Crystal structure of *bis*-[*N*,*N*'-*bis*-(3-allyl salicylidene)-*o*-phenylene diamine]thorium (IV), $C_{52}H_{44}N_4O_4Th$

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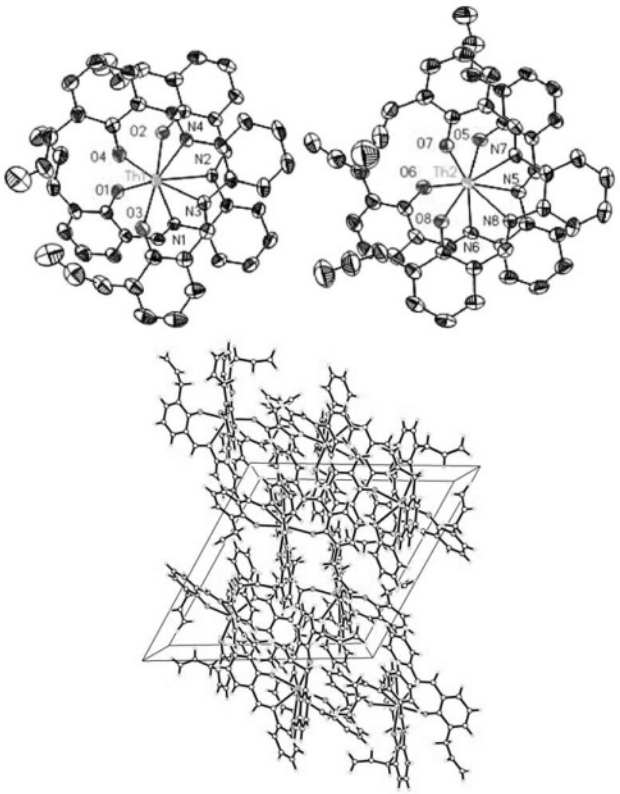
Received March 09, 2012, accepted June 12, 2012, available online September 06, 2012, CCDC no. 845810



Abstract

$C_{52}H_{44}N_4O_4Th$, triclinic, $P\overline{1}$ (no. 2), a = 16.3338(3) Å, b = 17.1662(3) Å, c = 18.5769(6) Å, α = 101.145(1)°, β = 95.195(1)°, γ = 117.054(1)°, V = 4455.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.0314, $wR_{ref}(F^2)$ = 0.0914, T = 296 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.20×0.20×0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	33.97 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II CCD, φ and ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	47678, 15646
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 12434
$N(param)_{refined}$:	1099
Programs:	SHELX [8]

Source of material

The ligand was prepared by refluxing an ethanolic mixture of 3-allyl salicyladehyde and *o*-phenylenediamine in the ratio of 2:1 for 2 h. The title compound was synthesized from a mixture the ligand (0.792 g, 2 mmol) and thorium nitrate tetrahydrate (0.552 g; 1 mmol). Both components were refluxed for 3 h in absolute ethanol (15 mL). The resulting precipitate was filtered and a yellow solid was obtained. Yellow single crystals were obtained by recrystallization of the solid in DMF and absolute ethanol(1:1).

Experimental details

H atoms were included in their idealized positions, with C–H = 0.96Å, and refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C) for other H atoms.

Discussion

Thorium, which is a rare but widely distributed element, has not only extensive application in variable areas, such as catalysts, agriculture, optics, radio techniques, aeronautics and aerospace, metallurgy and chemical industry, and material fields [1], but also it is radioactive element which might be almost substitute uranium as nuclear fuel [2]. So studying the thorium complexes is of interesting significance. The schiff base is an interesting class of chelating agents for metal atoms, especially, the salophen or salen metal complexes have been noted extensively because of their catalytic activity [3, 4]. In our work, we prepare the title compound (I) via refluxing the ethanol solution of the schiff base and thorium nitrate tetrahydrate [5, 6]. The complex of the title compound (I) consists of one Th(IV) atom coordinated by two *N*,*N*'-*bis*-(3-allylsalicylidene)*o*-phenylenediamine molecules, which is similar to the structure of *bis*-[*N*,*N*'-*o*-phenylene (salicylaldiminato)]Th(IV) reported by Hill [7]. As shown in the Fig. top, there are two crystallographic different complexes in the crystal structure as indicated by the bond distances and angles. The Th1–O (O1, O2, O3, O4) and Th1–N (N1, N2, N3, N4) bond lengths are different from the Th2–O (O5, O6, O7, O8) and Th2–N (N5, N6, N7, N8) bond distances obtained from the experimental data. The average bond distances of Th–O and Th–N were 2.269(3)Å (Th1–O), 2.271(3)Å (Th2–O), 2.6605(4)Å (Th1–N) and 2.656(4)Å (Th2–N), respectively. The angles of O–Th–O (∠O–Th–O) and N–Th–N all are below 90° except of these angles of O4–Th1–O1 (∠O4–Th1–O1 = 88.02(12)°), O2–Th1–O3 (∠O2–Th1–O3 = 172.09(12)°), O6–Th2–O7 (∠O6–Th2–O7 = 95.36(13)°), O5–Th2–O8 (∠O5–Th2–O8 = 163.94(13)°), N1–Th1–N4 (∠N1–Th1–N4 = 136.67(13)°) and N6–Th2–N7 (∠N6–Th2–N7 = 129.47(14)°) in the two crystal structures. In the crystals structure, the solvent and the hydrogen-bonds were inexistence.

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Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	2*i*	–0.0857	0.5992	1.0426	0.155
H(1B)	2*i*	–0.0896	0.5176	0.9801	0.155
H(2)	2*i*	0.0305	0.6153	0.9415	0.109
H(3A)	2*i*	0.0370	0.7529	1.0560	0.091
H(3B)	2*i*	0.0460	0.7655	0.9753	0.091
H(7)	2*i*	0.4234	0.8790	1.0876	0.087
H(8)	2*i*	0.3345	0.8677	1.1786	0.106
H(9)	2*i*	0.1745	0.8065	1.1440	0.096
H(10)	2*i*	0.4379	0.8548	0.9641	0.066
H(13)	2*i*	0.4388	0.7253	0.6682	0.081
H(14)	2*i*	0.5897	0.8479	0.7057	0.103
H(15)	2*i*	0.6338	0.9528	0.8180	0.108
H(16)	2*i*	0.5273	0.9410	0.8933	0.092
H(17A)	2*i*	–0.1638	0.3188	0.7836	0.194
H(17B)	2*i*	–0.1018	0.3773	0.8663	0.194
H(18)	2*i*	–0.0123	0.4900	0.8219	0.128
H(19A)	2*i*	–0.0735	0.4975	0.7055	0.096
H(19B)	2*i*	–0.1240	0.3913	0.6778	0.096
H(23)	2*i*	0.2254	0.4575	0.6073	0.075
H(24)	2*i*	0.0798	0.3292	0.5634	0.087
H(25)	2*i*	–0.0480	0.3252	0.6064	0.088
H(26)	2*i*	0.3246	0.6008	0.6903	0.062
H(27A)	2*i*	0.1457	0.9458	1.0139	0.218
H(27B)	2*i*	0.0928	0.9970	0.9849	0.218
H(28)	2*i*	0.2154	1.0823	0.9439	0.143
H(29A)	2*i*	0.3006	0.9838	0.9742	0.117
H(29B)	2*i*	0.3530	1.0887	1.0119	0.117
H(33)	2*i*	0.4432	1.0994	0.7280	0.094
H(34)	2*i*	0.4952	1.2178	0.8335	0.112
H(35)	2*i*	0.4302	1.1917	0.9365	0.113
H(36)	2*i*	0.3515	0.9487	0.6616	0.071
H(39)	2*i*	0.1091	0.5923	0.5121	0.087
H(40)	2*i*	0.2303	0.6197	0.4475	0.104
H(41)	2*i*	0.3695	0.7524	0.4886	0.106
H(42)	2*i*	0.3947	0.8545	0.6000	0.088
H(43A)	2*i*	–0.1668	0.8605	0.8618	0.230
H(43B)	2*i*	–0.0648	0.9432	0.8649	0.230
H(44)	2*i*	–0.0091	0.8509	0.8381	0.159
H(45A)	2*i*	–0.1770	0.6993	0.8391	0.104
H(45B)	2*i*	–0.0772	0.7083	0.8583	0.104
H(49)	2*i*	–0.1513	0.5710	0.5452	0.084
H(50)	2*i*	–0.2813	0.5519	0.5925	0.099
H(51)	2*i*	–0.2653	0.6173	0.7172	0.092
H(52)	2*i*	0.0107	0.6342	0.5562	0.067

Table 2. continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
	2*i*	0.3384	0.2231	0.1519	0.225
H(53B)	2*i*	0.3008	0.2394	0.0760	0.225
H(54)	2*i*	0.4136	0.3713	0.1001	0.204
H(55A)	2*i*	0.4969	0.3758	0.2323	0.113
H(55B)	2*i*	0.4919	0.4572	0.2103	0.113
H(59)	2*i*	0.8249	0.4947	0.1194	0.083
H(60)	2*i*	0.6992	0.3580	0.0556	0.096
H(61)	2*i*	0.5543	0.3182	0.0849	0.093
H(62)	2*i*	0.8938	0.6309	0.2139	0.069
H(64)	2*i*	0.9954	0.7640	0.2085	0.089
H(65)	2*i*	1.1345	0.8973	0.2609	0.108
H(66)	2*i*	1.1497	0.9893	0.3745	0.114
H(67)	2*i*	1.0294	0.9501	0.4375	0.098
H(69A)	2*i*	0.3763	0.5797	0.5375	0.243
H(69B)	2*i*	0.3873	0.5247	0.5954	0.243
H(70)	2*i*	0.5373	0.5703	0.5829	0.187
H(71A)	2*i*	0.5111	0.6841	0.5020	0.147
H(71B)	2*i*	0.5323	0.6108	0.4559	0.147
H(75)	2*i*	0.9013	0.8692	0.6126	0.109
H(76)	2*i*	0.8002	0.8368	0.6932	0.123
H(77)	2*i*	0.6423	0.7382	0.6464	0.112
H(78)	2*i*	0.9364	0.8520	0.4944	0.084
H(79A)	2*i*	0.3141	0.7673	0.3302	0.280
H(79B)	2*i*	0.4265	0.8303	0.3523	0.280
H(80)	2*i*	0.4496	0.7277	0.3257	0.168
H(81A)	2*i*	0.2986	0.5698	0.2908	0.115
H(81B)	2*i*	0.4026	0.5972	0.3240	0.115
H(85)	2*i*	0.4217	0.5453	0.0179	0.088
H(86)	2*i*	0.2710	0.4843	0.0384	0.104
H(87)	2*i*	0.2449	0.5118	0.1584	0.101
H(88)	2*i*	0.5819	0.6412	0.0587	0.072
H(91)	2*i*	0.9418	0.9280	0.1794	0.084
H(92)	2*i*	0.9628	0.8669	0.0637	0.104
H(93)	2*i*	0.8483	0.7279	–0.0094	0.103
H(94)	2*i*	0.7119	0.6481	0.0300	0.089
H(95A)	2*i*	0.6563	0.9700	0.6333	0.266
H(95B)	2*i*	0.5996	1.0255	0.6282	0.266
H(96)	2*i*	0.6001	1.0090	0.5068	0.184
H(97A)	2*i*	0.6196	0.8865	0.4533	0.123
H(97B)	2*i*	0.6942	0.9132	0.5250	0.123
H(101)	2*i*	0.9213	1.1126	0.3427	0.080
H(102)	2*i*	0.9136	1.1892	0.4560	0.092
H(103)	2*i*	0.8022	1.1136	0.5194	0.093
H(104)	2*i*	0.8641	0.9797	0.2444	0.066

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Th(1)	2*i*	0.18402(1)	0.75303(1)	0.786404(9)	0.0463(1)	0.0519(1)	0.0368(1)	0.02602(8)	0.01074(8)	0.01049(7)
Th(2)	2*i*	0.69618(1)	0.71968(1)	0.302000(9)	0.0496(1)	0.0425(1)	0.0440(1)	0.02015(8)	0.00429(8)	0.00735(8)
C(1)	2*i*	–0.0624(5)	0.5792(6)	1.0035(5)	0.101(6)	0.133(7)	0.140(7)	0.038(5)	0.032(5)	0.051(6)
C(2)	2*i*	0.0098(5)	0.6387(5)	0.9809(4)	0.080(4)	0.113(4)	0.086(4)	0.050(4)	0.028(3)	0.028(4)
C(3)	2*i*	0.0602(4)	0.7378(4)	1.0121(3)	0.083(3)	0.098(4)	0.060(3)	0.052(3)	0.030(3)	0.023(3)
C(4)	2*i*	0.1640(4)	0.7775(4)	1.0333(3)	0.084(3)	0.074(3)	0.044(2)	0.050(3)	0.021(2)	0.016(2)
C(5)	2*i*	0.2165(4)	0.7820(3)	0.9771(3)	0.063(3)	0.052(2)	0.044(3)	0.035(2)	0.009(2)	0.012(2)
C(6)	2*i*	0.3147(4)	0.8230(3)	0.9977(3)	0.061(3)	0.054(2)	0.046(2)	0.031(2)	0.005(2)	0.005(2)
C(7)	2*i*	0.3586(5)	0.8540(4)	1.0739(3)	0.080(4)	0.074(3)	0.055(3)	0.040(3)	–0.007(3)	0.000(3)
C(8)	2*i*	0.3059(5)	0.8473(5)	1.1282(3)	0.106(4)	0.104(4)	0.041(3)	0.051(4)	–0.001(3)	0.000(3)
C(9)	2*i*	0.2096(5)	0.8099(5)	1.1069(3)	0.105(4)	0.097(4)	0.046(3)	0.057(3)	0.016(3)	0.013(3)
C(10)	2*i*	0.3745(4)	0.8316(3)	0.9445(3)	0.052(3)	0.049(3)	0.056(3)	0.024(2)	–0.001(2)	0.004(2)
C(11)	2*i*	0.4199(4)	0.8233(3)	0.8285(3)	0.047(3)	0.055(3)	0.067(3)	0.026(2)	0.014(2)	0.016(2)
C(12)	2*i*	0.3930(4)	0.7595(3)	0.7603(3)	0.048(3)	0.055(3)	0.067(3)	0.028(2)	0.019(2)	0.021(2)
C(13)	2*i*	0.4563(4)	0.7680(4)	0.7139(4)	0.062(3)	0.070(3)	0.085(4)	0.037(3)	0.033(3)	0.029(3)
C(14)	2*i*	0.5466(4)	0.8417(4)	0.7366(4)	0.064(3)	0.087(4)	0.108(4)	0.031(3)	0.041(3)	0.030(3)
C(15)	2*i*	0.5729(5)	0.9045(5)	0.8033(4)	0.055(3)	0.074(4)	0.122(5)	0.018(3)	0.028(3)	0.020(3)
C(16)	2*i*	0.5098(4)	0.8967(4)	0.8486(4)	0.054(3)	0.064(3)	0.096(4)	0.018(3)	0.018(3)	0.012(3)
C(17)	2*i*	–0.1141(6)	0.3717(7)	0.8152(6)	0.130(8)	0.180(9)	0.153(8)	0.040(7)	0.018(6)	0.090(7)
C(18)	2*i*	–0.0607(5)	0.4391(5)	0.7873(5)	0.073(4)	0.111(5)	0.117(5)	0.027(4)	0.012(4)	0.039(4)
C(19)	2*i*	–0.0678(4)	0.4443(4)	0.7084(4)	0.060(3)	0.072(3)	0.096(4)	0.019(3)	0.001(3)	0.033(3)

Table 3. continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(20)	2*i*	0.0162(4)	0.4494(3)	0.6775(3)	0.068(3)	0.054(3)	0.060(3)	0.022(2)	–0.005(2)	0.023(2)
C(21)	2*i*	0.1038(4)	0.5296(3)	0.7039(3)	0.061(3)	0.049(2)	0.044(3)	0.024(2)	0.004(2)	0.020(2)
C(22)	2*i*	0.1826(4)	0.5322(3)	0.6758(3)	0.072(3)	0.053(2)	0.043(2)	0.033(2)	0.008(2)	0.016(2)
C(23)	2*i*	0.1731(4)	0.4564(3)	0.6244(3)	0.091(4)	0.056(3)	0.046(3)	0.040(3)	0.009(3)	0.014(2)
C(24)	2*i*	0.0862(5)	0.3793(4)	0.5985(3)	0.102(4)	0.051(3)	0.054(3)	0.035(3)	–0.007(3)	0.007(2)
C(25)	2*i*	0.0101(5)	0.3771(4)	0.6247(3)	0.086(4)	0.052(3)	0.063(3)	0.021(3)	–0.011(3)	0.015(2)
C(26)	2*i*	0.2749(4)	0.6097(3)	0.7022(3)	0.064(3)	0.059(3)	0.044(3)	0.038(2)	0.018(2)	0.016(2)
C(27)	2*i*	0.1456(7)	0.9893(8)	0.9909(7)	0.147(9)	0.146(9)	0.21(1)	0.039(7)	0.015(8)	0.053(8)
C(28)	2*i*	0.2210(7)	1.0405(6)	0.9663(5)	0.132(6)	0.137(6)	0.108(5)	0.087(5)	0.008(5)	0.023(5)
C(29)	2*i*	0.3077(6)	1.0416(5)	0.9688(4)	0.123(5)	0.097(4)	0.080(4)	0.075(4)	–0.004(4)	–0.004(3)
C(30)	2*i*	0.3438(5)	1.0591(4)	0.8972(4)	0.101(4)	0.066(3)	0.074(3)	0.054(3)	0.000(3)	0.001(3)
C(31)	2*i*	0.3114(4)	0.9855(4)	0.8319(3)	0.072(3)	0.053(3)	0.070(3)	0.039(3)	0.005(3)	0.012(2)
C(32)	2*i*	0.3523(4)	1.0007(4)	0.7697(3)	0.064(3)	0.058(3)	0.072(3)	0.036(2)	0.005(3)	0.020(2)
C(33)	2*i*	0.4190(4)	1.0890(4)	0.7708(4)	0.077(4)	0.060(3)	0.096(4)	0.032(3)	0.004(3)	0.025(3)
C(34)	2*i*	0.4494(5)	1.1599(4)	0.8329(5)	0.094(4)	0.058(3)	0.113(5)	0.033(3)	–0.011(4)	0.016(3)
C(35)	2*i*	0.4104(5)	1.1433(4)	0.8944(5)	0.110(5)	0.058(3)	0.104(4)	0.048(3)	–0.014(4)	–0.003(3)
C(36)	2*i*	0.3282(4)	0.9302(4)	0.7027(3)	0.061(3)	0.064(3)	0.066(3)	0.035(3)	0.017(3)	0.028(2)
C(37)	2*i*	0.2673(4)	0.7860(4)	0.6223(3)	0.073(3)	0.073(3)	0.042(3)	0.048(3)	0.022(2)	0.024(2)
C(38)	2*i*	0.1798(4)	0.7069(4)	0.5954(3)	0.081(3)	0.068(3)	0.038(2)	0.048(3)	0.018(2)	0.016(2)
C(39)	2*i*	0.1664(5)	0.6452(4)	0.5302(3)	0.092(4)	0.087(3)	0.045(3)	0.053(3)	0.014(3)	0.008(3)
C(40)	2*i*	0.2389(5)	0.6621(5)	0.4911(3)	0.110(4)	0.117(4)	0.052(3)	0.073(3)	0.029(3)	0.011(3)
C(41)	2*i*	0.3224(5)	0.7404(5)	0.5162(4)	0.100(4)	0.126(5)	0.060(3)	0.067(4)	0.039(3)	0.025(3)
C(42)	2*i*	0.3371(5)	0.8019(5)	0.5824(3)	0.083(4)	0.098(4)	0.058(3)	0.054(3)	0.032(3)	0.032(3)
C(43)	2*i*	–0.1045(8)	0.8814(8)	0.8576(7)	0.19(1)	0.168(9)	0.20(1)	0.085(8)	0.037(9)	0.000(9)
C(44)	2*i*	–0.0722(7)	0.8231(7)	0.8411(5)	0.119(6)	0.146(6)	0.102(5)	0.065(5)	0.020(5)	–0.037(5)
C(45)	2*i*	–0.1155(5)	0.7228(5)	0.8263(4)	0.066(4)	0.127(4)	0.064(3)	0.050(3)	0.013(3)	0.009(3)
C(46)	2*i*	–0.1255(4)	0.6767(4)	0.7453(3)	0.059(3)	0.079(3)	0.059(3)	0.039(3)	0.013(2)	0.018(2)
C(47)	2*i*	–0.0438(4)	0.6885(3)	0.7174(3)	0.058(3)	0.060(3)	0.050(3)	0.034(2)	0.007(2)	0.018(2)
C(48)	2*i*	–0.0546(4)	0.6465(3)	0.6418(3)	0.061(3)	0.054(2)	0.049(3)	0.028(2)	0.006(2)	0.015(2)
C(49)	2*i*	–0.1446(4)	0.5968(4)	0.5957(3)	0.068(3)	0.065(3)	0.058(3)	0.021(3)	0.001(3)	0.008(3)
C(50)	2*i*	–0.2220(4)	0.5858(4)	0.6235(4)	0.057(3)	0.082(4)	0.076(4)	0.014(3)	–0.003(3)	0.010(3)
C(51)	2*i*	–0.2120(4)	0.6255(4)	0.6983(4)	0.055(3)	0.084(4)	0.077(3)	0.024(3)	0.013(3)	0.018(3)
C(52)	2*i*	0.0243(4)	0.6581(3)	0.6078(3)	0.076(4)	0.049(3)	0.042(3)	0.031(3)	0.007(3)	0.011(2)
C(53)	2*i*	0.3451(6)	0.2604(6)	0.1201(7)	0.109(7)	0.167(9)	0.19(1)	0.019(6)	0.007(7)	–0.034(8)
C(54)	2*i*	0.4178(6)	0.3436(6)	0.1376(6)	0.114(6)	0.150(7)	0.146(7)	0.011(5)	0.017(5)	–0.034(6)
C(55)	2*i*	0.4962(5)	0.4028(4)	0.1911(4)	0.087(4)	0.060(3)	0.110(5)	0.030(3)	–0.001(3)	–0.006(3)
C(56)	2*i*	0.5898(4)	0.4304(3)	0.1653(3)	0.081(3)	0.045(2)	0.070(3)	0.029(2)	–0.004(3)	0.009(2)
C(57)	2*i*	0.6665(4)	0.5170(3)	0.2032(3)	0.075(3)	0.045(2)	0.054(3)	0.031(2)	0.002(2)	0.013(2)
C(58)	2*i*	0.7542(4)	0.5416(3)	0.1840(3)	0.077(3)	0.049(2)	0.049(3)	0.034(2)	0.010(2)	0.016(2)
C(59)	2*i*	0.7656(5)	0.4794(4)	0.1298(3)	0.097(4)	0.062(3)	0.059(3)	0.044(3)	0.019(3)	0.016(2)
C(60)	2*i*	0.6916(5)	0.3977(4)	0.0927(3)	0.119(4)	0.058(3)	0.063(3)	0.047(3)	0.016(3)	0.007(3)
C(61)	2*i*	0.6048(5)	0.3743(4)	0.1107(3)	0.102(4)	0.045(3)	0.068(3)	0.030(3)	–0.004(3)	0.001(2)
C(62)	2*i*	0.8363(4)	0.6265(3)	0.2209(3)	0.072(3)	0.060(3)	0.050(3)	0.040(3)	0.010(2)	0.018(2)
C(63)	2*i*	0.9283(4)	0.7758(3)	0.2923(3)	0.053(3)	0.055(3)	0.067(3)	0.027(2)	0.001(2)	0.014(2)
C(64)	2*i*	1.0018(4)	0.8009(4)	0.2548(4)	0.060(3)	0.072(3)	0.083(4)	0.028(3)	0.008(3)	0.017(3)
C(65)	2*i*	1.0849(4)	0.8808(5)	0.2860(4)	0.056(3)	0.083(4)	0.113(5)	0.023(3)	0.013(3)	0.017(3)
C(66)	2*i*	1.0939(5)	0.9355(5)	0.3539(4)	0.059(3)	0.072(4)	0.116(5)	0.010(3)	–0.001(3)	0.007(3)
C(67)	2*i*	1.0222(4)	0.9120(4)	0.3916(4)	0.062(3)	0.066(3)	0.093(4)	0.024(3)	–0.005(3)	–0.002(3)
C(68)	2*i*	0.9380(4)	0.8314(3)	0.3620(3)	0.048(3)	0.056(3)	0.070(3)	0.025(2)	–0.003(2)	0.009(2)
C(69)	2*i*	0.4127(7)	0.5616(8)	0.5638(6)	0.170(9)	0.169(9)	0.173(9)	0.026(8)	0.094(8)	–0.043(8)
C(70)	2*i*	0.5010(6)	0.5884(7)	0.5565(5)	0.160(7)	0.128(6)	0.112(6)	0.019(6)	0.055(5)	0.006(5)
C(71)	2*i*	0.5420(6)	0.6479(6)	0.5057(4)	0.139(5)	0.101(5)	0.081(4)	0.018(4)	0.033(4)	0.020(4)
C(72)	2*i*	0.6477(5)	0.7103(4)	0.5375(4)	0.119(4)	0.066(3)	0.063(3)	0.043(3)	0.023(3)	0.020(3)
C(73)	2*i*	0.7101(5)	0.7311(4)	0.4874(3)	0.095(4)	0.057(3)	0.054(3)	0.045(3)	0.009(3)	0.015(2)
C(74)	2*i*	0.8055(5)	0.7926(4)	0.5157(3)	0.090(3)	0.068(3)	0.054(3)	0.050(3)	0.001(3)	0.004(2)
C(75)	2*i*	0.8376(6)	0.8301(5)	0.5937(4)	0.110(4)	0.100(4)	0.058(3)	0.059(4)	0.000(3)	–0.002(3)
C(76)	2*i*	0.7779(6)	0.8107(5)	0.6419(4)	0.139(5)	0.109(5)	0.052(3)	0.063(4)	0.009(3)	0.003(3)
C(77)	2*i*	0.6833(6)	0.7512(5)	0.6135(4)	0.137(5)	0.089(4)	0.059(3)	0.057(4)	0.025(3)	0.022(3)
C(78)	2*i*	0.8740(4)	0.8185(4)	0.4692(3)	0.073(4)	0.068(3)	0.065(4)	0.043(3)	–0.008(3)	–0.002(3)
C(79)	2*i*	0.374(1)	0.7732(8)	0.3345(9)	0.28(1)	0.17(1)	0.23(1)	0.09(1)	0.10(1)	0.05(1)
C(80)	2*i*	0.3843(8)	0.7000(7)	0.3153(5)	0.145(6)	0.147(6)	0.117(6)	0.059(6)	0.074(5)	0.019(6)
C(81)	2*i*	0.3637(5)	0.6091(5)	0.2899(4)	0.069(4)	0.106(4)	0.088(4)	0.021(4)	0.026(3)	0.027(4)
C(82)	2*i*	0.3796(4)	0.5860(4)	0.2118(4)	0.055(3)	0.066(3)	0.078(3)	0.023(2)	0.006(3)	0.015(3)
C(83)	2*i*	0.4723(4)	0.6207(3)	0.2008(3)	0.058(3)	0.049(2)	0.061(3)	0.027(2)	0.005(2)	0.012(2)
C(84)	2*i*	0.4882(4)	0.6054(3)	0.1265(3)	0.064(3)	0.056(3)	0.057(3)	0.034(2)	0.002(2)	0.008(2)
C(85)	2*i*	0.4116(4)	0.5549(4)	0.0665(3)	0.074(3)	0.075(3)	0.063(3)	0.040(3)	–0.008(3)	0.001(3)
C(86)	2*i*	0.3216(5)	0.5193(4)	0.0786(4)	0.067(3)	0.083(4)	0.087(4)	0.031(3)	–0.018(3)	–0.002(3)
C(87)	2*i*	0.3062(5)	0.5355(4)	0.1508(4)	0.060(3)	0.078(4)	0.095(4)	0.026(3)	–0.003(3)	0.011(3)
C(88)	2*i*	0.5799(4)	0.6490(4)	0.1093(3)	0.077(4)	0.062(3)	0.047(3)	0.044(3)	0.006(3)	0.006(2)

Table 3. continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(89)	2*i*	0.7425(4)	0.7421(4)	0.1273(3)	0.068(3)	0.071(3)	0.051(3)	0.046(2)	0.019(2)	0.022(2)
C(90)	2*i*	0.8126(4)	0.8258(4)	0.1731(3)	0.063(3)	0.070(3)	0.059(3)	0.043(2)	0.019(2)	0.027(2)
C(91)	2*i*	0.8949(4)	0.8722(4)	0.1493(3)	0.067(3)	0.087(3)	0.078(3)	0.045(3)	0.030(3)	0.038(3)
C(92)	2*i*	0.9078(5)	0.8352(5)	0.0801(4)	0.082(4)	0.122(4)	0.087(4)	0.060(3)	0.044(3)	0.049(3)
C(93)	2*i*	0.8392(5)	0.7523(5)	0.0365(4)	0.096(4)	0.119(4)	0.071(4)	0.070(3)	0.038(3)	0.030(3)
C(94)	2*i*	0.7573(5)	0.7049(5)	0.0596(3)	0.086(4)	0.091(4)	0.062(3)	0.056(3)	0.023(3)	0.016(3)
C(95)	2*i*	0.628(1)	0.9941(9)	0.6053(6)	0.29(1)	0.18(1)	0.186(9)	0.10(1)	0.14(1)	0.035(9)
C(96)	2*i*	0.6289(8)	0.9837(7)	0.5326(6)	0.196(7)	0.133(6)	0.153(7)	0.087(5)	0.091(6)	0.038(6)
C(97)	2*i*	0.6697(6)	0.9377(5)	0.4913(4)	0.151(5)	0.083(4)	0.084(4)	0.064(4)	0.051(4)	0.015(3)
C(98)	2*i*	0.7484(5)	0.9898(4)	0.4519(3)	0.090(4)	0.065(3)	0.061(3)	0.048(3)	0.009(3)	0.008(2)
C(99)	2*i*	0.7573(4)	0.9403(3)	0.3850(3)	0.057(3)	0.048(2)	0.053(3)	0.030(2)	0.002(2)	0.008(2)
C(100)	2*i*	0.8225(4)	0.9862(3)	0.3440(3)	0.054(3)	0.049(2)	0.064(3)	0.027(2)	0.002(2)	0.014(2)
C(101)	2*i*	0.8793(4)	1.0811(4)	0.3706(3)	0.067(3)	0.053(3)	0.074(3)	0.025(2)	–0.006(3)	0.019(2)
C(102)	2*i*	0.8733(5)	1.1272(4)	0.4370(4)	0.088(4)	0.047(3)	0.077(4)	0.028(3)	–0.015(3)	0.002(3)
C(103)	2*i*	0.8072(5)	1.0811(4)	0.4753(4)	0.106(4)	0.060(3)	0.065(3)	0.047(3)	0.001(3)	0.004(3)
C(104)	2*i*	0.8302(4)	0.9421(3)	0.2730(3)	0.051(3)	0.054(3)	0.069(3)	0.028(2)	0.014(2)	0.027(2)
O(1)	2*i*	0.1726(2)	0.7485(2)	0.9063(2)	0.052(2)	0.075(2)	0.037(2)	0.027(2)	0.011(2)	0.013(2)
O(2)	2*i*	0.1106(2)	0.5980(2)	0.7538(2)	0.054(2)	0.053(2)	0.054(2)	0.023(2)	0.011(2)	0.013(2)
O(3)	2*i*	0.2448(3)	0.9049(2)	0.8312(2)	0.078(3)	0.057(2)	0.062(2)	0.035(2)	0.022(2)	0.010(2)
O(4)	2*i*	0.0386(2)	0.7378(3)	0.7625(2)	0.054(2)	0.089(3)	0.044(2)	0.042(2)	0.006(2)	0.006(2)
O(5)	2*i*	0.6542(3)	0.5708(2)	0.2566(2)	0.065(2)	0.048(2)	0.070(2)	0.023(2)	0.009(2)	0.003(2)
O(6)	2*i*	0.6781(3)	0.6906(2)	0.4152(2)	0.081(3)	0.059(2)	0.048(2)	0.023(2)	0.004(2)	0.014(2)
O(7)	2*i*	0.5427(2)	0.6697(2)	0.2588(2)	0.048(2)	0.065(2)	0.054(2)	0.022(2)	0.005(2)	0.009(2)
O(8)	2*i*	0.7028(2)	0.8522(2)	0.3628(2)	0.062(2)	0.047(2)	0.064(2)	0.024(2)	0.013(2)	0.007(2)
N(1)	2*i*	0.3505(3)	0.8110(3)	0.8729(2)	0.047(2)	0.049(2)	0.056(3)	0.024(2)	0.008(2)	0.010(2)
N(2)	2*i*	0.2965(3)	0.6898(3)	0.7403(2)	0.049(2)	0.056(2)	0.045(2)	0.028(2)	0.015(2)	0.014(2)
N(3)	2*i*	0.2780(3)	0.8443(3)	0.6933(2)	0.058(3)	0.058(2)	0.051(2)	0.033(2)	0.014(2)	0.015(2)
N(4)	2*i*	0.1114(3)	0.6973(3)	0.6399(2)	0.063(3)	0.053(2)	0.039(2)	0.030(2)	0.011(2)	0.012(2)
N(5)	2*i*	0.8389(3)	0.6974(3)	0.2627(2)	0.057(3)	0.050(2)	0.052(2)	0.028(2)	0.003(2)	0.010(2)
N(6)	2*i*	0.8602(3)	0.8015(3)	0.3970(2)	0.060(3)	0.053(2)	0.054(3)	0.030(2)	–0.006(2)	–0.002(2)
N(7)	2*i*	0.6599(3)	0.6978(3)	0.1557(2)	0.060(3)	0.056(2)	0.046(2)	0.036(2)	0.011(2)	0.011(2)
N(8)	2*i*	0.7953(3)	0.8561(3)	0.2443(2)	0.049(2)	0.053(2)	0.052(2)	0.028(2)	0.011(2)	0.015(2)

Acknowledgments. We gratefully acknowledge the service provided by the *X*-ray facility at Department of Chemistry and Chemical Engneering, Hengyang Normal University. Financial support of this work by the National Science Foundation (no.11175080) and by the Nature Science Fund of the Hunan Province (no. 10JJ6025) are gratefully acknowledged.

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