Crystal structure of (*N*,*N*,*N*′,*N*′-tetrakis((2-benzimidazolyl)methyl)-1,2-cyclohexanediamine)nickel(II) dipicrate dimethylformamide sesquisolvate, $Ni[C_6H_{10}N_2(C_8H_7N_2)_4][C_6H_2(NO_2)_3O]_2 \cdot 1.5\,(CH_3)_2NCHO$

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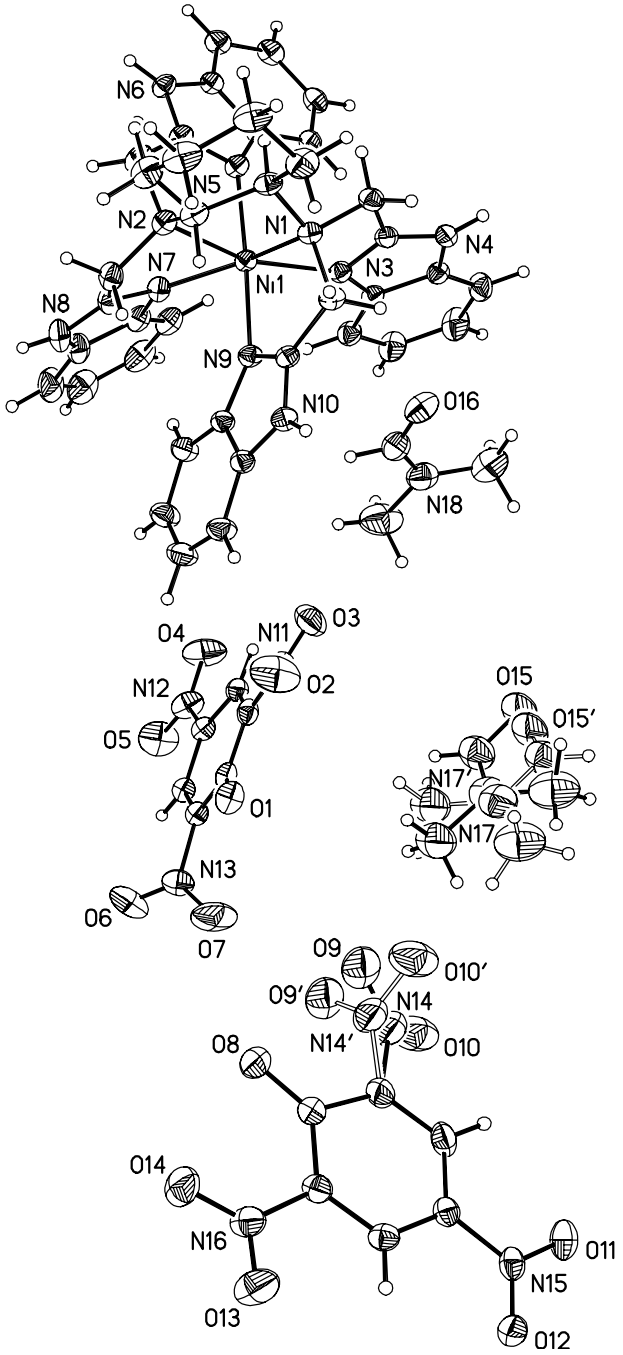

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Abstract

$C_{54.50}H_{52.50}N_{17.50}NiO_{15.50}$, monoclinic, *P*12/*c*1 (no. 13), *a* = 20.460(1) Å, *b* = 12.1971(6) Å, *c* = 24.942(1) Å, β = 110.864(1)°, *V* = 5816.2 Å^3, *Z* = 4, $R_{gt}(F)$ = 0.055, $wR_{ref}(F^2)$ = 0.169, *T* = 293 K.

Source of material

A mixture of $Ni(pic)_2 \cdot 6H_2O$ (0.6227 g, 1 mmol; pic = picrate) and *N*,*N*,*N*′,*N*′-tetrakis((2-benzimidazoly)methyl)-1,2-cyclohexanediamine (0.6340 g, 1 mmol; CDTB) was dissolved in about 15 mL of DMF and then stirred at room temperature for 2 h. The undissolved materials were removed by filtration. Ethanol was added slowly to the filtrate along the glass wall. The resulting biphasic solution was set aside to crystallize. After one week, the brown block-shaped single crystals were obtained.

Experimental details

All non-hydrogen atoms were refined anisotropically. The H atoms attached at carbon and nitrogen were placed in calculated positions with *d*(C—H) = 0.93 Å (aromatic) or 0.97 Å (aliphatic), *d*(N—H) = 0.86 Å and U_{iso}(H) = 1.2U_{eq}© or N) in the riding model approximation. The H atoms of the 1.5 solvated DMF molecules being disordered were also placed in calculated positions, with *d*(C—H) = 0.93 Å or 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C).

Discussion

Transition metal polybenzimidazole complexes play an important role in mimicking the biological activities of proteins because they contain the particular imidazole units of histidine [1]. In this regard, a variety of transition metal complexes involving polybenzimidazole ligands have been synthesized and studied extensively [2-4]. In our series of studies on the properties of transition metal complexes with polybenzimidazole ligands, we synthesized a complex of hydrated nickel(II) with CDTB and determined the crystal structure.

The crystal structure of the title complex is similar to that of the complex of hydrated nickel(II) picrate with *N*,*N*,*N*′,*N*′-tetrakis((2-benzimidazoly)methyl)-1,2-ethanediamine (EDTB) reported earlier [5]. Four benzimidazole imine nitrogen atoms (N3, N5, N7, N9) and two amine nitrogen atoms (N1, N2) in CDTB coordinate to the central Ni(II) ion directly, forming a distorted octahedral environment. Two benzimidazole imine nitrogen atoms (N5 and N9) are located at the axial positions, another two benzimidazole imine nitrogen atoms (N3 and N7) and two amine nitrogen atoms (N1 and N2) are located on the equatorial positions. The Ni—benzimidazole bond lengths are significantly shorter than the Ni—amine bond lengths, partially due to the greater π-bonding ability of benzimidazole pendants compared

to alkylamines, which are exclusively σ-donors [6]. The similar case was also observed in the complex of hydrated nickel picrate with EDTB. The bond angles around Ni range from 77.6(1)° to 121.9(1)° for the *cis* groups and from 157.5(1)° to 176.9(1)° for the *trans* groups. The largest deviation from the ideal octahedral geometry is the N3–Ni–N7 angle of 121.9(1)°. In addition, there are also extensive hydrogen bonds in the crystal structure. Two picrate anions and one DMF molecule are linked to the complex cation $[Ni(CDTB)]^{2+}$ by intermolecular hydrogen bonds. The N4···O1^{i}, N10···O1^{ii}, N6···O8^{iii}, N8···O15, N8···O15′ distances and the angles of N4–H4′···O1^{i}, N10–H10′···O1^{ii}, N6–H6′···O8^{iii}, N8–H8′···O15 and N8–H8′···O15′ are 2.868(4) Å, 2.764(4) Å, 2.663(4) Å, 2.67(2) Å, 2.81(2) Å; 162.4°, 161.6°, 147.2°, 176.3°, 160.7°, respectively (symmetry operations: (i) $x,-y+1,z-½$; (ii) $-x+1,-y+1,-z+1$; (iii) $-x,-y+2,-z+1$).

Table 1. Data collection and handling.

Crystal:	brown block, size 0.31 × 0.31 × 0.41 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	4.18 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ/ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	51116, 13329
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 8676
$N(param)_{refined}$:	852
Programs:	SHELXS-97 [7], SHELXL-97 [8], SHELXTL [9]

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

Atom	Site	Occ.	x	y	z	U_{iso}
H(51)	4*g*	0.508	0.0045	0.5790	0.3805	0.138
H(52A)	4*g*	0.508	0.1250	0.5989	0.5117	0.219
H(52B)	4*g*	0.508	0.0487	0.5609	0.4759	0.219
H(52C)	4*g*	0.508	0.0645	0.6853	0.4905	0.219
H(53A)	4*g*	0.508	0.1825	0.6204	0.4124	0.251
H(53B)	4*g*	0.508	0.1922	0.6864	0.4687	0.251
H(53C)	4*g*	0.508	0.1542	0.7407	0.4086	0.251
H(51′)	4*g*	0.492	0.1583	0.6499	0.3796	0.138
H(52D)	4*g*	0.492	0.0243	0.6686	0.4482	0.219
H(52E)	4*g*	0.492	0.0553	0.5539	0.4727	0.219
H(52F)	4*g*	0.492	0.0169	0.5694	0.4065	0.219
H(53D)	4*g*	0.492	0.1678	0.7378	0.4880	0.251
H(53E)	4*g*	0.492	0.2086	0.6366	0.4770	0.251
H(53F)	4*g*	0.492	0.1633	0.6241	0.5158	0.251
H(4′)	4*g*		0.4290	0.7182	0.1049	0.065
H(6′)	4*g*		0.0396	0.8385	0.0488	0.065
H(8′)	4*g*		0.0879	0.5824	0.2745	0.093
H(10′)	4*g*		0.4315	0.7369	0.3725	0.065
H(1)	4*g*		0.2512	0.9450	0.1655	0.069
H(2A)	4*g*		0.3624	1.0218	0.2623	0.097
H(2B)	4*g*		0.3491	1.0533	0.1984	0.097
H(3A)	4*g*		0.3128	1.1973	0.2444	0.107
H(3B)	4*g*		0.2484	1.1520	0.1933	0.107
H(4A)	4*g*		0.2801	1.0902	0.3092	0.107
H(4B)	4*g*		0.2193	1.1708	0.2760	0.107
H(5A)	4*g*		0.1609	1.0316	0.2140	0.096
H(5B)	4*g*		0.1751	0.9939	0.2772	0.096
H(6)	4*g*		0.2659	0.8834	0.2778	0.068
H(7A)	4*g*		0.3959	0.8667	0.1691	0.069
H(7B)	4*g*		0.3190	0.8666	0.1242	0.069
H(10)	4*g*		0.4536	0.5076	0.0659	0.089
H(11)	4*g*		0.4195	0.3289	0.0676	0.111
H(12)	4*g*		0.3398	0.2793	0.1086	0.099
H(13)	4*g*		0.2914	0.4093	0.1515	0.076
H(15A)	4*g*		0.1233	0.9240	0.1575	0.080
H(15B)	4*g*		0.0838	0.8185	0.1652	0.080
H(18)	4*g*		0.2480	0.6227	0.0397	0.062
H(19)	4*g*		0.1941	0.5907	–0.0573	0.071
H(20)	4*g*		0.0838	0.6565	–0.1074	0.079
H(21)	4*g*		0.0220	0.7552	–0.0616	0.075
H(23A)	4*g*		0.1229	0.7900	0.2574	0.076
H(23B)	4*g*		0.2003	0.7521	0.2911	0.076
H(26)	4*g*		0.1682	0.4222	0.1208	0.085
H(27)	4*g*		0.1196	0.2528	0.1254	0.111
H(28)	4*g*		0.0646	0.2198	0.1895	0.128
H(29)	4*g*		0.0539	0.3546	0.2497	0.123
H(31A)	4*g*		0.4228	0.7853	0.2532	0.066
H(31B)	4*g*		0.3926	0.8746	0.2833	0.066
H(34)	4*g*		0.2413	0.4581	0.2792	0.080
H(35)	4*g*		0.2660	0.3598	0.3634	0.096
H(36)	4*g*		0.3508	0.4179	0.4467	0.099
H(37)	4*g*		0.4168	0.5717	0.4486	0.085
H(41)	4*g*		0.3926	0.0671	0.4171	0.073
H(43)	4*g*		0.3807	–0.1446	0.5366	0.064
H(47)	4*g*		0.1669	0.8943	0.8717	0.087
H(49)	4*g*		0.2224	0.9614	1.0389	0.069
H(54)	4*g*	0.50	0.4477	0.5303	0.2779	0.105
H(55A)	4*g*	0.50	0.5657	0.5011	0.2140	0.186
H(55B)	4*g*	0.50	0.5312	0.3916	0.1844	0.186
H(55C)	4*g*	0.50	0.5918	0.3885	0.2444	0.186
H(56A)	4*g*	0.50	0.4437	0.3583	0.2840	0.219
H(56B)	4*g*	0.50	0.5113	0.2936	0.2875	0.219
H(56C)	4*g*	0.50	0.4475	0.2987	0.2295	0.219

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

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(15)	4*g*	0.508(5)	0.0532(8)	0.613(1)	0.3303(4)	0.128(9)	0.197(4)	0.043(6)	–0.009(5)	0.023(5)	–0.014(5)
N(17)	4*g*	0.508	0.096(1)	0.633(1)	0.4298(9)	0.160(7)	0.086(3)	0.115(4)	0.027(3)	0.056(4)	0.000(3)
C(51)	4*g*	0.508	0.0468(6)	0.6054(8)	0.3796(4)	0.144(6)	0.113(5)	0.095(4)	0.005(5)	0.052(5)	–0.005(4)
C(52)	4*g*	0.508	0.0825(8)	0.618(1)	0.4811(4)	0.21(1)	0.136(6)	0.113(7)	0.063(7)	0.084(8)	0.008(7)
C(53)	4*g*	0.508	0.1617(6)	0.673(1)	0.4299(6)	0.22(1)	0.101(6)	0.162(9)	0.014(7)	0.04(1)	0.000(8)
O(15′)	4*g*	0.492	0.0774(8)	0.612(1)	0.3491(4)	0.128(9)	0.197(4)	0.043(6)	–0.009(5)	0.023(5)	–0.014(5)
N(17′)	4*g*	0.492	0.110(1)	0.633(1)	0.436(1)	0.160(7)	0.086(3)	0.115(4)	0.027(3)	0.056(4)	0.000(3)
C(51′)	4*g*	0.492	0.1157(7)	0.6315(9)	0.3828(5)	0.144(6)	0.113(5)	0.095(4)	0.005(5)	0.052(5)	–0.005(4)
C(52′)	4*g*	0.492	0.0467(7)	0.604(1)	0.4412(6)	0.21(1)	0.136(6)	0.113(7)	0.063(7)	0.084(8)	0.008(7)
C(53′)	4*g*	0.492	0.1666(8)	0.660(1)	0.4826(5)	0.22(1)	0.101(6)	0.162(9)	0.014(7)	0.04(1)	0.000(8)
Ni(1)	4*g*		0.25016(2)	0.69452(3)	0.18680(1)	0.0450(2)	0.0510(2)	0.0380(2)	0.0016(2)	0.0110(2)	–0.0049(2)
O(1)	4*g*		0.4932(1)	0.1581(2)	0.5993(1)	0.068(2)	0.067(2)	0.088(2)	–0.014(1)	0.022(1)	–0.030(1)
O(2)	4*g*		0.4801(3)	0.2973(3)	0.5156(2)	0.208(5)	0.078(2)	0.144(4)	–0.059(3)	0.027(3)	0.001(2)
O(3)	4*g*		0.4598(2)	0.2305(3)	0.4322(2)	0.150(3)	0.097(2)	0.134(3)	0.022(2)	0.091(3)	0.041(2)

Table 3. Continued.

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(4)	4*g*		0.3150(2)	–0.0890(3)	0.3766(1)	0.172(3)	0.113(3)	0.053(2)	0.013(2)	–0.010(2)	–0.022(2)
O(5)	4*g*		0.3099(2)	–0.2014(3)	0.4404(2)	0.143(3)	0.095(2)	0.106(3)	–0.047(2)	0.010(2)	–0.036(2)
O(6)	4*g*		0.4200(2)	–0.1064(3)	0.6408(1)	0.172(3)	0.114(3)	0.077(2)	–0.038(3)	0.053(2)	0.002(2)
O(7)	4*g*		0.5192(2)	–0.0322(4)	0.6598(2)	0.142(3)	0.177(4)	0.073(2)	–0.036(3)	–0.028(2)	0.012(2)
O(8)	4*g*		0.0266(2)	1.1027(3)	0.9217(1)	0.081(2)	0.145(3)	0.068(2)	0.045(2)	0.029(1)	0.018(2)
O(9)	4*g*	0.395(4)	0.0267(5)	1.069(1)	0.8150(4)	0.079(3)	0.164(4)	0.090(3)	–0.009(3)	0.010(2)	–0.024(3)
O(10)	4*g*	0.395	0.0505(5)	0.8898(9)	0.8051(4)	0.112(4)	0.181(5)	0.105(3)	–0.033(3)	0.003(3)	0.041(3)
N(14)	4*g*	0.395	0.0564(4)	0.972(1)	0.8311(4)	0.112(4)	0.186(5)	0.080(3)	0.071(4)	0.037(3)	0.015(4)
O(9′)	4*g*	0.605	–0.0115(3)	0.9804(6)	0.8184(2)	0.079(3)	0.164(4)	0.090(3)	–0.009(3)	0.010(2)	–0.024(3)
O(10′)	4*g*	0.605	0.0680(4)	1.0912(6)	0.8065(3)	0.112(4)	0.181(5)	0.105(3)	–0.033(3)	0.003(3)	0.041(3)
N(14′)	4*g*	0.605	0.0481(4)	1.0163(6)	0.8370(3)	0.112(4)	0.186(5)	0.080(3)	0.071(4)	0.037(3)	0.015(4)
O(11)	4*g*		0.2767(1)	0.8075(2)	0.9294(1)	0.079(2)	0.079(2)	0.101(2)	–0.005(1)	0.050(2)	–0.025(2)
O(12)	4*g*		0.3058(1)	0.8415(2)	1.0199(1)	0.061(1)	0.083(2)	0.082(2)	0.006(1)	0.028(1)	0.014(1)
O(13)	4*g*		0.1636(2)	1.0669(3)	1.0868(1)	0.141(3)	0.144(3)	0.061(2)	0.066(2)	0.005(2)	–0.028(2)
O(14)	4*g*		0.0611(2)	1.1130(3)	1.0343(1)	0.100(2)	0.137(3)	0.078(2)	0.038(2)	0.030(2)	–0.025(2)
N(1)	4*g*		0.3234(1)	0.8304(2)	0.2051(1)	0.054(1)	0.046(1)	0.045(1)	0.002(1)	0.013(1)	–0.001(1)
N(2)	4*g*		0.1873(1)	0.8144(2)	0.2122(1)	0.054(1)	0.066(2)	0.039(1)	0.007(1)	0.011(1)	–0.012(1)
N(3)	4*g*		0.3235(1)	0.6323(2)	0.1549(1)	0.050(1)	0.046(1)	0.049(1)	0.004(1)	0.017(1)	0.001(1)
N(4)	4*g*		0.4016(1)	0.6780(2)	0.1159(1)	0.057(2)	0.055(2)	0.057(2)	0.005(1)	0.027(1)	0.007(1)
N(5)	4*g*		0.1857(1)	0.7432(2)	0.10509(9)	0.051(1)	0.057(1)	0.040(1)	0.006(1)	0.010(1)	–0.008(1)
N(6)	4*g*		0.0789(1)	0.8053(2)	0.0559(1)	0.048(1)	0.063(2)	0.044(1)	0.008(1)	0.007(1)	–0.007(1)
N(7)	4*g*		0.1670(1)	0.5976(2)	0.1922(1)	0.050(1)	0.068(2)	0.047(1)	–0.004(1)	0.015(1)	–0.012(1)
N(8)	4*g*		0.1068(2)	0.5696(3)	0.2494(1)	0.061(2)	0.102(2)	0.081(2)	–0.015(2)	0.040(2)	–0.016(2)
N(9)	4*g*		0.3112(1)	0.6510(2)	0.2702(1)	0.047(1)	0.052(1)	0.043(1)	–0.004(1)	0.008(1)	–0.000(1)
N(10)	4*g*		0.3970(1)	0.6999(2)	0.3497(1)	0.051(1)	0.060(2)	0.042(1)	–0.003(1)	0.005(1)	–0.006(1)
N(11)	4*g*		0.4633(2)	0.2211(3)	0.4809(2)	0.075(2)	0.072(2)	0.111(3)	0.004(2)	0.039(2)	0.015(2)
N(12)	4*g*		0.3312(2)	–0.1179(3)	0.4261(2)	0.090(2)	0.074(2)	0.066(2)	0.006(2)	0.004(2)	–0.024(2)
N(13)	4*g*		0.4610(2)	–0.0529(3)	0.6277(1)	0.098(2)	0.071(2)	0.054(2)	–0.004(2)	0.017(2)	–0.011(2)
N(15)	4*g*		0.2663(2)	0.8516(2)	0.9697(1)	0.061(2)	0.053(2)	0.080(2)	–0.007(1)	0.039(2)	–0.004(1)
N(16)	4*g*		0.1170(2)	1.0724(2)	1.0399(1)	0.095(2)	0.067(2)	0.058(2)	0.025(2)	0.021(2)	–0.006(1)
C(1)	4*g*		0.2821(2)	0.9321(2)	0.2052(1)	0.068(2)	0.047(2)	0.052(2)	0.010(1)	0.014(2)	–0.001(1)
C(2)	4*g*		0.3262(2)	1.0358(3)	0.2254(2)	0.089(3)	0.047(2)	0.103(3)	–0.002(2)	0.030(2)	–0.006(2)
C(3)	4*g*		0.2826(3)	1.1341(3)	0.2306(2)	0.111(3)	0.056(2)	0.085(3)	0.010(2)	0.017(2)	–0.011(2)
C(4)	4*g*		0.2458(2)	1.1075(3)	0.2718(2)	0.114(3)	0.062(2)	0.074(3)	0.015(2)	0.014(2)	–0.023(2)
C(5)	4*g*		0.1973(2)	1.0113(3)	0.2498(2)	0.092(3)	0.073(2)	0.073(2)	0.016(2)	0.027(2)	–0.024(2)
C(6)	4*g*		0.2353(2)	0.9088(3)	0.2399(1)	0.063(2)	0.055(2)	0.044(2)	0.007(1)	0.010(1)	–0.013(1)
C(7)	4*g*		0.3511(2)	0.8293(2)	0.1575(1)	0.069(2)	0.046(2)	0.058(2)	0.002(1)	0.026(2)	0.004(1)
C(8)	4*g*		0.3595(2)	0.7123(2)	0.1432(1)	0.053(2)	0.050(2)	0.048(2)	0.006(1)	0.017(1)	0.004(1)
C(9)	4*g*		0.3927(2)	0.5654(3)	0.1087(1)	0.053(2)	0.053(2)	0.056(2)	0.010(1)	0.021(1)	0.004(1)
C(10)	4*g*		0.4216(2)	0.4883(3)	0.0830(2)	0.078(2)	0.073(2)	0.085(2)	0.009(2)	0.048(2)	–0.005(2)
C(11)	4*g*		0.4008(2)	0.3830(4)	0.0842(2)	0.099(3)	0.071(3)	0.122(4)	0.012(2)	0.058(3)	–0.022(2)
C(12)	4*g*		0.3526(2)	0.3526(3)	0.1091(2)	0.086(3)	0.052(2)	0.117(3)	0.006(2)	0.044(2)	–0.012(2)
C(13)	4*g*		0.3235(2)	0.4293(3)	0.1346(2)	0.061(2)	0.054(2)	0.077(2)	0.005(2)	0.026(2)	0.000(2)
C(14)	4*g*		0.3440(2)	0.5373(2)	0.1338(1)	0.049(2)	0.048(2)	0.051(2)	0.008(1)	0.016(1)	0.002(1)
C(15)	4*g*		0.1263(2)	0.8448(3)	0.1606(1)	0.059(2)	0.082(2)	0.049(2)	0.021(2)	0.007(2)	–0.016(2)
C(16)	4*g*		0.1310(2)	0.7983(2)	0.1069(1)	0.050(2)	0.055(2)	0.042(1)	0.005(1)	0.010(1)	–0.008(1)
C(17)	4*g*		0.1672(2)	0.7096(2)	0.0478(1)	0.051(2)	0.044(2)	0.040(1)	–0.006(1)	0.015(1)	–0.003(1)
C(18)	4*g*		0.2034(2)	0.6494(2)	0.0199(1)	0.057(2)	0.052(2)	0.048(2)	–0.002(1)	0.020(1)	–0.002(1)
C(19)	4*g*		0.1708(2)	0.6308(3)	–0.0379(1)	0.076(2)	0.059(2)	0.049(2)	–0.009(2)	0.030(2)	–0.010(1)
C(20)	4*g*		0.1039(2)	0.6703(3)	–0.0683(1)	0.076(2)	0.078(2)	0.039(2)	–0.012(2)	0.014(2)	–0.011(2)
C(21)	4*g*		0.0669(2)	0.7295(3)	–0.0416(1)	0.059(2)	0.076(2)	0.043(2)	–0.009(2)	0.006(1)	–0.002(2)
C(22)	4*g*		0.1003(2)	0.7486(2)	0.0168(1)	0.052(2)	0.053(2)	0.041(1)	–0.004(1)	0.013(1)	–0.004(1)
C(23)	4*g*		0.1634(2)	0.7539(3)	0.2537(1)	0.063(2)	0.079(2)	0.052(2)	0.002(2)	0.025(2)	–0.016(2)
C(24)	4*g*		0.1449(2)	0.6403(3)	0.2315(1)	0.052(2)	0.079(2)	0.054(2)	–0.004(2)	0.021(2)	–0.013(2)
C(25)	4*g*		0.1399(2)	0.4908(3)	0.1835(1)	0.042(2)	0.070(2)	0.061(2)	–0.007(1)	0.006(1)	–0.010(2)
C(26)	4*g*		0.1456(2)	0.4093(3)	0.1466(2)	0.055(2)	0.073(2)	0.071(2)	–0.003(2)	0.005(2)	–0.018(2)
C(27)	4*g*		0.1166(2)	0.3088(4)	0.1497(2)	0.064(2)	0.077(3)	0.111(3)	–0.009(2)	0.001(2)	–0.028(2)
C(28)	4*g*		0.0829(2)	0.2891(4)	0.1881(3)	0.070(3)	0.088(3)	0.147(5)	–0.026(2)	0.021(3)	–0.011(3)
C(29)	4*g*		0.0761(2)	0.3685(4)	0.2237(2)	0.064(2)	0.110(4)	0.136(4)	–0.029(2)	0.039(3)	–0.002(3)
C(30)	4*g*		0.1036(2)	0.4723(4)	0.2201(2)	0.051(2)	0.092(3)	0.085(3)	–0.017(2)	0.025(2)	–0.011(2)
C(31)	4*g*		0.3814(2)	0.8079(2)	0.2607(1)	0.053(2)	0.050(2)	0.053(2)	–0.005(1)	0.008(1)	–0.001(1)
C(32)	4*g*		0.3622(2)	0.7215(2)	0.2938(1)	0.045(2)	0.049(2)	0.044(2)	0.002(1)	0.010(1)	–0.002(1)
C(33)	4*g*		0.3141(2)	0.5758(3)	0.3138(1)	0.051(2)	0.057(2)	0.045(2)	–0.000(1)	0.013(1)	0.004(1)
C(34)	4*g*		0.2760(2)	0.4814(3)	0.3128(2)	0.064(2)	0.070(2)	0.058(2)	–0.014(2)	0.012(2)	0.007(2)
C(35)	4*g*		0.2910(2)	0.4233(3)	0.3631(2)	0.081(2)	0.079(2)	0.074(2)	–0.015(2)	0.020(2)	0.020(2)
C(36)	4*g*		0.3426(2)	0.4580(4)	0.4132(2)	0.087(3)	0.091(3)	0.062(2)	–0.005(2)	0.018(2)	0.025(2)
C(37)	4*g*		0.3818(2)	0.5494(3)	0.4149(1)	0.073(2)	0.082(2)	0.046(2)	–0.002(2)	0.007(2)	0.008(2)
C(38)	4*g*		0.3674(2)	0.6075(3)	0.3642(1)	0.054(2)	0.059(2)	0.047(2)	–0.000(1)	0.014(1)	0.001(1)
C(39)	4*g*		0.4622(2)	0.0938(3)	0.5587(1)	0.042(2)	0.054(2)	0.068(2)	–0.001(1)	0.019(1)	–0.013(2)

Table 3. Continued.

Atom	Site	Occ.	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(40)	4*g*		0.4430(2)	0.1174(3)	0.4989(2)	0.053(2)	0.049(2)	0.084(2)	0.003(1)	0.033(2)	0.000(2)
C(41)	4*g*		0.4029(2)	0.0486(3)	0.4555(1)	0.061(2)	0.068(2)	0.059(2)	0.018(2)	0.027(2)	0.004(2)
C(42)	4*g*		0.3784(2)	–0.0484(3)	0.4703(1)	0.056(2)	0.054(2)	0.051(2)	0.004(1)	0.014(1)	–0.014(1)
C(43)	4*g*		0.3970(2)	–0.0792(2)	0.5269(1)	0.056(2)	0.047(2)	0.057(2)	–0.001(1)	0.020(1)	–0.010(1)
C(44)	4*g*		0.4395(2)	–0.0123(3)	0.5685(1)	0.052(2)	0.055(2)	0.051(2)	0.002(1)	0.017(1)	–0.008(1)
C(45)	4*g*		0.0801(2)	1.0445(3)	0.9344(1)	0.063(2)	0.083(2)	0.056(2)	0.013(2)	0.025(2)	0.011(2)
C(46)	4*g*		0.0995(2)	0.9885(3)	0.8916(1)	0.065(2)	0.135(3)	0.045(2)	0.014(2)	0.021(2)	0.009(2)
C(47)	4*g*		0.1580(2)	0.9286(3)	0.9017(2)	0.065(2)	0.102(3)	0.060(2)	–0.006(2)	0.035(2)	–0.011(2)
C(48)	4*g*		0.2046(2)	0.9190(2)	0.9574(1)	0.057(2)	0.053(2)	0.059(2)	–0.005(1)	0.026(2)	–0.001(1)
C(49)	4*g*		0.1908(2)	0.9681(2)	1.0015(1)	0.067(2)	0.050(2)	0.053(2)	0.002(1)	0.018(2)	–0.000(1)
C(50)	4*g*		0.1301(2)	1.0275(2)	0.9905(1)	0.075(2)	0.050(2)	0.053(2)	0.006(2)	0.026(2)	–0.001(1)
O(16)	4*g*	0.50	0.497(3)	0.6220(5)	0.251(2)	0.076(8)	0.089(3)	0.099(4)	0.01(2)	0.007(4)	–0.01(2)
N(18)	4*g*	0.50	0.502(1)	0.4359(6)	0.2479(8)	0.076(4)	0.080(4)	0.099(4)	–0.01(1)	0.009(3)	0.01(1)
C(54)	4*g*	0.50	0.4803(4)	0.5331(9)	0.2598(4)	0.058(5)	0.110(6)	0.078(6)	–0.014(5)	0.006(4)	0.007(6)
C(55)	4*g*	0.50	0.5516(6)	0.429(1)	0.2205(5)	0.107(8)	0.13(1)	0.116(9)	0.023(8)	0.020(7)	–0.005(8)
C(56)	4*g*	0.50	0.4738(7)	0.339(1)	0.2635(7)	0.14(1)	0.103(8)	0.15(1)	–0.035(8)	0.000(9)	0.032(9)

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