1(4)
C(301)	0.8602(3)	0.4197(5)	0.1179(3)	2.0(3)
C(302)	0.9363(4)	0.3931(5)	0.1151(3)	2.2(3)
C(303)	0.9896(3)	0.4652(5)	0.0924(3)	2.3(3)
C(304)	0.9628(4)	0.5630(5)	0.0698(3)	2.5(4)
C(305)	0.8870(4)	0.5931(5)	0.0726(3)	2.3(3)
C(306)	0.8368(3)	0.5197(5)	0.0971(3)	1.8(3)
C(307)	1.0732(4)	0.4429(6)	0.0933(3)	3.4(4)
C(308)	0.8618(4)	0.7015(5)	0.0507(3)	3.4(4)
H(1)	0.823	0.368	0.135	2.6
H(2)	1.000	0.612	0.051	3.0
H(3)	0.718	-0.090	0.388	4.7
H(4)	0.715	-0.131	0.320	4.7
H(5)	0.789	-0.077	0.346	4.7
H(6)	0.609	0.329	0.403	4.9
H(7)	0.534	0.268	0.387	4.9
H(8)	0.589	0.222	0.437	4.9
H(9)	0.537	0.088	0.213	6.7
H(10)	0.530	-0.031	0.191	6.7
H(11)	0.598	0.003	0.232	6.7
H(12)	0.565	-0.112	-0.011	8.6
H(13)	0.574	-0.015	-0.055	8.6
H(14)	0.643	-0.090	-0.042	8.6
H(15)	0.805	-0.050	0.201	5.2
H(16)	0.822	-0.082	0.134	5.2
H(17)	0.875	-0.120	0.186	5.2
H(18)	1.102	0.003	0.080	5.5
H(19)	1.059	0.063	0.028	5.5
H(20)	1.120	0.123	0.067	5.5
H(21)	1.045	0.109	0.303	5.7
H(22)	1.064	0.227	0.287	5.7
H(23)	0.986	0.200	0.315	5.7
H(24)	0.471	0.441	0.157	4.4
H(25)	0.505	0.338	0.127	4.4
H(26)	0.522	0.363	0.196	4.4
H(27)	0.648	0.696	-0.020	4.1

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(Table S3-2, contd.)

H(28)	0.612	0.586	-0.038	4.1
H(29)	0.562	0.675	-0.008	4.1
H(30)	0.671	0.699	0.255	5.1
H(31)	0.690	0.785	0.206	5.1
H(32)	0.606	0.758	0.221	5.1
H(33)	1.084	0.373	0.111	4.1
H(34)	1.095	0.446	0.054	4.1
H(35)	1.099	0.495	0.119	4.1
H(36)	0.887	0.759	0.074	3.8
H(37)	0.874	0.713	0.008	3.8
H(38)	0.808	0.711	0.056	3.8
H(39)	0.654	0.072	0.407	3.8
H(40)	0.558	-0.064	0.091	5.8
H(41)	0.977	-0.050	0.123	4.0
H(42)	0.931	0.018	0.076	4.0
H(43)	1.077	0.055	0.192	4.7
H(44)	1.094	0.174	0.176	4.7
H(45)	0.888	0.101	0.251	3.7
H(46)	0.947	0.009	0.245	3.7
H(47)	0.575	0.454	0.043	3.5
H(48)	0.524	0.542	0.072	3.5
H(49)	0.669	0.742	0.093	3.5
H(50)	0.585	0.721	0.107	3.5
H(51)	0.552	0.582	0.196	3.7
H(52)	0.619	0.516	0.224	3.7
H(53)	0.809	0.435	0.337	5.2
H(54)	0.756	0.456	0.281	5.2
H(55)	0.725	0.400	0.339	5.2
H(56)	0.811	0.190	-0.065	5.3
H(57)	0.830	0.312	-0.074	5.3
H(58)	0.868	0.247	-0.021	5.3
H(59)	0.846	0.305	0.265	4.5
H(60)	0.753	0.378	0.003	4.5

[a]Estimated standard deviations are given in parentheses. [b]All non-hydrogen atoms were assigned anisotropic thermal parameters given as the isotropic equivalent displacement parameter defined as $B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a^*_i \cdot a^*_j \, a_i \cdot a_j$. [c]All carbon-bound hydrogen atoms were calculated with C-H = 0.95 Å and those of methanol molecules were determined by difference Fourier syntheses. All hydrogen atoms were not refined with the appropriate B_{iso}.

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Table S3-3. Final Anisotropic Thermal Parameters for 4[a,b]

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(1)	0.0419(5)	0.0330(5)	0.0322(5)	-0.0006(4)	-0.0038(4)	-0.0018(4)
Fe(1)	0.0386(6)	0.0378(7)	0.0280(6)	-0.0005(5)	0.0022(5)	0.0054(5)
O(1)	0.048(3)	0.044(3)	0.034(3)	0.004(2)	0.001(2)	0.006(3)
O(2)	0.041(3)	0.050(3)	0.038(3)	0.002(2)	0.002(2)	0.011(3)
O(3)	0.042(3)	0.039(3)	0.040(3)	-0.011(3)	-0.001(2)	0.003(2)
O(4)	0.071(4)	0.038(3)	0.050(3)	-0.010(3)	-0.019(3)	-0.003(3)
O(5)	0.043(3)	0.054(3)	0.034(3)	-0.000(3)	0.003(2)	-0.011(3)
O(6)	0.063(3)	0.039(3)	0.037(3)	0.002(3)	0.015(3)	-0.002(2)
O(101)	0.050(3)	0.050(3)	0.026(3)	0.006(3)	-0.007(2)	-0.005(2)
O(102)	0.035(3)	0.034(3)	0.037(3)	-0.002(2)	0.000(2)	-0.006(3)
O(103)	0.048(3)	0.050(3)	0.027(3)	0.009(2)	0.004(2)	0.004(3)
O(104)	0.039(3)	0.045(3)	0.033(3)	-0.001(2)	-0.002(2)	-0.000(3)
O(201)	0.040(3)	0.033(3)	0.032(3)	0.003(2)	-0.001(2)	0.001(2)
O(202)	0.044(3)	0.035(3)	0.028(3)	0.000(2)	-0.008(2)	0.000(2)
O(203)	0.041(3)	0.029(3)	0.027(3)	0.004(2)	-0.002(2)	-0.002(2)
O(204)	0.032(3)	0.064(3)	0.034(3)	-0.000(3)	-0.003(2)	-0.014(3)
N(101)	0.033(3)	0.033(4)	0.025(4)	0.002(3)	0.001(3)	-0.000(3)
N(201)	0.026(3)	0.030(3)	0.022(3)	-0.002(3)	-0.004(3)	0.003(3)
C(1)	0.058(5)	0.046(5)	0.045(5)	-0.004(4)	-0.007(4)	0.011(4)
C(2)	0.033(4)	0.040(5)	0.027(5)	-0.007(4)	-0.012(4)	0.003(4)
C(3)	0.051(5)	0.035(5)	0.033(5)	-0.006(4)	-0.005(4)	0.004(4)
C(4)	0.031(4)	0.047(5)	0.034(5)	-0.013(4)	-0.003(4)	-0.009(4)
C(5)	0.044(5)	0.058(5)	0.053(5)	-0.004(4)	0.012(4)	0.002(4)
C(6)	0.070(6)	0.077(6)	0.073(6)	-0.033(5)	0.006(5)	0.013(5)
C(7)	0.043(5)	0.042(5)	0.051(6)	0.001(4)	-0.011(4)	0.012(4)
C(8)	0.079(6)	0.041(5)	0.060(6)	-0.025(4)	-0.019(5)	0.003(5)
C(9)	0.076(6)	0.030(5)	0.056(6)	0.003(5)	-0.035(5)	-0.004(5)
C(10)	0.15(1)	0.052(6)	0.088(7)	-0.028(6)	-0.045(6)	-0.006(5)
C(21)	0.059(6)	0.079(7)	0.049(5)	-0.012(5)	-0.005(4)	-0.002(5)
C(22)	0.075(6)	0.068(6)	0.032(5)	0.017(5)	0.010(4)	0.007(4)
C(101)	0.032(4)	0.031(5)	0.041(5)	-0.004(4)	0.005(4)	-0.001(4)
C(102)	0.033(4)	0.041(5)	0.032(5)	0.006(4)	0.001(4)	-0.004(4)
C(103)	0.026(4)	0.049(5)	0.028(5)	-0.004(4)	-0.004(4)	-0.001(4)
C(104)	0.079(6)	0.025(5)	0.067(6)	0.005(4)	0.006(5)	0.003(4)
C(105)	0.060(5)	0.060(5)	0.053(5)	0.035(4)	0.013(4)	0.010(4)
C(106)	0.066(5)	0.057(5)	0.045(5)	-0.006(4)	-0.024(4)	0.011(4)
C(107)	0.041(4)	0.033(4)	0.034(4)	0.014(4)	0.004(4)	0.002(4)
C(108)	0.056(5)	0.034(5)	0.045(5)	0.021(4)	-0.005(4)	-0.001(4)
C(109)	0.044(5)	0.050(5)	0.037(5)	0.022(4)	0.002(4)	0.001(4)
C(110)	0.050(5)	0.052(5)	0.040(5)	0.020(4)	-0.000(4)	0.012(4)
C(111)	0.041(5)	0.042(5)	0.025(4)	0.010(4)	-0.006(4)	0.011(4)
C(112)	0.059(5)	0.036(5)	0.030(4)	0.003(4)	0.003(4)	0.012(4)

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(Table S3-3, contd.)

C(201)	0.032(5)	0.030(5)	0.037(5)	-0.012(4)	-0.000(4)	0.001(4)
C(202)	0.039(5)	0.017(4)	0.035(5)	-0.001(4)	-0.003(4)	0.008(4)
C(203)	0.029(5)	0.031(4)	0.029(5)	-0.004(4)	0.001(4)	-0.007(4)
C(204)	0.028(4)	0.054(5)	0.053(5)	0.001(4)	0.001(4)	0.000(4)
C(205)	0.047(5)	0.042(5)	0.052(5)	0.008(4)	-0.012(4)	0.011(4)
C(206)	0.053(5)	0.053(5)	0.065(6)	0.004(4)	0.010(4)	-0.019(5)
C(207)	0.021(4)	0.046(5)	0.034(4)	0.003(4)	0.003(3)	-0.005(4)
C(208)	0.026(4)	0.033(4)	0.048(5)	0.008(3)	-0.007(3)	-0.005(4)
C(209)	0.034(4)	0.036(4)	0.033(4)	0.002(4)	-0.003(3)	0.003(4)
C(210)	0.032(4)	0.032(4)	0.052(5)	0.008(3)	-0.004(4)	-0.001(4)
C(211)	0.036(5)	0.036(4)	0.040(5)	0.001(4)	0.005(4)	-0.016(4)
C(212)	0.030(4)	0.056(5)	0.032(4)	0.008(4)	0.002(3)	-0.011(4)
C(301)	0.025(4)	0.033(5)	0.018(4)	-0.001(4)	0.006(3)	-0.001(3)
C(302)	0.031(5)	0.031(5)	0.024(4)	0.005(4)	0.001(3)	0.003(3)
C(303)	0.026(4)	0.036(5)	0.024(4)	0.003(4)	-0.001(3)	-0.002(4)
C(304)	0.029(5)	0.045(5)	0.023(4)	-0.008(4)	0.006(3)	-0.006(4)
C(305)	0.047(5)	0.026(4)	0.014(4)	-0.002(4)	0.003(3)	0.000(3)
C(306)	0.025(4)	0.026(4)	0.017(4)	0.001(4)	-0.006(3)	-0.004(3)
C(307)	0.036(5)	0.050(5)	0.042(5)	-0.010(4)	-0.001(3)	0.006(4)
C(308)	0.050(5)	0.037(5)	0.041(4)	-0.002(4)	0.013(4)	0.003(4)

[a]Estmated standard deviations are given in parentheses. [b]Parameters have the form $\exp(-2\pi^2(U_{11}h^2a^{*2} + \cdots + 2U_{12}hka^*b^*\cos\gamma + \cdots))$

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Table S3-4. Bond Lengths for Non-hydrogen Atoms of **4**[a]

atom	atom	distance	atom	atom	distance
Zn(1)	O(3)	2.132(4)	N(101)	C(103)	1.414(7)
Zn(1)	O(4)	1.955(5)	N(101)	C(302)	1.453(7)
Zn(1)	O(6)	2.110(4)	N(201)	C(202)	1.396(7)
Zn(1)	O(101)	1.975(4)	N(201)	C(203)	1.426(7)
Zn(1)	O(201)	1.966(4)	N(201)	C(306)	1.457(7)
Fe(1)	O(1)	2.031(4)	C(1)	C(2)	1.501(9)
Fe(1)	O(2)	2.039(4)	C(2)	C(3)	1.387(9)
Fe(1)	O(3)	2.255(4)	C(3)	C(4)	1.391(9)
Fe(1)	O(5)	2.198(4)	C(4)	C(5)	1.512(9)
Fe(1)	O(102)	2.091(4)	C(6)	C(7)	1.49(1)
Fe(1)	O(202)	2.072(4)	C(7)	C(8)	1.38(1)
O(1)	C(2)	1.275(7)	C(8)	C(9)	1.40(1)
O(2)	C(4)	1.266(7)	C(9)	C(10)	1.50(1)
O(3)	C(7)	1.282(8)	C(101)	C(107)	1.520(9)
O(4)	C(9)	1.254(8)	C(102)	C(109)	1.525(9)
O(5)	C(21)	1.420(8)	C(103)	C(111)	1.522(9)
O(6)	C(22)	1.411(8)	C(104)	C(107)	1.531(9)
O(101)	C(101)	1.255(7)	C(105)	C(109)	1.532(9)
O(102)	C(101)	1.267(7)	C(106)	C(111)	1.514(8)
O(103)	C(102)	1.200(7)	C(107)	C(108)	1.539(9)
O(104)	C(103)	1.223(7)	C(107)	C(112)	1.517(9)
O(201)	C(201)	1.271(7)	C(108)	C(109)	1.535(9)
O(202)	C(201)	1.252(7)	C(109)	C(110)	1.511(9)
O(203)	C(202)	1.215(7)	C(110)	C(111)	1.530(9)
O(204)	C(203)	1.199(7)	C(111)	C(112)	1.534(9)
N(101)	C(102)	1.415(8)	C(201)	C(207)	1.521(9)

(Table S3-4, contd.)

C(202)	C(209)	1.529(9)
C(203)	C(211)	1.519(9)
C(204)	C(207)	1.544(9)
C(205)	C(209)	1.526(8)
C(206)	C(211)	1.529(9)
C(207)	C(208)	1.545(8)
C(207)	C(212)	1.540(9)
C(208)	C(209)	1.525(8)
C(209)	C(210)	1.519(8)
C(210)	C(211)	1.521(9)
C(211)	C(212)	1.533(9)
C(301)	C(302)	1.382(8)
C(301)	C(306)	1.381(8)
C(302)	C(303)	1.389(8)
C(303)	C(304)	1.389(8)
C(303)	*C(307)*	*1.498(8)*
C(304)	C(305)	1.388(8)
C(305)	C(306)	1.377(8)
C(305)	C(308)	1.491(9)

[a]Estimated standard deviations are given in parentheses.

Table S3-5. Bond Angles for Non-hydrogen Atoms of 4[a]

atom	atom	atom	angle	atom	atom	atom	angle
O(3)	Zn(1)	O(4)	90.8(2)	Fe(1)	O(2)	C(4)	124.7(4)
O(3)	Zn(1)	O(6)	169.2(2)	Zn(1)	O(3)	Fe(1)	105.5(2)
O(3)	Zn(1)	O(101)	96.7(2)	Zn(1)	O(3)	C(7)	123.3(4)
O(3)	Zn(1)	O(201)	87.2(2)	Fe(1)	O(3)	C(7)	131.1(4)
O(4)	Zn(1)	O(6)	91.6(2)	Zn(1)	O(4)	C(9)	127.3(5)
O(4)	Zn(1)	O(101)	100.7(2)	Fe(1)	O(5)	C(21)	122.5(4)
O(4)	Zn(1)	O(201)	116.9(2)	Zn(1)	O(6)	C(22)	127.9(4)
O(6)	Zn(1)	O(101)	93.2(2)	Zn(1)	O(101)	C(101)	113.4(4)
O(6)	Zn(1)	O(201)	82.3(2)	Fe(1)	O(102)	C(101)	138.1(4)
O(101)	Zn(1)	O(201)	142.2(2)	Zn(1)	O(201)	C(201)	128.7(4)
O(1)	Fe(1)	O(2)	87.0(2)	Fe(1)	O(202)	C(201)	133.6(4)
O(1)	Fe(1)	O(3)	91.4(2)	C(102)	N(101)	C(103)	124.2(6)
O(1)	Fe(1)	O(5)	96.7(2)	C(102)	N(101)	C(302)	116.9(5)
O(1)	Fe(1)	O(102)	91.3(2)	C(103)	N(101)	C(302)	118.9(5)
O(1)	Fe(1)	O(202)	174.9(2)	C(202)	N(201)	C(203)	125.6(5)
O(2)	Fe(1)	O(3)	111.2(2)	C(202)	N(201)	C(306)	117.6(5)
O(2)	Fe(1)	O(5)	87.3(2)	C(203)	N(201)	C(306)	116.5(5)
O(2)	Fe(1)	O(102)	167.3(2)	O(1)	C(2)	C(1)	115.7(6)
O(2)	Fe(1)	O(202)	90.0(2)	O(1)	C(2)	C(3)	124.3(6)
O(3)	Fe(1)	O(5)	160.3(2)	C(1)	C(2)	C(3)	120.0(6)
O(3)	Fe(1)	O(102)	81.4(2)	C(2)	C(3)	C(4)	125.1(6)
O(3)	Fe(1)	O(202)	85.8(2)	O(2)	C(4)	C(3)	125.4(6)
O(5)	Fe(1)	O(102)	80.4(2)	O(2)	C(4)	C(5)	115.9(7)
O(5)	Fe(1)	O(202)	87.3(2)	C(3)	C(4)	C(5)	118.7(7)
O(102)	Fe(1)	O(202)	92.5(2)	O(3)	C(7)	C(6)	116.4(7)
Fe(1)	O(1)	C(2)	127.5(4)	O(3)	C(7)	C(8)	123.7(7)

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(Table S3-5, contd.)

C(6)	C(7)	C(8)	119.8(7)	C(108)	C(109)	C(110)	110.5(6)
C(7)	C(8)	C(9)	128.6(7)	C(109)	C(110)	C(111)	109.8(5)
O(4)	C(9)	C(8)	125.9(7)	C(103)	C(111)	C(106)	108.3(6)
O(4)	C(9)	C(10)	115.7(8)	C(103)	C(111)	C(110)	108.4(5)
C(8)	C(9)	C(10)	118.5(8)	C(103)	C(111)	C(112)	110.7(5)
O(101)	C(101)	O(102)	122.6(6)	C(106)	C(111)	C(110)	110.8(5)
O(101)	C(101)	C(107)	118.9(6)	C(106)	C(111)	C(112)	109.8(5)
O(102)	C(101)	C(107)	118.5(6)	C(110)	C(111)	C(112)	108.9(5)
O(103)	C(102)	N(101)	119.6(6)	C(107)	C(112)	C(111)	117.1(5)
O(103)	C(102)	C(109)	123.3(6)	O(201)	C(201)	O(202)	125.4(6)
N(101)	C(102)	C(109)	117.1(6)	O(201)	C(201)	C(207)	116.3(6)
O(104)	C(103)	N(101)	118.5(6)	O(202)	C(201)	C(207)	118.2(6)
O(104)	C(103)	C(111)	123.5(6)	O(203)	C(202)	N(201)	120.0(6)
N(101)	C(103)	C(111)	118.0(6)	O(203)	C(202)	C(209)	122.5(6)
C(101)	C(107)	C(104)	103.2(5)	N(201)	C(202)	C(209)	117.4(6)
C(101)	C(107)	C(108)	111.0(5)	O(204)	C(203)	N(201)	119.0(6)
C(101)	C(107)	C(112)	112.7(5)	O(204)	C(203)	C(211)	124.8(6)
C(104)	C(107)	C(108)	110.0(5)	N(201)	C(203)	C(211)	116.0(6)
C(104)	C(107)	C(112)	110.4(5)	C(201)	C(207)	C(204)	104.2(5)
C(108)	C(107)	C(112)	109.4(5)	C(201)	C(207)	C(208)	111.7(5)
C(107)	C(108)	C(109)	115.6(5)	C(201)	C(207)	C(212)	112.2(5)
C(102)	C(109)	C(105)	107.3(6)	C(204)	C(207)	C(208)	110.0(5)
C(102)	C(109)	C(108)	109.4(5)	C(204)	C(207)	C(212)	109.1(5)
C(102)	C(109)	C(110)	109.7(6)	C(208)	C(207)	C(212)	109.6(5)
C(105)	C(109)	C(108)	109.4(6)	C(207)	C(208)	C(209)	114.9(5)
C(105)	C(109)	C(110)	110.6(6)	C(202)	C(209)	C(205)	107.7(5)

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(Table S3-5, contd.)

C(202)	C(209)	C(208)	110.0(5)	C(301)	C(306)	C(305)	121.7(6)
C(202)	C(209)	C(210)	108.9(5)				
C(205)	C(209)	C(208)	108.9(5)				
C(205)	C(209)	C(210)	111.0(5)				
C(208)	C(209)	C(210)	110.3(5)				
C(209)	C(210)	C(211)	109.8(5)				
C(203)	C(211)	C(206)	107.4(5)				
C(203)	C(211)	C(210)	108.5(5)				
C(203)	C(211)	C(212)	111.1(5)				
C(206)	C(211)	C(210)	110.4(6)				
C(206)	C(211)	C(212)	109.0(5)				
C(210)	C(211)	C(212)	110.4(5)				
C(207)	C(212)	C(211)	116.3(5)				
C(302)	C(301)	C(306)	119.2(6)				
N(101)	C(302)	C(301)	120.1(6)				
N(101)	C(302)	C(303)	118.5(5)				
C(301)	C(302)	C(303)	121.5(6)				
C(302)	C(303)	C(304)	117.1(6)				
C(302)	C(303)	C(307)	123.0(6)				
C(304)	C(303)	C(307)	119.9(6)				
C(303)	C(304)	C(305)	122.9(6)				
C(304)	C(305)	C(306)	117.5(6)				
C(304)	C(305)	C(308)	120.8(6)				
C(306)	C(305)	C(308)	121.7(6)				
N(201)	C(306)	C(301)	119.5(5)				
N(201)	C(306)	C(305)	118.7(6)				

[a]Estimated deviations are given in parentheses.

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Table S4-1. Crystallographic and Experimental Data for **5**

formula	$C_{44}H_{60}N_2O_{14}ZnNi$
formula weight	965.04
color	pale green
size, mm	0.48 x 0.31 x 0.18
cryst. system	monoclinic
space group	$P2_1/c$ (No. 14)
no. refs used for cell determination	22 ($21 < 2\theta < 25°$)
lattice const.	a = 17.817(2) Å
	b = 12.241(3) Å
	c = 21.786(2) Å
	β = 91.043(9)°
	V = 4751(1) Å^3
Z	4
D_{calc}, g cm^{-3}	1.343
μ (Mo $K\alpha$), cm^{-1}	9.66 (trans. 0.89 ~ 1.00)
	An absorption correction by ψ-scan method was applied.
radiation	Mo $K\alpha$ (λ = 0.71069 Å)
monochromator	graphite
temp,°C	-79
2θ range, deg	$3 < 2\theta < 46$
h, k, l range	+h, +k, ±l
scan method	ω - 2θ
scan speed,° min^{-1}	variable (2 ~ 8)
scan width	0.80 + 0.35 tanθ
std. reflections	3 every ~200 (3600 sec)
solution	direct methods (SIR92)

(Table S4-1, continue)

refinement	full-matrix least-squares All non-hydrogen atoms were refined with aniotropic temperature factors.
function minimized	$\Sigma w(\|F_o\| - \|F_c\|)^2$
weighting scheme	$1/\sigma^2(F_o)$
anomalous dispersion	all non-hydrogen atoms
hydrogen atoms	All carbon-bound hydrogen atoms were calculated with C-H = 0.95 Å and those of methanol molecules were determined by difference Fourier syntheses. All hydrogen atoms were not refined
no. reflections measured	6958
no. unique reflections	4497 ($I > 3\sigma(I)$)
p-factor	0.03
no. variables	560
data / param ratio	8.03
R [a]	0.050
Rw [b]	0.058
GOF [c]	1.82
max shift/error in final cycle	0.002
ρ_{max}, eÅ^3	0.65 around Ni(1)

[a] $R = \Sigma| |F_o| - |F_c| |/\Sigma|F_o|$.

[b] $R_w = [\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2]^{1/2}$ ($w = 1/\sigma^2(F_o)$).

[c] GOF = $[\Sigma w(|F_o| - |F_c|)^2/(N_o - N_p]^{1/2}$ (N_o = no. data, N_p = no. variables)

Table S4-2. Final Positional Parameters and B_{eq} for $5^{a,b,c}$

atom	x	y	z	B_{eq}
Zn(1)	0.21411(4)	0.19328(6)	0.57190(3)	2.77(4)
Ni(1)	0.21009(4)	0.21469(7)	0.72725(3)	2.29(4)
O(1)	0.2300(2)	0.0715(3)	0.7680(2)	2.8(2)
O(2)	0.1292(2)	0.2485(3)	0.7867(2)	2.9(2)
O(3)	0.1562(2)	0.1343(3)	0.6510(2)	2.9(2)
O(4)	0.1597(3)	0.0893(4)	0.5189(2)	4.1(3)
O(5)	0.2868(2)	0.2992(4)	0.7858(2)	2.8(2)
O(6)	0.2562(3)	0.2777(4)	0.4958(2)	4.0(2)
O(101)	0.3086(2)	0.1128(4)	0.5867(2)	3.2(2)
O(102)	0.3064(2)	0.1929(3)	0.6778(2)	2.4(2)
O(103)	0.4770(2)	0.2330(3)	0.5387(2)	3.0(2)
O(104)	0.4336(2)	0.3376(4)	0.7341(2)	2.8(2)
O(201)	0.1634(2)	0.3323(3)	0.5857(2)	2.8(2)
O(202)	0.1840(2)	0.3596(3)	0.6862(2)	2.6(2)
O(203)	0.2355(2)	0.5062(4)	0.5021(2)	2.7(2)
O(204)	0.2850(2)	0.6076(4)	0.6983(2)	3.3(2)
N(101)	0.4593(2)	0.2876(4)	0.6371(2)	2.3(2)
N(201)	0.2593(2)	0.5564(4)	0.6005(2)	2.0(2)
C(1)	0.2349(4)	-0.0621(6)	0.8449(3)	3.7(3)
C(2)	0.2090(3)	0.0465(5)	0.8214(3)	2.7(3)
C(3)	0.1635(3)	0.1104(6)	0.8580(3)	2.9(3)
C(4)	0.1278(3)	0.2065(6)	0.8402(3)	2.7(3)
C(5)	0.0828(4)	0.2688(6)	0.8863(3)	4.3(4)
C(6)	0.0630(4)	0.0395(7)	0.7055(3)	4.7(4)
C(7)	0.1052(4)	0.0611(6)	0.6487(3)	3.5(4)
C(8)	0.0877(4)	0.0014(6)	0.5971(3)	4.7(4)
C(9)	0.1157(5)	0.0197(7)	0.5365(4)	5.6(5)
C(10)	0.0904(7)	-0.0592(8)	0.4852(4)	9.7(7)
C(21)	0.2707(4)	0.4060(7)	0.8091(3)	4.5(4)
C(22)	0.3160(4)	0.2488(7)	0.4580(3)	4.9(4)
C(101)	0.3312(3)	0.1221(5)	0.6417(3)	2.4(3)
C(102)	0.4822(3)	0.2105(5)	0.5930(3)	2.6(3)
C(103)	0.4576(3)	0.2676(5)	0.7012(3)	2.5(3)
C(104)	0.3421(4)	-0.0658(6)	0.6735(3)	3.9(4)
C(105)	0.5731(4)	0.0636(6)	0.5713(3)	4.3(4)
C(106)	0.5213(4)	0.1737(6)	0.7883(3)	4.0(4)
C(107)	0.3891(3)	0.0386(5)	0.6647(3)	2.5(3)
C(108)	0.4502(4)	0.0171(5)	0.6180(3)	3.3(3)
C(109)	0.5138(3)	0.1019(5)	0.6154(3)	2.9(3)
C(110)	0.5471(3)	0.1175(5)	0.6801(3)	3.2(3)
C(111)	0.4881(3)	0.1583(5)	0.7237(3)	2.7(3)
C(112)	0.4252(4)	0.0722(5)	0.7267(3)	3.1(3)
C(201)	0.1517(3)	0.3809(5)	0.6357(3)	2.5(3)

(Table S4-2, contd.)

C(202)	0.2125(3)	0.5501(5)	0.5479(3)	2.3(3)
C(203)	0.2391(3)	0.6034(5)	0.6572(3)	2.6(3)
C(204)	0.0197(3)	0.4033(6)	0.6554(3)	3.5(3)
C(205)	0.1125(4)	0.6421(6)	0.4876(3)	3.9(4)
C(206)	0.1604(4)	0.7400(6)	0.7093(3)	3.9(4)
C(207)	0.0898(3)	0.4678(5)	0.6352(3)	2.5(3)
C(208)	0.0768(3)	0.5148(5)	0.5712(3)	3.0(3)
C(209)	0.1346(3)	0.6004(5)	0.5519(3)	2.7(3)
C(210)	0.1366(3)	0.6922(5)	0.5983(3)	3.2(3)
C(211)	0.1603(3)	0.6493(5)	0.6616(3)	2.6(3)
C(212)	0.1048(3)	0.5591(5)	0.6813(3)	3.0(3)
C(301)	0.3599(3)	0.4214(5)	0.6168(2)	2.1(3)
C(302)	0.4351(3)	0.3935(5)	0.6143(2)	2.1(3)
C(303)	0.4879(3)	0.4656(5)	0.5917(3)	2.2(3)
C(304)	0.4620(3)	0.5651(5)	0.5682(2)	2.2(3)
C(305)	0.3875(3)	0.5953(5)	0.5699(2)	2.2(3)
C(306)	0.3378(3)	0.5234(5)	0.5949(2)	2.1(3)
C(307)	0.5707(3)	0.4409(6)	0.5940(3)	3.0(3)
C(308)	0.3627(3)	0.7054(5)	0.5466(3)	3.0(3)
H(1)	0.323	0.369	0.634	2.6
H(2)	0.499	0.614	0.550	2.8
H(3)	0.156	0.084	0.901	3.7
H(4)	0.054	-0.058	0.604	6.1
H(5)	0.580	0.369	0.611	3.6
H(6)	0.593	0.442	0.554	3.6
H(7)	0.599	0.492	0.619	3.6
H(8)	0.387	0.763	0.570	3.5
H(9)	0.374	0.715	0.504	3.5
H(10)	0.309	0.715	0.551	3.5
H(11)	-0.024	0.450	0.657	4.1
H(12)	0.009	0.345	0.628	4.1
H(13)	0.028	0.373	0.696	4.1
H(14)	0.176	0.714	0.749	4.7
H(15)	0.192	0.799	0.698	4.7
H(16)	0.110	0.771	0.714	4.7
H(17)	0.148	0.696	0.473	4.3
H(18)	0.111	0.584	0.458	4.3
H(19)	0.064	0.677	0.486	4.3
H(20)	0.303	-0.054	0.703	4.9
H(21)	0.318	-0.088	0.636	4.9
H(22)	0.372	-0.125	0.688	4.9
H(23)	0.595	-0.005	0.583	5.2
H(24)	0.553	0.055	0.530	5.2
H(25)	0.613	0.116	0.569	5.2
H(26)	0.542	0.107	0.805	4.8
H(27)	0.562	0.227	0.788	4.8