Crystal structure of *catena*-(hexakis(μ_2-3,5-dinitrobenzoate-*O*,*O'*)-tetrakis(dimethylsulfoxide-*O*)dilanthanum(III), $La_2[(C_7H_3N_2O_6)_6(C_2H_6SO)_4]$

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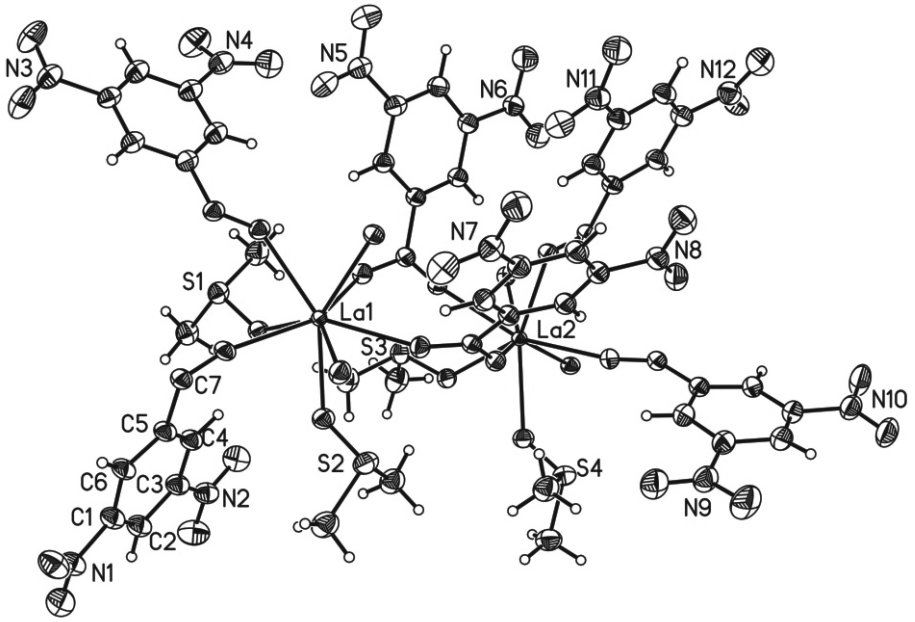

Abstract

$C_{50}H_{42}La_2N_{12}O_{40}S_4$, triclinic, $P\bar{1}$ (no. 2), a = 14.293(6) Å, b = 14.334(6) Å, c = 20.28(1) Å, α = 97.899(9)°, β = 95.891(9)°, γ = 119.560(6)°, V = 3509.4 Å^3, Z = 2, $R_{gt}(F)$ = 0.099, $wR_{ref}(F^2)$ = 0.189, T = 296 K.

Source of material

The title compound was synthesized from a mixture of 0.437 g of $La(NO_3)_3 \cdot 6H_2O$, 0.437 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 a 25 mL Teflon-lined stainless steel vessel, 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, 32.18 %; H, 2.32 %; N, 9.11 %; S, 6.75 %; calculated for $C_{50}H_{42}La_2N_{12}O_{40}S_4$: C, 32.34 %; H, 2.28 %; N, 9.05 %; S, 6.91 %.

Experimental details

The *R* values are moderately high, probably because of the statistical disorder of organic acids and poor crystal quality.

Discussion

Lanthanide complexes containing carboxylic acid ligands have been studied owing to their intresting coordination patterns and catalytic properties, and the effective approaches to synthesize novel polynuclear lanthanide complexes with unique structures and properties under the hydrothermal/solvothermal method [1-3].

The title crystal structure presents as a novel non-electrolyte complex with 1D chain. It is similar to that of $Pr_2[(C_7H_3N_2O_6)_6(C_2H_6SO)_4]$ [4]. The asymmetric unit contains two lanthanum (III) ions, both of which have approximately distorted square antiprismatic coordination. Each La^{3+} is coordinated by six sites occupied by the oxygen atoms from carboxyl group belonging to six 3,5-dinitrobenzoate molecules, and the other two by the oxygen atoms from coordinated DMSO molecules. The nitro groups of 3,5-dinitrobenzoate do not coordinated the La^{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 La^{3+}. There is a link between La1 and La2 with four 3,5-dinitrobenzoate, forming a dimer unit $La_2[(C_7H_3N_2O_6)_4(C_2H_6SO)_4]^{2+}$. Each La^{3+} links to another adjacent La^{3+} with two other carboxyl groups in the dimer unit, following the generic rule that a pair of La^{3+} are alternately connected by four or two carboxylate groups to form an infinite chain of 8-coordinated La^{3+} ions. The La atoms are coordinated by six oxygen atoms from the adjacent 3,5-dinitrobenzoate and two other oxygen atoms from the adjacent DMSO. The La—O distances vary from 2.419(9) Å to 2.554(8) Å and the mean of 2.503 Å, which is within a normal range [5].

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Table 1. Data collection and handling.

Crystal:	colorless block, size 0.24 × 0.26 × 0.38 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	14.29 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II CCD, φ/ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	17425, 12054
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 10529
$N(param)_{refined}$:	981
Programs:	SHELXS-97, SHELXL-97, SHELXTL [5]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	2*i*	0.3257	0.2158	1.0346	0.062
H(4)	2*i*	0.1100	0.2899	0.9513	0.055
H(6)	2*i*	0.2179	0.3811	1.1518	0.055
H(10)	2*i*	–0.3317	0.2401	1.0691	0.055
H(12)	2*i*	–0.6332	0.0286	0.9553	0.064
H(14)	2*i*	–0.3853	0.2225	0.8691	0.059
H(15A)	2*i*	–0.2687	0.1628	0.7965	0.090
H(15B)	2*i*	–0.3118	0.0391	0.7973	0.090
H(15C)	2*i*	–0.2117	0.1041	0.7632	0.090
H(16A)	2*i*	–0.1000	0.0397	0.8280	0.084
H(16B)	2*i*	–0.1949	–0.0265	0.8654	0.084
H(16C)	2*i*	–0.0755	0.0551	0.9071	0.084
H(17A)	2*i*	0.3837	0.5400	0.9626	0.102
H(17B)	2*i*	0.4469	0.5469	0.9030	0.102
H(17C)	2*i*	0.3555	0.4323	0.9122	0.102
H(18A)	2*i*	0.2887	0.3878	0.7912	0.097
H(18B)	2*i*	0.3588	0.5033	0.7741	0.097
H(18C)	2*i*	0.2308	0.4371	0.7507	0.097
H(21)	2*i*	–0.2668	0.3807	0.8065	0.052
H(23)	2*i*	–0.4931	0.3908	0.6745	0.058
H(25)	2*i*	–0.2407	0.3810	0.6120	0.051
H(28)	2*i*	0.1097	0.7410	0.8845	0.052
H(30)	2*i*	0.0685	0.9671	0.8077	0.056
H(32)	2*i*	0.1202	0.7558	0.6893	0.053
H(33A)	2*i*	0.0861	0.2047	0.7089	0.095
H(33B)	2*i*	–0.0355	0.1246	0.7144	0.095
H(33C)	2*i*	0.0188	0.2515	0.7415	0.095
H(34A)	2*i*	–0.0154	0.1235	0.5302	0.103
H(34B)	2*i*	–0.0791	0.0370	0.5729	0.103
H(34C)	2*i*	0.0490	0.1118	0.5928	0.103
H(35A)	2*i*	0.4211	0.5245	0.6034	0.099
H(35B)	2*i*	0.4905	0.6105	0.6716	0.099
H(35C)	2*i*	0.5089	0.6454	0.6019	0.099
H(36A)	2*i*	0.3417	0.7243	0.7280	0.095
H(36B)	2*i*	0.4599	0.7911	0.7127	0.095
H(36C)	2*i*	0.4253	0.6851	0.7416	0.095
H(38)	2*i*	–0.1390	0.6821	0.6729	0.057
H(40)	2*i*	–0.2841	0.8222	0.5833	0.059
H(42)	2*i*	–0.1919	0.6405	0.4675	0.058
H(46)	2*i*	0.2475	0.8493	0.4468	0.056
H(48)	2*i*	0.4908	1.1235	0.5748	0.064
H(50)	2*i*	0.3235	0.8477	0.6421	0.060

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}
La(1)	2*i*	0.00755(5)	0.45135(5)	0.89555(3)	0.0234(3)	0.0231(3)	0.0264(3)	0.0126(2)	0.0064(2)	0.0069(2)
La(2)	2*i*	0.04880(5)	0.48207(5)	0.60476(3)	0.0243(3)	0.0242(3)	0.0258(3)	0.0139(2)	0.0064(2)	0.0051(2)
C(1)	2*i*	0.284(1)	0.302(1)	1.1010(7)	0.048(3)	0.048(3)	0.058(3)	0.030(2)	0.004(3)	0.011(3)
C(2)	2*i*	0.283(1)	0.248(1)	1.0393(7)	0.049(3)	0.049(3)	0.060(3)	0.030(2)	0.006(3)	0.009(3)
C(3)	2*i*	0.213(1)	0.243(1)	0.9844(7)	0.047(2)	0.046(2)	0.059(2)	0.029(2)	0.009(2)	0.010(2)
C(4)	2*i*	0.153(1)	0.292(1)	0.9898(7)	0.045(2)	0.044(2)	0.056(2)	0.028(2)	0.009(2)	0.012(2)
C(5)	2*i*	0.157(1)	0.346(1)	1.0527(7)	0.043(2)	0.041(2)	0.054(2)	0.029(2)	0.009(2)	0.011(2)
C(6)	2*i*	0.219(1)	0.349(1)	1.1089(7)	0.047(3)	0.045(3)	0.056(3)	0.032(2)	0.006(3)	0.011(3)
C(7)	2*i*	0.092(1)	0.405(1)	1.0602(7)	0.042(2)	0.041(2)	0.051(2)	0.026(2)	0.010(2)	0.013(2)
C(8)	2*i*	–0.219(1)	0.325(1)	0.9754(7)	0.040(2)	0.039(2)	0.050(2)	0.023(2)	0.013(2)	0.010(2)
C(9)	2*i*	–0.339(1)	0.240(1)	0.9687(7)	0.042(2)	0.041(2)	0.052(2)	0.021(2)	0.013(2)	0.010(2)
C(10)	2*i*	–0.378(1)	0.209(1)	1.0267(7)	0.042(3)	0.042(3)	0.055(3)	0.021(2)	0.017(3)	0.009(3)
C(11)	2*i*	–0.488(1)	0.130(1)	1.0198(7)	0.043(3)	0.043(3)	0.057(3)	0.022(2)	0.018(3)	0.009(3)
C(12)	2*i*	–0.560(1)	0.083(1)	0.9592(7)	0.046(3)	0.047(3)	0.059(3)	0.018(3)	0.016(3)	0.009(3)
C(13)	2*i*	–0.518(1)	0.121(1)	0.9039(7)	0.044(3)	0.047(3)	0.058(3)	0.020(2)	0.013(2)	0.008(2)
C(14)	2*i*	–0.410(1)	0.199(1)	0.9076(7)	0.044(2)	0.045(2)	0.055(2)	0.020(2)	0.014(2)	0.009(2)
C(15)	2*i*	–0.248(1)	0.109(1)	0.7999(7)	0.051(4)	0.048(4)	0.059(4)	0.012(3)	0.005(4)	0.008(4)
C(16)	2*i*	–0.129(1)	0.042(1)	0.8686(8)	0.058(5)	0.041(4)	0.061(5)	0.021(4)	0.008(4)	0.009(4)
C(17)	2*i*	0.377(1)	0.508(1)	0.9163(8)	0.055(4)	0.062(4)	0.070(4)	0.019(4)	0.008(4)	0.008(4)
C(18)	2*i*	0.291(1)	0.454(1)	0.7860(8)	0.055(4)	0.058(4)	0.066(4)	0.019(4)	0.009(4)	0.012(4)
C(19)	2*i*	–0.133(1)	0.379(1)	0.7254(6)	0.041(2)	0.039(2)	0.047(2)	0.023(2)	0.011(2)	0.013(2)
C(20)	2*i*	–0.238(1)	0.380(1)	0.7115(6)	0.040(2)	0.040(2)	0.048(2)	0.025(2)	0.011(2)	0.012(2)
C(21)	2*i*	–0.293(1)	0.382(1)	0.7629(7)	0.041(2)	0.042(2)	0.050(2)	0.023(2)	0.012(2)	0.011(2)
C(22)	2*i*	–0.390(1)	0.386(1)	0.7482(7)	0.043(2)	0.047(2)	0.053(2)	0.023(2)	0.013(2)	0.009(2)
C(23)	2*i*	–0.429(1)	0.389(1)	0.6841(7)	0.044(2)	0.048(2)	0.054(2)	0.025(2)	0.009(2)	0.012(2)
C(24)	2*i*	–0.371(1)	0.388(1)	0.6355(7)	0.043(2)	0.045(2)	0.051(2)	0.024(2)	0.009(2)	0.013(2)
C(25)	2*i*	–0.277(1)	0.383(1)	0.6471(7)	0.041(2)	0.043(2)	0.048(2)	0.024(2)	0.010(2)	0.012(2)
C(26)	2*i*	0.118(1)	0.627(1)	0.7732(6)	0.039(2)	0.038(2)	0.047(2)	0.025(2)	0.012(2)	0.012(2)
C(27)	2*i*	0.111(1)	0.731(1)	0.7845(6)	0.041(2)	0.040(2)	0.046(2)	0.025(2)	0.010(2)	0.011(2)
C(28)	2*i*	0.104(1)	0.772(1)	0.8478(7)	0.044(2)	0.041(2)	0.047(2)	0.023(2)	0.011(2)	0.011(2)
C(29)	2*i*	0.087(1)	0.861(1)	0.8551(7)	0.046(2)	0.044(2)	0.051(2)	0.025(2)	0.013(2)	0.010(2)
C(30)	2*i*	0.081(1)	0.909(1)	0.8023(7)	0.048(2)	0.044(2)	0.053(2)	0.027(2)	0.011(2)	0.010(2)
C(31)	2*i*	0.094(1)	0.867(1)	0.7403(7)	0.046(2)	0.044(2)	0.051(2)	0.025(2)	0.010(2)	0.012(2)
C(32)	2*i*	0.110(1)	0.781(1)	0.7311(7)	0.044(2)	0.042(2)	0.049(2)	0.024(2)	0.011(2)	0.011(2)
C(33)	2*i*	0.015(1)	0.196(1)	0.7070(8)	0.061(4)	0.050(4)	0.064(4)	0.018(3)	0.010(4)	0.011(4)

Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(34)	2*i*	–0.018(1)	0.109(1)	0.5750(9)	0.064(6)	0.046(5)	0.072(6)	0.013(5)	0.010(5)	0.006(5)
C(35)	2*i*	0.455(1)	0.600(1)	0.6261(8)	0.048(5)	0.072(6)	0.070(6)	0.028(5)	0.006(5)	0.012(5)
C(36)	2*i*	0.400(1)	0.719(1)	0.7123(8)	0.053(4)	0.054(4)	0.063(4)	0.016(4)	0.005(4)	0.007(4)
C(37)	2*i*	–0.097(1)	0.587(1)	0.5663(6)	0.041(2)	0.041(2)	0.048(2)	0.027(2)	0.011(2)	0.011(2)
C(38)	2*i*	–0.166(1)	0.695(1)	0.6333(7)	0.047(2)	0.048(2)	0.052(2)	0.028(2)	0.010(2)	0.010(2)
C(39)	2*i*	–0.214(1)	0.756(1)	0.6367(7)	0.047(2)	0.050(2)	0.054(2)	0.028(2)	0.010(2)	0.010(2)
C(40)	2*i*	–0.252(1)	0.779(1)	0.5801(7)	0.050(2)	0.050(2)	0.057(3)	0.032(2)	0.010(2)	0.011(2)
C(41)	2*i*	–0.241(1)	0.736(1)	0.5176(7)	0.048(2)	0.052(2)	0.055(3)	0.030(2)	0.009(2)	0.014(2)
C(42)	2*i*	–0.196(1)	0.670(1)	0.5102(7)	0.047(2)	0.050(2)	0.053(2)	0.029(2)	0.010(2)	0.011(2)
C(43)	2*i*	–0.155(1)	0.649(1)	0.5694(7)	0.043(2)	0.045(2)	0.050(2)	0.029(2)	0.011(2)	0.011(2)
C(44)	2*i*	0.178(1)	0.713(1)	0.5297(7)	0.042(2)	0.041(2)	0.050(2)	0.024(2)	0.010(2)	0.013(2)
C(45)	2*i*	0.269(1)	0.831(1)	0.5424(7)	0.041(2)	0.041(2)	0.052(2)	0.024(2)	0.011(2)	0.012(2)
C(46)	2*i*	0.289(1)	0.885(1)	0.4904(7)	0.045(3)	0.043(3)	0.056(3)	0.024(2)	0.012(3)	0.015(3)
C(47)	2*i*	0.374(1)	0.994(1)	0.5039(7)	0.047(3)	0.045(3)	0.059(3)	0.021(3)	0.013(3)	0.016(3)
C(48)	2*i*	0.438(1)	1.049(1)	0.5660(7)	0.048(3)	0.044(3)	0.061(3)	0.020(3)	0.011(3)	0.013(3)
C(49)	2*i*	0.421(1)	0.988(1)	0.6163(7)	0.048(3)	0.047(2)	0.058(3)	0.019(2)	0.009(2)	0.012(2)
C(50)	2*i*	0.337(1)	0.884(1)	0.6064(7)	0.046(2)	0.045(2)	0.055(2)	0.021(2)	0.010(2)	0.014(2)
N(1)	2*i*	0.361(1)	0.315(1)	1.1597(6)	0.053(3)	0.050(3)	0.063(3)	0.031(2)	0.001(3)	0.009(3)
N(2)	2*i*	0.213(1)	0.191(1)	0.9168(6)	0.050(2)	0.049(2)	0.062(3)	0.030(2)	0.009(2)	0.006(2)
N(3)	2*i*	–0.529(1)	0.098(1)	1.0830(6)	0.048(3)	0.046(3)	0.061(3)	0.017(3)	0.019(3)	0.009(3)
N(4)	2*i*	–0.593(1)	0.079(1)	0.8379(6)	0.047(3)	0.051(3)	0.062(3)	0.019(2)	0.012(2)	0.005(2)
N(5)	2*i*	–0.4465(9)	0.3883(9)	0.8035(6)	0.044(2)	0.048(2)	0.057(2)	0.022(2)	0.013(2)	0.009(2)
N(6)	2*i*	–0.4068(9)	0.3950(9)	0.5663(6)	0.044(2)	0.049(2)	0.054(2)	0.024(2)	0.007(2)	0.014(2)
N(7)	2*i*	0.079(1)	0.902(1)	0.9221(6)	0.052(2)	0.045(2)	0.054(3)	0.023(2)	0.013(2)	0.008(2)
N(8)	2*i*	0.0879(9)	0.9154(9)	0.6815(6)	0.048(2)	0.046(2)	0.054(2)	0.026(2)	0.009(2)	0.012(2)
N(9)	2*i*	0.498(1)	1.039(1)	0.6828(7)	0.052(3)	0.050(3)	0.064(3)	0.016(3)	0.007(3)	0.011(3)
N(10)	2*i*	0.389(1)	1.055(1)	0.4495(7)	0.052(3)	0.049(3)	0.063(3)	0.018(3)	0.013(3)	0.017(3)
N(11)	2*i*	–0.220(1)	0.802(1)	0.7036(6)	0.052(2)	0.053(2)	0.057(2)	0.028(2)	0.010(2)	0.008(2)
N(12)	2*i*	–0.276(1)	0.762(1)	0.4562(6)	0.055(3)	0.058(3)	0.060(3)	0.029(2)	0.009(3)	0.012(3)
O(1)	2*i*	–0.0503(7)	0.2504(7)	0.8726(4)	0.043(2)	0.039(2)	0.053(2)	0.023(2)	0.011(2)	0.012(2)
O(2)	2*i*	0.1725(7)	0.4375(7)	0.8802(5)	0.044(2)	0.042(2)	0.057(2)	0.025(2)	0.013(2)	0.012(2)
O(3)	2*i*	0.0509(7)	0.4182(7)	1.0088(4)	0.041(2)	0.040(2)	0.050(2)	0.028(2)	0.009(2)	0.012(2)
O(4)	2*i*	–0.1841(7)	0.3430(7)	0.9216(4)	0.040(2)	0.039(2)	0.048(2)	0.022(2)	0.013(2)	0.010(2)
O(5)	2*i*	–0.1067(7)	0.3656(7)	0.7832(4)	0.042(2)	0.041(2)	0.047(2)	0.021(2)	0.011(2)	0.012(2)
O(6)	2*i*	0.1044(7)	0.5781(7)	0.8212(4)	0.044(2)	0.039(2)	0.047(2)	0.021(2)	0.013(2)	0.013(2)
O(7)	2*i*	–0.0819(7)	0.3855(7)	0.6785(4)	0.039(2)	0.039(2)	0.047(2)	0.024(2)	0.014(2)	0.012(2)
O(8)	2*i*	0.1352(7)	0.5991(7)	0.7180(4)	0.042(2)	0.039(2)	0.047(2)	0.023(1)	0.012(2)	0.012(2)
O(9)	2*i*	0.1501(9)	0.1818(9)	0.8680(6)	0.069(4)	0.059(4)	0.067(4)	0.031(3)	0.006(3)	0.001(3)
O(10)	2*i*	0.269(1)	0.147(1)	0.9130(6)	0.072(4)	0.074(4)	0.084(5)	0.044(4)	0.007(4)	–0.008(4)
O(11)	2*i*	0.410(1)	0.266(1)	1.1532(6)	0.075(2)	0.075(2)	0.076(2)	0.040(1)	0.014(1)	0.016(1)
O(12)	2*i*	0.378(1)	0.377(1)	1.2118(6)	0.069(5)	0.071(5)	0.073(5)	0.035(4)	–0.011(4)	0.007(4)
O(13)	2*i*	–0.466(1)	0.133(1)	1.1345(6)	0.071(5)	0.072(5)	0.069(5)	0.014(4)	0.026(4)	0.018(4)
O(14)	2*i*	–0.628(1)	0.029(1)	1.0738(6)	0.060(4)	0.070(5)	0.083(5)	0.005(4)	0.031(4)	0.012(4)
O(15)	2*i*	–0.5715(9)	0.133(1)	0.7964(6)	0.061(4)	0.064(4)	0.068(4)	0.016(3)	–0.002(3)	0.004(3)
O(16)	2*i*	–0.673(1)	–0.013(1)	0.8292(6)	0.057(5)	0.070(5)	0.084(5)	0.002(4)	0.004(4)	–0.009(4)
O(17)	2*i*	–0.4075(8)	0.3972(8)	0.8600(5)	0.052(3)	0.055(3)	0.061(3)	0.019(3)	0.019(3)	0.004(3)
O(18)	2*i*	–0.5406(9)	0.373(1)	0.7859(6)	0.055(4)	0.075(4)	0.078(4)	0.028(3)	0.017(3)	0.006(4)
O(19)	2*i*	–0.3583(9)	0.3937(9)	0.5235(5)	0.057(3)	0.066(4)	0.059(3)	0.023(3)	0.003(3)	0.014(3)
O(20)	2*i*	–0.4855(9)	0.408(1)	0.5570(6)	0.061(4)	0.074(4)	0.075(4)	0.029(3)	0.002(3)	0.018(3)
O(21)	2*i*	0.2482(7)	0.5332(7)	0.6277(4)	0.039(2)	0.044(2)	0.053(2)	0.022(2)	0.010(2)	0.011(2)
O(22)	2*i*	0.0571(7)	0.3141(7)	0.6166(4)	0.042(2)	0.040(2)	0.054(2)	0.022(2)	0.013(2)	0.014(2)
O(23)	2*i*	–0.0654(7)	0.5725(7)	0.6200(4)	0.042(2)	0.042(2)	0.048(2)	0.026(1)	0.011(2)	0.011(2)
O(24)	2*i*	0.1581(7)	0.6703(7)	0.5803(4)	0.042(2)	0.041(2)	0.048(2)	0.022(2)	0.010(2)	0.014(2)
O(25)	2*i*	–0.1764(9)	0.7924(9)	0.7541(5)	0.061(3)	0.063(3)	0.060(3)	0.028(3)	0.011(3)	0.002(3)
O(26)	2*i*	–0.276(1)	0.847(1)	0.7065(6)	0.074(2)	0.074(2)	0.074(2)	0.039(1)	0.014(1)	0.015(1)
O(27)	2*i*	–0.293(1)	0.840(1)	0.4647(6)	0.078(2)	0.078(2)	0.079(2)	0.041(1)	0.015(1)	0.017(1)
O(28)	2*i*	–0.2897(9)	0.706(1)	0.4008(6)	0.069(5)	0.078(5)	0.069(5)	0.046(4)	0.003(4)	0.016(4)
O(29)	2*i*	0.041(1)	0.962(1)	0.9266(6)	0.073(2)	0.073(2)	0.074(2)	0.038(1)	0.015(1)	0.015(1)
O(30)	2*i*	0.099(1)	0.871(1)	0.9688(6)	0.074(4)	0.065(4)	0.062(4)	0.027(4)	0.013(4)	0.000(4)
O(31)	2*i*	0.052(1)	0.9782(9)	0.6893(6)	0.071(4)	0.063(3)	0.073(4)	0.032(3)	0.004(3)	0.014(3)
O(32)	2*i*	0.1046(9)	0.8879(8)	0.6299(5)	0.062(3)	0.054(3)	0.059(3)	0.023(3)	0.006(3)	0.017(3)
O(33)	2*i*	0.326(1)	1.012(1)	0.3984(6)	0.078(5)	0.062(5)	0.073(5)	0.011(4)	0.010(4)	0.029(4)
O(34)	2*i*	0.466(1)	1.1454(9)	0.4588(6)	0.066(4)	0.054(4)	0.088(5)	0.014(4)	0.019(4)	0.028(4)
O(35)	2*i*	0.570(1)	1.138(1)	0.6922(7)	0.071(5)	0.061(5)	0.084(5)	0.000(4)	–0.004(4)	0.004(4)
O(36)	2*i*	0.485(1)	0.9850(9)	0.7252(6)	0.064(4)	0.060(4)	0.070(4)	0.012(4)	–0.004(4)	0.008(4)
O(37)	2*i*	0.1667(7)	0.6287(7)	0.9658(4)	0.044(2)	0.043(2)	0.048(2)	0.018(2)	0.011(2)	0.012(2)
O(38)	2*i*	–0.0877(7)	0.5600(7)	0.8802(4)	0.042(2)	0.038(2)	0.047(2)	0.027(2)	0.012(2)	0.011(2)
O(39)	2*i*	–0.1276(7)	0.3302(7)	0.5305(4)	0.042(2)	0.041(2)	0.046(2)	0.021(2)	0.009(2)	0.012(2)

Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(40)	2*i*	0.0829(7)	0.4440(7)	0.4912(4)	0.039(2)	0.041(2)	0.047(2)	0.024(2)	0.013(2)	0.009(2)
S(1)	2*i*	–0.1571(3)	0.1494(3)	0.8781(2)	0.047(1)	0.035(1)	0.052(1)	0.019(1)	0.010(1)	0.009(1)
S(2)	2*i*	0.2785(3)	0.5180(3)	0.8635(2)	0.047(2)	0.052(2)	0.079(2)	0.025(1)	0.021(1)	0.017(1)
S(3)	2*i*	–0.0307(3)	0.2079(3)	0.6282(2)	0.055(2)	0.042(2)	0.076(2)	0.024(1)	0.016(1)	0.019(1)
S(4)	2*i*	0.3527(3)	0.6383(3)	0.6285(2)	0.037(1)	0.055(2)	0.059(2)	0.019(1)	0.005(1)	0.013(1)

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