Crystal structure of *catena*-(hexakis(μ_2-3,5-dinitrobenzoate-*O*,*O'*)-tetrakis(dimethylsulfoxide-*O*)dineodymium(III), $Nd_2[(C_7H_3N_2O_6)_6(C_2H_6SO)_4]$

Fu-Lin Zhou[*,I] and Zhi-Hua Du[II]

[I] Department of Applied Chemistry, Yuncheng University, Yuncheng 044000, Shanxi, P. R. China
[II] Plant Protection and Plant Quarantine Station, Agriculture and Animal Husbandry Bureau, Wulanchabu 012000, Inner Mongolia, P. R. China

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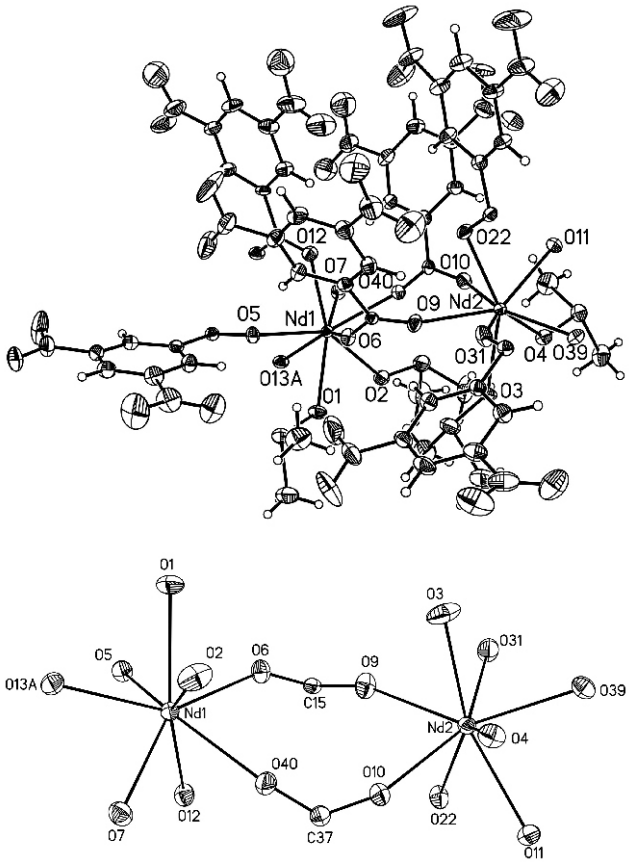

Abstract

$C_{50}H_{42}N_{12}Nd_2O_{40}S_4$, triclinic, $P\bar{1}$ (no. 2), a = 14.216(4) Å, b = 14.255(6) Å, c = 20.026(9) Å, α = 76.705(7)°, β = 84.256(6)°, γ = 60.370(4)°, V = 3432.5 Å^3, Z = 2, $R_{gt}(F)$ = 0.058, $wR_{ref}(F^2)$ = 0.160, T = 296 K.

Source of material

The title compound was synthesized from a mixture of 0.437 g of $Nd(NO_3)_3 \cdot 6H_2O$, 0.425 g of 3,5-binitrobenzoic acid, 4 mL of EtOH, 2 mL of dimethyl sulfoxide, and 2 mL of H_2O. This mixture was sealed in 25 mL of Teflon-lined stainless steel vessels, and heated at 120° for about 5 days under autogenous pressure, then cooled to room temperature. The resulting columnar colorless crystals were collected and dried in air at ambient temperature.

Elemental analysis — found: C, 32.34 %; H, 2.23 %; N, 8.92 %, S, 6.94 %; calculated for $C_{50}H_{42}N_{12}Nd_2O_{40}S_4$: C, 32.15 %; H, 2.27 %; N, 9.00 %; S, 6.87 %.

Discussion

The studies of metal-organic frameworks (MOFs) based on the lanthanide family tend to be growing rapidly nowadays, not only for their fascinating coordination geometry and versatile architecture, but also for their potential utilization as luminescent and sensory materials [1-3]. One of the most effective approaches to synthesize novel polynuclear lanthanide complexes with unique structures and properties is the hydrothermal/solvothermal method by incorporating appropriate lanthanide ions with carboxylic acid ligands [4,5].

In this paper, we report the synthesis and crystal structure of a novel compound of $Nd_2[(C_7H_3N_2O_6)_6(C_2H_6SO)_4]$. The crystal structure showed it as a novel non-electrolyte complex with 1D chain. The title crystal structure is similar to that of $Pr_2[(C_7H_3N_2O_6)_6(C_2H_6SO)_4]$ [6]. The X-ray structure analysis shows that an asymmetric unit contains two neodymium (III) ions, both of which have approximately distorted square antiprism geometry. Each Nd^{3+} is coordinated by six sites occupied by the oxygen atoms from carboxyl groups belonging to six 3,5-dinitrobenzoate molecules, and the other two by the oxygen atoms from coordinated DMSO molecules (figure, top). The nitro groups of 3,5-dinitrobenzoate do not coordinate the Nd^{3+}. Carboxyl groups of 3,5-dinitrobenzoate are dissociated and act as the bidentate bridging ligands, of which two oxygen atoms are coordinated to different Nd^{3+}. There is a link between Nd1 and Nd2 with four 3,5-dinitrobenzoate, forming a dimer unit $Nd_2[(C_7H_3N_2O_6)_4(C_2H_6SO)_4]^{2+}$; meanwhile, each Nd^{3+} links to another adjacent Nd^{3+} with two other carboxyl groups in the dimer unit, following the generic rule that a pair of Nd^{3+} are alternately connected by four or two carboxylate groups to form an infinite chain of 8-coordinated Nd^{3+} ions (figure, bottom). In the compound, the Nd is coordinated with six oxygen atoms from the adjacent 3,5-dinitrobenzoate and two other oxygen atoms from the adjacent DMSO. The d(Nd—O) vary from 2.348(6) Å to 2.495(6) Å and the mean of 2.440 Å, which are within normal ranges [7].

* Correspondence author (e-mail: fulinzhou@yeah.net)

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.20 × 0.24 × 0.26 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	17.28 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II CCD, φ/ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	17140, 11798
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 10282
$N(param)_{refined}$:	973
Programs:	SHELXS-97, SHELXL-97, SHELXTL [7]

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

Atom	Site	x	y	z	U_{iso}
H(50A)	2*i*	0.8634	0.7440	0.1164	0.045
H(1A)	2*i*	1.3836	0.5531	0.4187	0.109
H(1B)	2*i*	1.3597	0.6647	0.3684	0.109
H(1C)	2*i*	1.3905	0.5601	0.3393	0.109
H(2A)	2*i*	1.1074	0.7471	0.2779	0.113
H(2B)	2*i*	1.2266	0.6746	0.2561	0.113
H(2C)	2*i*	1.1961	0.7792	0.2852	0.113
H(3A)	2*i*	1.3393	0.1094	0.4708	0.116
H(3B)	2*i*	1.4218	0.1287	0.4194	0.116
H(3C)	2*i*	1.3898	0.0402	0.4135	0.116
H(4A)	2*i*	1.2715	0.2496	0.2537	0.133
H(4B)	2*i*	1.3501	0.1248	0.2842	0.133
H(4C)	2*i*	1.3800	0.2148	0.2900	0.133
H(5A)	2*i*	1.2885	0.4498	0.2536	0.130
H(5B)	2*i*	1.3656	0.4978	0.2231	0.130
H(5C)	2*i*	1.3896	0.3829	0.2115	0.130
H(6A)	2*i*	1.3311	0.5503	0.0351	0.134
H(6B)	2*i*	1.4139	0.4404	0.0825	0.134
H(6C)	2*i*	1.3927	0.5543	0.0941	0.134
H(7A)	2*i*	1.0650	0.1619	0.2053	0.103
H(7B)	2*i*	1.1795	0.1085	0.2395	0.103
H(7C)	2*i*	1.1498	0.0385	0.2048	0.103
H(8A)	2*i*	1.3659	0.0581	0.0917	0.085
H(8B)	2*i*	1.3293	–0.0232	0.1369	0.085
H(8C)	2*i*	1.3593	0.0468	0.1715	0.085
H(10A)	2*i*	0.8985	0.8467	0.5571	0.045
H(12A)	2*i*	0.9783	0.8435	0.3606	0.046
H(14A)	2*i*	0.8699	1.1209	0.4295	0.059
H(16A)	2*i*	1.0671	0.7634	0.0712	0.042
H(18A)	2*i*	1.1647	0.9688	–0.0442	0.058
H(20A)	2*i*	1.1052	0.7754	–0.1304	0.048
H(24A)	2*i*	0.6648	0.6156	0.1503	0.044
H(26A)	2*i*	0.3913	0.7844	0.0337	0.060
H(28A)	2*i*	0.6811	0.7102	–0.0523	0.042
H(31A)	2*i*	0.8729	0.3853	0.3866	0.040
H(33A)	2*i*	0.6142	0.3890	0.3207	0.062
H(35A)	2*i*	0.8489	0.3843	0.1896	0.042
H(36A)	2*i*	0.8606	0.7555	0.3143	0.041
H(39A)	2*i*	0.3965	0.8232	0.4166	0.058
H(41A)	2*i*	0.6674	0.6429	0.5345	0.048
H(43A)	2*i*	0.6837	0.6759	0.3291	0.044
H(46A)	2*i*	0.6005	0.9706	0.1942	0.055

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}
Nd(1)	2*i*	1.06571(3)	0.48293(3)	0.39393(2)	0.0197(2)	0.0227(2)	0.0232(2)	–0.0088(2)	–0.0001(2)	–0.0046(2)
Nd(2)	2*i*	1.05429(3)	0.45281(3)	0.10539(2)	0.0205(2)	0.0237(2)	0.0245(2)	–0.0112(2)	0.0023(2)	–0.0066(2)
S(1)	2*i*	1.2133(2)	0.6374(2)	0.3720(1)	0.047(1)	0.054(2)	0.053(2)	–0.034(1)	0.013(1)	–0.016(1)
S(2)	2*i*	1.2561(2)	0.2124(2)	0.3680(2)	0.038(1)	0.038(1)	0.083(2)	–0.012(1)	0.004(1)	–0.025(1)
S(3)	2*i*	1.2536(2)	0.5219(2)	0.1387(2)	0.036(1)	0.050(2)	0.100(2)	–0.022(1)	–0.003(1)	–0.031(2)
S(4)	2*i*	1.1909(2)	0.1532(2)	0.1231(1)	0.043(1)	0.029(1)	0.043(1)	–0.015(1)	–0.001(1)	–0.0061(9)
O(1)	2*i*	1.2130(5)	0.5327(5)	0.3706(3)	0.035(3)	0.037(3)	0.049(4)	–0.025(3)	0.000(3)	–0.002(3)
O(2)	2*i*	1.2375(5)	0.3195(5)	0.3808(4)	0.026(3)	0.037(4)	0.077(5)	–0.008(3)	0.001(3)	–0.027(3)
O(3)	2*i*	1.2281(5)	0.4390(6)	0.1239(4)	0.026(3)	0.045(4)	0.095(6)	–0.018(3)	0.001(3)	–0.033(4)
O(4)	2*i*	1.1963(5)	0.2547(5)	0.1295(3)	0.032(3)	0.026(3)	0.042(3)	–0.013(3)	0.003(3)	–0.005(2)
O(5)	2*i*	0.9906(5)	0.6656(4)	0.4217(3)	0.039(3)	0.023(3)	0.032(3)	–0.015(3)	0.002(2)	–0.006(2)
O(6)	2*i*	1.0325(5)	0.6003(5)	0.2839(3)	0.038(3)	0.030(3)	0.027(3)	–0.013(3)	–0.002(2)	–0.004(2)
O(7)	2*i*	1.0379(5)	0.3361(5)	0.4666(3)	0.044(4)	0.034(3)	0.034(3)	–0.021(3)	0.005(3)	–0.006(3)
O(9)	2*i*	1.0214(5)	0.5796(5)	0.1799(3)	0.031(3)	0.035(3)	0.037(3)	–0.006(3)	–0.001(3)	–0.014(3)
O(10)	2*i*	1.0236(5)	0.3698(5)	0.2147(3)	0.048(4)	0.043(3)	0.025(3)	–0.028(3)	0.003(3)	–0.006(3)
O(11)	2*i*	0.9744(5)	0.3464(5)	0.0765(3)	0.034(3)	0.031(3)	0.035(3)	–0.019(3)	–0.002(2)	–0.006(2)
O(12)	2*i*	0.8655(5)	0.5703(5)	0.3843(3)	0.029(3)	0.035(3)	0.030(3)	–0.011(3)	–0.004(2)	–0.004(2)
O(13)	2*i*	0.8588(4)	0.5564(5)	0.4960(3)	0.025(3)	0.041(3)	0.035(3)	–0.015(3)	–0.005(2)	–0.006(3)
O(14)	2*i*	0.5035(7)	0.714(1)	0.6002(5)	0.047(5)	0.16(1)	0.051(5)	–0.041(6)	0.016(4)	–0.032(6)
O(15)	2*i*	0.365(1)	0.837(1)	0.5361(6)	0.105(3)	0.107(3)	0.106(3)	–0.050(2)	0.002(1)	–0.023(1)
O(16)	2*i*	0.383(1)	0.844(1)	0.2927(6)	0.098(3)	0.101(3)	0.099(3)	–0.048(2)	0.001(1)	–0.020(1)
O(17)	2*i*	0.5355(8)	0.7894(9)	0.2461(4)	0.072(6)	0.125(8)	0.044(5)	–0.049(6)	–0.018(4)	0.012(5)
O(18)	2*i*	0.7167(8)	0.8895(8)	0.3733(5)	0.079(7)	0.094(7)	0.061(6)	–0.014(5)	0.011(5)	–0.042(5)
O(19)	2*i*	0.5720(8)	0.982(1)	0.3142(6)	0.062(6)	0.123(9)	0.097(8)	0.013(6)	0.027(6)	–0.046(7)
O(20)	2*i*	0.7259(9)	0.877(1)	0.0307(5)	0.085(7)	0.13(1)	0.042(5)	–0.018(7)	–0.019(5)	–0.001(5)
O(21)	2*i*	0.5754(8)	0.968(1)	0.0748(6)	0.059(6)	0.118(9)	0.110(8)	0.016(6)	–0.051(6)	–0.030(7)
O(22)	2*i*	0.8541(4)	0.5615(5)	0.1158(3)	0.024(3)	0.040(3)	0.028(3)	–0.008(3)	0.000(2)	–0.009(3)
O(23)	2*i*	0.5307(7)	0.8125(8)	–0.1354(4)	0.063(6)	0.096(7)	0.047(5)	–0.011(5)	–0.010(4)	0.005(5)
O(24)	2*i*	0.3797(7)	0.847(1)	–0.0886(5)	0.038(5)	0.16(1)	0.087(7)	–0.025(6)	–0.027(5)	0.018(7)
O(25)	2*i*	0.3593(7)	0.737(1)	0.1528(6)	0.036(5)	0.16(1)	0.098(8)	–0.026(6)	0.029(5)	–0.005(7)
O(26)	2*i*	0.5026(8)	0.6217(8)	0.2110(5)	0.074(6)	0.086(7)	0.060(6)	–0.024(5)	0.027(5)	0.006(5)
O(27)	2*i*	1.1592(9)	1.0121(8)	–0.1717(5)	0.118(8)	0.072(6)	0.100(7)	–0.074(6)	–0.015(6)	0.027(5)
O(28)	2*i*	1.2037(9)	0.8623(9)	–0.2045(5)	0.096(7)	0.086(7)	0.060(6)	–0.045(6)	0.026(5)	–0.001(5)
O(29)	2*i*	1.159(1)	0.9714(9)	0.0754(6)	0.17(1)	0.089(7)	0.114(9)	–0.087(8)	–0.029(8)	–0.033(6)
O(30)	2*i*	1.0994(9)	0.8678(9)	0.1374(5)	0.116(8)	0.108(8)	0.064(6)	–0.063(7)	0.001(6)	–0.041(6)
O(31)	2*i*	1.0359(6)	0.6268(5)	0.0368(3)	0.074(5)	0.041(4)	0.034(3)	–0.040(4)	0.005(3)	–0.007(3)

Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(32)	2*i*	0.9993(9)	0.9847(8)	0.2771(5)	0.105(8)	0.061(6)	0.069(6)	−0.037(6)	0.024(5)	−0.002(5)
O(33)	2*i*	0.933(1)	1.1367(8)	0.3127(6)	0.17(1)	0.052(6)	0.105(8)	−0.068(7)	0.024(8)	0.005(5)
O(34)	2*i*	0.8183(8)	1.1450(7)	0.5469(6)	0.080(6)	0.062(6)	0.15(1)	−0.033(5)	0.019(6)	−0.071(6)
O(35)	2*i*	0.811(1)	1.0086(9)	0.6077(6)	0.15(1)	0.083(7)	0.078(7)	−0.045(7)	0.042(7)	−0.050(6)
O(36)	2*i*	0.5843(8)	0.374(1)	0.2079(6)	0.052(6)	0.18(1)	0.124(9)	−0.076(7)	−0.001(5)	−0.055(8)
O(37)	2*i*	0.605(1)	0.408(1)	0.4408(6)	0.104(3)	0.106(3)	0.105(3)	−0.052(2)	0.003(1)	−0.022(1)
O(38)	2*i*	0.7462(9)	0.393(1)	0.4754(5)	0.096(8)	0.16(1)	0.051(5)	−0.079(8)	0.024(5)	−0.033(6)
O(39)	2*i*	1.1323(5)	0.4179(5)	−0.0041(3)	0.027(3)	0.034(3)	0.037(3)	−0.012(3)	0.006(2)	−0.007(3)
O(40)	2*i*	1.0286(5)	0.3908(5)	0.3202(3)	0.034(3)	0.046(4)	0.033(3)	−0.022(3)	0.005(2)	−0.016(3)
O(8)	2*i*	0.6929(7)	0.4004(7)	0.1343(5)	0.063(5)	0.076(6)	0.062(5)	−0.036(5)	−0.017(4)	−0.011(4)
C(50)	2*i*	0.8277(7)	0.7740(7)	0.1540(5)	0.042(5)	0.032(5)	0.038(5)	−0.017(4)	−0.001(4)	−0.008(4)
N(1)	2*i*	0.4771(7)	0.8068(8)	−0.0863(5)	0.031(5)	0.062(6)	0.058(6)	−0.011(4)	−0.011(4)	0.006(5)
N(2)	2*i*	0.4558(7)	0.6852(8)	0.1592(5)	0.034(5)	0.065(6)	0.062(6)	−0.017(4)	0.019(4)	−0.005(5)
N(3)	2*i*	0.6644(8)	0.3861(8)	0.1922(6)	0.050(6)	0.062(6)	0.080(8)	−0.023(5)	−0.018(5)	−0.020(5)
N(4)	2*i*	0.6949(9)	0.3944(9)	0.4322(5)	0.065(6)	0.082(7)	0.064(6)	−0.053(6)	0.036(5)	−0.030(5)
N(5)	2*i*	0.4822(8)	0.7996(9)	0.2960(5)	0.044(5)	0.091(8)	0.053(6)	−0.031(5)	−0.020(5)	0.018(5)
N(6)	2*i*	0.4627(8)	0.762(1)	0.5451(6)	0.042(5)	0.13(1)	0.071(8)	−0.034(6)	0.019(5)	−0.046(7)
N(7)	2*i*	0.8328(8)	1.0529(9)	0.5557(7)	0.052(6)	0.062(7)	0.094(9)	−0.017(5)	0.001(6)	−0.050(6)
N(8)	2*i*	0.9562(9)	1.0400(8)	0.3200(6)	0.079(7)	0.038(5)	0.077(7)	−0.032(5)	−0.001(6)	0.010(5)
N(9)	2*i*	1.1271(8)	0.9039(7)	0.0833(6)	0.056(6)	0.045(5)	0.076(7)	−0.022(5)	−0.016(5)	−0.023(5)
N(10)	2*i*	1.1700(8)	0.9204(9)	−0.1624(6)	0.053(6)	0.063(6)	0.071(7)	−0.038(5)	−0.004(5)	0.015(5)
N(11)	2*i*	0.6723(8)	0.9057(8)	0.0796(5)	0.058(6)	0.048(5)	0.059(6)	−0.013(5)	−0.022(5)	−0.001(4)
N(12)	2*i*	0.6684(8)	0.9178(8)	0.3211(5)	0.052(6)	0.053(6)	0.065(7)	−0.017(5)	0.020(5)	−0.025(5)
C(1)	2*i*	1.353(1)	0.599(1)	0.3749(7)	0.060(8)	0.10(1)	0.080(9)	−0.056(8)	0.014(6)	−0.027(8)
C(2)	2*i*	1.182(1)	0.719(1)	0.2883(7)	0.080(9)	0.061(8)	0.080(9)	−0.041(7)	0.009(7)	0.005(6)
C(3)	2*i*	1.364(1)	0.111(1)	0.4244(7)	0.071(9)	0.047(7)	0.09(1)	−0.013(6)	−0.011(7)	−0.002(6)
C(4)	2*i*	1.322(1)	0.199(1)	0.2903(7)	0.09(1)	0.077(9)	0.073(9)	−0.015(8)	0.006(8)	−0.040(8)
C(5)	2*i*	1.334(1)	0.455(1)	0.2156(7)	0.08(1)	0.11(1)	0.08(1)	−0.046(9)	0.000(8)	−0.039(9)
C(6)	2*i*	1.360(1)	0.516(1)	0.0809(8)	0.09(1)	0.12(1)	0.11(1)	−0.08(1)	0.024(9)	−0.04(1)
C(7)	2*i*	1.141(1)	0.111(1)	0.2023(6)	0.09(1)	0.055(7)	0.066(8)	−0.048(7)	0.020(7)	−0.005(6)
C(8)	2*i*	1.3269(9)	0.0466(8)	0.1318(6)	0.055(7)	0.031(5)	0.061(7)	−0.004(5)	−0.006(5)	−0.010(5)
C(9)	2*i*	0.8765(7)	0.9925(8)	0.4999(5)	0.029(5)	0.038(5)	0.064(7)	−0.011(4)	0.002(4)	−0.026(5)
C(10)	2*i*	0.9042(7)	0.8826(7)	0.5130(5)	0.032(5)	0.038(5)	0.045(5)	−0.018(4)	0.003(4)	−0.014(4)
C(11)	2*i*	0.9400(6)	0.8271(6)	0.4606(4)	0.024(4)	0.027(4)	0.042(5)	−0.014(3)	0.001(3)	−0.008(4)
C(12)	2*i*	0.9536(8)	0.8802(7)	0.3968(5)	0.044(5)	0.031(4)	0.037(5)	−0.017(4)	0.003(4)	−0.006(4)
C(13)	2*i*	0.9302(8)	0.9882(8)	0.3873(5)	0.049(6)	0.030(5)	0.054(6)	−0.020(4)	0.000(5)	0.001(4)
C(14)	2*i*	0.8889(8)	1.0467(8)	0.4375(6)	0.037(5)	0.027(5)	0.081(8)	−0.014(4)	−0.001(5)	−0.010(5)
C(15)	2*i*	0.9870(6)	0.6278(6)	0.2277(4)	0.023(4)	0.023(4)	0.026(4)	−0.013(3)	0.003(3)	−0.006(3)
C(16)	2*i*	1.0842(7)	0.7927(7)	0.0282(5)	0.038(5)	0.024(4)	0.041(5)	−0.013(4)	−0.003(4)	−0.004(4)
C(17)	2*i*	1.1178(7)	0.8697(8)	0.0214(5)	0.031(5)	0.037(5)	0.060(6)	−0.014(4)	−0.006(4)	−0.019(4)
C(18)	2*i*	1.1440(8)	0.9153(8)	−0.0402(6)	0.047(6)	0.033(5)	0.074(7)	−0.025(5)	−0.007(5)	−0.010(5)
C(19)	2*i*	1.1382(8)	0.8780(8)	−0.0954(5)	0.049(6)	0.043(5)	0.053(6)	−0.031(5)	−0.002(5)	0.001(4)
C(20)	2*i*	1.1063(8)	0.8000(7)	−0.0915(5)	0.047(5)	0.037(5)	0.039(5)	−0.024(4)	0.000(4)	−0.005(4)
C(21)	2*i*	1.0762(7)	0.7594(7)	−0.0292(4)	0.032(4)	0.028(4)	0.034(4)	−0.016(4)	0.000(3)	−0.005(3)
C(22)	2*i*	1.0419(6)	0.6722(6)	−0.0225(4)	0.029(4)	0.022(4)	0.033(5)	−0.014(3)	0.000(3)	−0.003(3)
C(23)	2*i*	0.6917(7)	0.6526(6)	0.0501(4)	0.029(4)	0.027(4)	0.035(4)	−0.014(4)	0.002(3)	−0.005(3)
C(24)	2*i*	0.6318(7)	0.6493(7)	0.1072(5)	0.028(5)	0.033(5)	0.040(5)	−0.009(4)	0.004(4)	−0.007(4)
C(25)	2*i*	0.5202(8)	0.6975(8)	0.0996(5)	0.032(5)	0.043(5)	0.048(6)	−0.016(4)	0.009(4)	−0.004(4)
C(26)	2*i*	0.4662(8)	0.7515(9)	0.0376(5)	0.030(5)	0.051(6)	0.058(6)	−0.014(5)	0.003(4)	−0.005(5)
C(27)	2*i*	0.5301(7)	0.7534(8)	−0.0180(5)	0.023(4)	0.048(5)	0.045(5)	−0.013(4)	−0.001(4)	−0.004(4)
C(28)	2*i*	0.6408(7)	0.7061(7)	−0.0132(5)	0.022(4)	0.034(5)	0.041(5)	−0.008(4)	0.002(3)	−0.007(4)
C(29)	2*i*	0.8131(6)	0.5965(6)	0.0567(4)	0.027(4)	0.025(4)	0.031(4)	−0.013(3)	0.007(3)	−0.008(3)
C(30)	2*i*	0.8780(7)	0.3835(6)	0.2860(4)	0.035(5)	0.021(4)	0.035(4)	−0.015(3)	0.001(3)	−0.006(3)
C(31)	2*i*	0.8355(7)	0.3855(7)	0.3510(5)	0.034(5)	0.026(4)	0.040(5)	−0.016(4)	0.007(4)	−0.008(4)
C(32)	2*i*	0.7380(8)	0.3877(7)	0.3627(5)	0.038(5)	0.034(5)	0.053(6)	−0.015(4)	0.017(4)	−0.012(4)
C(33)	2*i*	0.6803(9)	0.3878(9)	0.3119(6)	0.041(6)	0.059(7)	0.065(7)	−0.031(5)	0.010(5)	−0.020(5)
C(34)	2*i*	0.7229(7)	0.3861(8)	0.2483(5)	0.030(5)	0.040(5)	0.061(6)	−0.015(4)	−0.010(4)	−0.009(4)
C(35)	2*i*	0.8217(7)	0.3846(7)	0.2338(5)	0.029(4)	0.034(5)	0.043(5)	−0.015(4)	0.001(4)	−0.008(4)
C(36)	2*i*	0.8258(7)	0.7813(7)	0.2718(4)	0.038(5)	0.027(4)	0.033(5)	−0.014(4)	0.003(4)	−0.003(3)
C(37)	2*i*	0.9835(6)	0.3833(6)	0.2725(4)	0.030(4)	0.019(4)	0.028(4)	−0.011(3)	0.001(3)	−0.005(3)
C(38)	2*i*	0.5330(8)	0.7541(8)	0.3642(5)	0.036(5)	0.053(6)	0.041(5)	−0.023(5)	−0.009(4)	0.003(4)
C(39)	2*i*	0.4713(7)	0.7789(8)	0.4205(6)	0.019(4)	0.046(6)	0.065(7)	−0.006(4)	−0.004(4)	−0.006(5)
C(40)	2*i*	0.5236(7)	0.7360(9)	0.4838(5)	0.026(5)	0.061(6)	0.050(6)	−0.019(5)	0.008(4)	−0.021(5)
C(41)	2*i*	0.6345(7)	0.6713(8)	0.4913(5)	0.031(5)	0.050(5)	0.040(5)	−0.021(4)	0.003(4)	−0.011(4)
C(42)	2*i*	0.6954(6)	0.6498(6)	0.4329(4)	0.015(4)	0.028(4)	0.039(4)	−0.010(3)	−0.004(3)	−0.004(3)
C(43)	2*i*	0.6434(7)	0.6911(7)	0.3686(4)	0.032(5)	0.044(5)	0.031(5)	−0.018(4)	−0.002(4)	−0.001(4)
C(44)	2*i*	0.8177(6)	0.5862(6)	0.4374(4)	0.019(4)	0.021(4)	0.034(4)	−0.011(3)	0.002(3)	−0.005(3)
C(45)	2*i*	0.7234(8)	0.8630(8)	0.1473(5)	0.044(5)	0.041(5)	0.042(5)	−0.019(4)	−0.008(4)	−0.006(4)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(46)	2*i*	0.6704(8)	0.9112(8)	0.1998(5)	0.030(5)	0.030(5)	0.063(6)	–0.004(4)	–0.005(4)	–0.004(4)
C(47)	2*i*	0.7239(7)	0.8689(7)	0.2621(5)	0.036(5)	0.032(5)	0.047(5)	–0.012(4)	0.006(4)	–0.008(4)
C(48)	2*i*	0.8765(7)	0.7318(7)	0.2175(4)	0.031(4)	0.029(4)	0.032(4)	–0.018(4)	0.002(3)	–0.003(3)
C(49)	2*i*	0.9661(6)	0.7080(6)	0.4730(4)	0.027(4)	0.024(4)	0.031(4)	–0.013(3)	0.000(3)	–0.004(3)

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