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Crystal structures of tetrabutylammonium bis(phthalocyaninato)terbium(III) methanol solvate hydrate (1:1:½), $[N(C_4H_9)_4][Tb(C_8H_4N_2)_2]\cdot CH_3OH\cdot ½\ H_2O$, and tetrabutylammonium bis(phthalocyaninato)dysprosium(III) methanol solvate hydrate (1:1:1), $[N(C_4H_9)_4][Dy(C_8H_4N_2)_2]\cdot CH_3OH\cdot H_2O$

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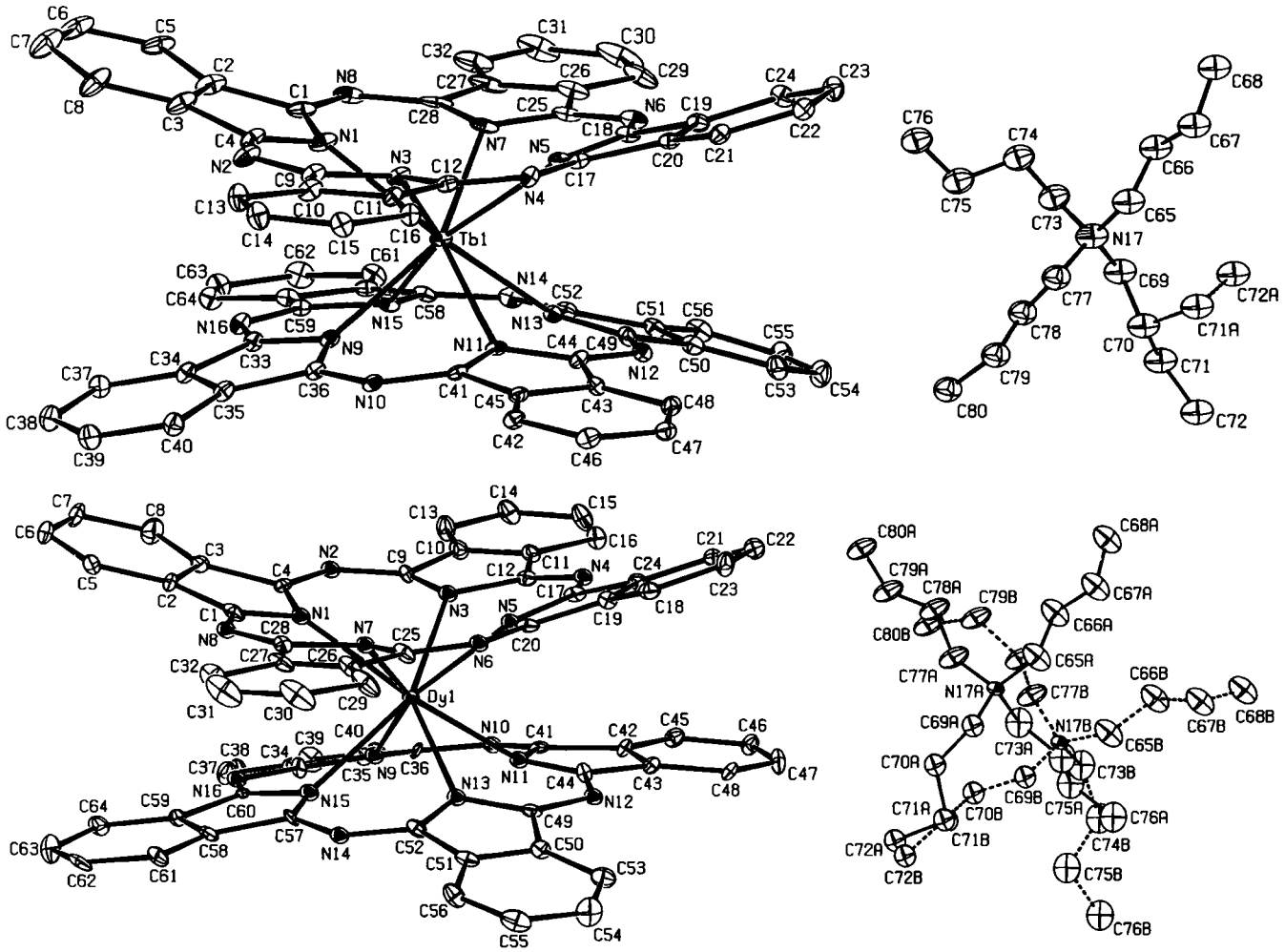

Abstract

$C_{81}H_{75}N_{17}O_{2.50}Tb$, orthorhombic, $Pna2_1$ (no. 33), a = 25.296(2) Å, b = 25.021(2) Å, c = 11.510(1) Å, V = 7285.0 Å^3, Z = 4, $R_{gt}(F)$ = 0.052, $wR_{ref}(F^2)$ = 0.149, T = 153 K.

$C_{81}H_{74}DyN_{17}O_2$, orthorhombic, $Pna2_1$ (no. 33), a = 25.216(2) Å, b = 25.039(2) Å, c = 11.4858(7) Å, V = 7252.0 Å^3, Z = 4, $R_{gt}(F)$ = 0.052, $wR_{ref}(F^2)$ = 0.090, T = 153 K.

Source of material

The title compounds were synthesized as described previously [1] with some minor changes as follows: The crude product (0.201 g, 0.16 mmol) was dissolved in a mixture of acetone/MeOH (8 ml; 1:1, *v*/*v*) at 323 K. After addition of KOH (0.100 g, 1.78 mmol), the solution was filtered hot and an excess of tetrabutylammonium bromide (0.218 g, 0.68 mmol) was added. Crystals were obtained by slow evaporation of the solution at 278 K.

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Experimental details

The Squeeze instruction in PLATON03 [2] was used to calculate the potential solvent accessible volumes in the unit cells; 677 Å^3 and 276 Å^3 were calculated for the Tb and Dy complexes, containing 57 and 36 electrons, respectively. The synthesis and crystallization of the title compounds were carried out in aerobic conditions. Regarding the calculated void and electron count, only very small solvent molecules can be included. Even if methanol or acetone cannot be excluded as additionally crystallized solvent, the probability for water co-crystallization is higher. Therefore, six water molecules (6 × 10 electrons) and four water molecules (4 × 10 electrons), respectively, per unit cell were included in all further calculations and their atomic coordinates were not determined. The different ratio of electron number per volume is probably caused by the different partial disorder which was found in the *tert*-butyl ammonium cations (figure, right). Semi-empirical absorption corrections were applied using MULABS (PLATON [2], $T_{min} = 0.723$, $T_{max} = 0.912$ (Tb); $T_{min} = 0.777$, $T_{max} = 0.793$ (Dy)).

Discussion

A few crystal structures of tetrabutylammonium bis(phthalocyaninato)lanthanide(III) complexes have been published [3,4]. They crystallize either in a tetragonal or a triclinic space group. In contrast, the title compounds crystallize in an orthorhombic space group. The $[NBu_4]^+$cation and the $[Ln^{III}pc_2]^-$ anion, alternate within stacks along the *c* axis. The solvent molecules are located between the columns formed by the stacks. The terbium and dysprosium ions are eight-coordinated by the isoindoline nitrogens (N_{iso}) of the two phthalocyanine rings forming a sandwich structure. The phthalocyanine rings are rotated by 46.7° and 46.6°, respectively, with respect to the others. Therefore, the coordination polyhedron of the metal ion is a slightly distorted square antiprism. The r.m.s. deviations from the least-squares plane through the four coordinating N_{iso} atoms of each ring amount for terbium to only 0.0002 Å and 0.0008 Å, respectively, and for dysprosium to 0.0007 Å and 0.0008 Å, respectively. The terbium ion is displaced almost equidistantly by 1.411 Å and 1.414 Å from these two planes, thus, the interplanar distance is 2.825 Å. The dysprosium ion is displaced by 1.381 Å and 1.404 Å from these two planes, thus, the interplanar distance is 2.785 Å. The coordination of the metal ion leads to a distortion of the phthalocyanine rings. Therefore, the entire macrocycles, defined by the carbon atoms C1 – C32 and the nitrogen atoms N1 – N8, the carbon atoms C33 – C64 and the nitrogen atoms N9 – N16, deviate from least-squares planes by 0.412 Å and 0.333 Å, respectively, for Tb and by 0.429 Å and 0.334 Å, respectively, for Dy. The *Ln*–N_{iso} bond distances range from 2.424(5) Å to 2.444(6) Å with an average of 2.435 Å (Tb) as well as from 2.399(7) Å to 2.435(7) Å with an average of 2.410 Å (Dy), which is comparable to the analogous tetrabutylammonium bis(phthalocyanato)lanthanide(III) complexes, when the difference in the ionic radii is considered [3,4]. The absolute structures were confirmed by the values of the Flack parameter of 0.02(1) (Tb) and –0.02(1) (Dy).

1. Tetrabutylammonium bis(phthalocyaninato)terbium(III) methanol solvate hydrate (1:1:½), $[N(C_4H_9)_4][Tb(C_8H_4N_2)_2]\cdot CH_3OH\cdot \frac{1}{2}H_2O$

Table 1. Data collection and handling.

Crystal:	red block, size 0.15 × 0.20 × 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	10.32 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS I, φ
$2\theta_{max}$:	49.9°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	56025, 12573
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 11320
$N(param)_{refined}$:	824
Programs:	PLATON [2], SHELXS-97 [5], SHELXL-97 [6]

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

Atom	Site	Occ.	*x*	*y*	*z*	U_{iso}
H(5)	4*a*		–0.6196	–0.7160	0.0869	0.082
H(6)	4*a*		–0.6443	–0.6268	0.0939	0.104
H(7)	4*a*		–0.7325	–0.6022	0.0782	0.109
H(8)	4*a*		–0.7977	–0.6628	0.0271	0.096
H(13)	4*a*		–0.9426	–0.7442	–0.0302	0.066
H(14)	4*a*		–1.0330	–0.7694	–0.0365	0.069
H(15)	4*a*		–1.0582	–0.8575	–0.0134	0.059
H(16)	4*a*		–0.9955	–0.9247	0.0220	0.048
H(21)	4*a*		–0.9194	–1.0583	0.1610	0.048
H(22)	4*a*		–0.8995	–1.1414	0.2481	0.059
H(23)	4*a*		–0.8111	–1.1656	0.2824	0.063
H(24)	4*a*		–0.7419	–1.1120	0.2196	0.056
H(29)	4*a*		–0.5917	–1.0415	0.1507	0.088
H(30)	4*a*		–0.5015	–1.0149	0.1573	0.136
H(31)	4*a*		–0.4769	–0.9272	0.1333	0.114
H(32)	4*a*		–0.5385	–0.8629	0.0918	0.099
H(37)	4*a*		–0.7697	–0.6969	–0.3603	0.056
H(38)	4*a*		–0.8458	–0.6535	–0.4311	0.063
H(39)	4*a*		–0.9277	–0.6988	–0.4326	0.065
H(40)	4*a*		–0.9357	–0.7839	–0.3629	0.056
H(45)	4*a*		–0.9878	–0.9455	–0.2583	0.047
H(46)	4*a*		–1.0304	–1.0283	–0.2562	0.056
H(47)	4*a*		–0.9835	–1.1061	–0.2204	0.050
H(48)	4*a*		–0.8944	–1.1044	–0.1864	0.049
H(53)	4*a*		–0.7353	–1.1476	–0.1816	0.062
H(54)	4*a*		–0.6538	–1.1927	–0.2046	0.075
H(55)	4*a*		–0.5747	–1.1467	–0.2041	0.070
H(56)	4*a*		–0.5722	–1.0544	–0.1808	0.063
H(61)	4*a*		–0.5260	–0.8942	–0.1953	0.057
H(62)	4*a*		–0.4802	–0.8166	–0.2407	0.072
H(63)	4*a*		–0.5244	–0.7375	–0.2895	0.066
H(64)	4*a*		–0.6172	–0.7349	–0.2930	0.054
H(65A)	4*a*		–0.7081	–0.8451	–0.4838	0.117
H(65B)	4*a*		–0.7601	–0.8102	–0.4992	0.117
H(66A)	4*a*		–0.6746	–0.8084	–0.6637	0.117
H(66B)	4*a*		–0.7257	–0.7703	–0.6690	0.117
H(67A)	4*a*		–0.7017	–0.7398	–0.4743	0.117

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(67B)	4*a*		−0.6467	−0.7704	−0.4912	0.117
H(68C)	4*a*		−0.6505	−0.6744	−0.5345	0.146
H(68B)	4*a*		−0.6762	−0.6930	−0.6549	0.146
H(68A)	4*a*		−0.6179	−0.7121	−0.6209	0.146
H(69A)	4*a*		−0.6935	−0.9076	−0.6763	0.117
H(69B)	4*a*		−0.7453	−0.9422	−0.7016	0.117
H(70A)	4*a*	0.5	−0.7414	−0.9719	−0.5007	0.117
H(70B)	4*a*	0.5	−0.6841	−0.9444	−0.4937	0.117
H(70C)	4*a*	0.5	−0.6977	−0.9957	−0.5792	0.117
H(70D)	4*a*	0.5	−0.7390	−0.9681	−0.4910	0.117
H(71A)	4*a*	0.5	−0.7144	−1.0295	−0.6448	0.117
H(71B)	4*a*	0.5	−0.6613	−0.9969	−0.6661	0.117
H(72C)	4*a*	0.5	−0.6723	−1.0853	−0.5378	0.146
H(72B)	4*a*	0.5	−0.6555	−1.0387	−0.4503	0.146
H(72A)	4*a*	0.5	−0.6188	−1.0527	−0.5595	0.146
H(71C)	4*a*	0.5	−0.6503	−0.9533	−0.4263	0.117
H(71D)	4*a*	0.5	−0.6806	−0.8983	−0.4515	0.117
H(72D)	4*a*	0.5	−0.6371	−0.8869	−0.6248	0.146
H(72E)	4*a*	0.5	−0.6148	−0.9467	−0.6223	0.146
H(72F)	4*a*	0.5	−0.5924	−0.9032	−0.5331	0.146
H(73A)	4*a*		−0.8067	−0.8871	−0.7440	0.129

Table 2. Continued.

Atom	Site	Occ.	x	y	z	U_{iso}
H(73B)	4*a*		−0.7601	−0.8453	−0.7649	0.129
H(74A)	4*a*		−0.8216	−0.7843	−0.7549	0.129
H(74B)	4*a*		−0.8194	−0.7930	−0.6168	0.129
H(75A)	4*a*		−0.8878	−0.8559	−0.7646	0.129
H(75B)	4*a*		−0.8887	−0.8567	−0.6257	0.129
H(76C)	4*a*		−0.9611	−0.8064	−0.7106	0.161
H(76B)	4*a*		−0.9188	−0.7635	−0.7549	0.161
H(76A)	4*a*		−0.9277	−0.7724	−0.6186	0.161
H(77A)	4*a*		−0.8287	−0.8777	−0.5069	0.112
H(77B)	4*a*		−0.7838	−0.9154	−0.4524	0.112
H(78A)	4*a*		−0.8449	−0.9405	−0.6590	0.112
H(78B)	4*a*		−0.7956	−0.9767	−0.6175	0.112
H(79A)	4*a*		−0.8764	−0.9485	−0.4595	0.112
H(79B)	4*a*		−0.8340	−0.9948	−0.4440	0.112
H(80C)	4*a*		−0.9109	−1.0376	−0.4646	0.141
H(80B)	4*a*		−0.8836	−1.0442	−0.5892	0.141
H(80A)	4*a*		−0.9292	−1.0006	−0.5707	0.141
H(81C)	4*a*		−1.0297	−0.8730	−0.4845	0.091
H(81B)	4*a*		−0.9790	−0.9096	−0.4605	0.091
H(81A)	4*a*		−0.9715	−0.8485	−0.4976	0.091
H(1)	4*a*		−0.9635	−0.8584	−0.3058	0.074

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}
C(1)	4*a*		−0.6931(3)	−0.8018(4)	0.0359(6)	0.040(5)	0.083(6)	0.026(4)	−0.022(4)	0.008(3)	−0.012(4)
C(2)	4*a*		−0.6947(4)	−0.7435(4)	0.0465(7)	0.049(5)	0.086(7)	0.046(4)	−0.033(5)	0.019(4)	−0.021(4)
C(3)	4*a*		−0.7474(4)	−0.7291(4)	0.0295(9)	0.047(5)	0.075(6)	0.060(6)	−0.030(4)	0.018(4)	−0.032(5)
C(4)	4*a*		−0.7773(3)	−0.7775(3)	0.0098(7)	0.038(4)	0.051(4)	0.046(4)	−0.016(4)	0.015(3)	−0.023(3)
C(5)	4*a*		−0.6552(4)	−0.7055(5)	0.0737(7)	0.060(5)	0.104(8)	0.041(4)	−0.046(6)	0.010(4)	−0.029(5)
C(6)	4*a*		−0.6702(5)	−0.6536(5)	0.080(1)	0.084(8)	0.11(1)	0.071(7)	−0.056(8)	0.029(6)	−0.050(7)
C(7)	4*a*		−0.7232(5)	−0.6387(5)	0.067(1)	0.090(8)	0.084(8)	0.100(9)	−0.040(7)	0.035(7)	−0.045(7)
C(8)	4*a*		−0.7623(4)	−0.6741(4)	0.039(1)	0.067(7)	0.074(7)	0.098(8)	−0.028(5)	0.043(6)	−0.048(6)
C(9)	4*a*		−0.8584(3)	−0.8211(3)	0.0019(7)	0.026(3)	0.051(4)	0.046(4)	−0.008(3)	0.011(3)	−0.014(3)
C(10)	4*a*		−0.9166(3)	−0.8223(3)	−0.0028(7)	0.030(4)	0.057(5)	0.053(5)	−0.001(3)	0.010(3)	−0.013(4)
C(11)	4*a*		−0.9314(3)	−0.8742(3)	0.0149(6)	0.033(4)	0.037(4)	0.040(4)	−0.003(3)	0.006(3)	−0.008(3)
C(12)	4*a*		−0.8836(3)	−0.9054(3)	0.0319(7)	0.024(4)	0.050(5)	0.031(4)	0.000(3)	0.004(3)	−0.011(3)
C(13)	4*a*		−0.9534(3)	−0.7803(3)	−0.0209(8)	0.045(5)	0.044(4)	0.076(5)	0.008(4)	0.016(4)	0.009(4)
C(14)	4*a*		−1.0066(3)	−0.7958(4)	−0.0240(8)	0.042(4)	0.054(5)	0.076(5)	0.013(4)	0.012(4)	0.012(4)
C(15)	4*a*		−1.0217(3)	−0.8485(3)	−0.0094(7)	0.031(4)	0.056(5)	0.061(5)	0.001(3)	0.001(3)	0.009(4)
C(16)	4*a*		−0.9848(3)	−0.8886(3)	0.0110(7)	0.028(4)	0.044(4)	0.049(4)	0.001(3)	0.010(3)	0.002(3)
C(17)	4*a*		−0.8405(2)	−0.9836(3)	0.0849(6)	0.023(3)	0.045(4)	0.028(3)	−0.004(3)	0.002(3)	−0.011(3)
C(18)	4*a*		−0.8425(3)	−1.0376(3)	0.1369(6)	0.035(4)	0.045(4)	0.025(3)	0.003(3)	0.005(3)	−0.006(3)
C(19)	4*a*		−0.7898(3)	−1.0519(3)	0.1533(6)	0.036(4)	0.054(4)	0.031(3)	0.005(3)	0.006(3)	−0.002(3)
C(20)	4*a*		−0.7569(3)	−1.0090(3)	0.1090(6)	0.022(3)	0.063(5)	0.026(3)	0.002(3)	−0.001(3)	−0.002(3)
C(21)	4*a*		−0.8838(3)	−1.0692(3)	0.1721(6)	0.038(4)	0.040(4)	0.044(4)	−0.001(3)	0.005(3)	−0.008(3)
C(22)	4*a*		−0.8718(3)	−1.1181(3)	0.2249(7)	0.050(5)	0.048(4)	0.050(4)	0.001(4)	0.001(4)	−0.003(4)
C(23)	4*a*		−0.8186(4)	−1.1329(3)	0.2439(8)	0.052(5)	0.047(5)	0.060(5)	0.006(4)	0.011(4)	0.004(4)
C(24)	4*a*		−0.7775(3)	−1.1012(3)	0.2081(7)	0.031(4)	0.061(5)	0.047(4)	0.012(3)	−0.002(3)	0.006(4)
C(25)	4*a*		−0.6748(3)	−0.9665(4)	0.0948(6)	0.028(4)	0.096(7)	0.019(3)	−0.005(4)	−0.001(3)	0.000(4)
C(26)	4*a*		−0.6181(3)	−0.9658(5)	0.1116(6)	0.023(4)	0.120(8)	0.028(4)	0.001(5)	0.001(3)	0.011(4)
C(27)	4*a*		−0.6025(3)	−0.9118(5)	0.0926(7)	0.024(4)	0.17(1)	0.025(4)	−0.015(5)	−0.009(3)	0.012(5)
C(28)	4*a*		−0.6495(3)	−0.8829(5)	0.0685(6)	0.027(4)	0.129(9)	0.010(3)	−0.017(5)	0.001(3)	−0.004(4)
C(29)	4*a*		−0.5815(3)	−1.0055(5)	0.1374(8)	0.036(5)	0.138(9)	0.046(5)	0.007(5)	−0.005(4)	0.037(6)
C(30)	4*a*		−0.5281(4)	−0.9889(8)	0.1425(9)	0.023(5)	0.26(2)	0.056(6)	0.021(8)	−0.009(4)	0.050(9)
C(31)	4*a*		−0.5131(4)	−0.9368(7)	0.127(1)	0.020(5)	0.20(2)	0.062(6)	−0.017(7)	−0.007(4)	0.033(8)
C(32)	4*a*		−0.5495(4)	−0.8989(6)	0.1024(8)	0.035(5)	0.17(1)	0.044(5)	−0.028(6)	−0.010(4)	0.009(6)
C(33)	4*a*		−0.7713(3)	−0.8019(3)	−0.2683(6)	0.028(3)	0.036(4)	0.043(4)	−0.002(3)	−0.004(3)	−0.003(3)
C(34)	4*a*		−0.8098(3)	−0.7656(3)	−0.3164(7)	0.042(4)	0.034(4)	0.050(4)	0.004(3)	0.001(3)	−0.011(3)
C(35)	4*a*		−0.8582(3)	−0.7919(3)	−0.3171(6)	0.026(3)	0.040(4)	0.048(4)	0.007(3)	0.004(3)	−0.012(3)
C(36)	4*a*		−0.8480(3)	−0.8453(3)	−0.2680(6)	0.026(3)	0.037(4)	0.040(4)	0.004(3)	−0.004(3)	−0.009(3)
C(37)	4*a*		−0.8032(3)	−0.7140(3)	−0.3599(7)	0.039(4)	0.046(4)	0.055(4)	−0.002(3)	−0.005(3)	0.002(4)

Table 3. Continued.

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(38)	4a		−0.8480(3)	−0.6890(3)	−0.4022(8)	0.042(4)	0.045(4)	0.070(6)	0.009(4)	0.001(4)	−0.001(4)
C(39)	4a		−0.8974(3)	−0.7164(3)	−0.4025(8)	0.041(4)	0.055(5)	0.066(5)	0.012(4)	−0.004(4)	0.005(4)
C(40)	4a		−0.9024(3)	−0.7663(3)	−0.3615(7)	0.038(4)	0.043(4)	0.059(5)	0.004(3)	−0.009(4)	0.000(4)
C(41)	4a		−0.8740(3)	−0.9340(3)	−0.2247(6)	0.028(4)	0.036(4)	0.029(3)	−0.007(3)	−0.005(3)	−0.011(3)
C(42)	4a		−0.9135(3)	−0.9757(3)	−0.2269(6)	0.039(4)	0.037(4)	0.027(3)	−0.009(3)	−0.003(3)	−0.006(3)
C(43)	4a		−0.8863(2)	−1.0224(3)	−0.2027(6)	0.024(3)	0.036(3)	0.034(3)	0.002(3)	−0.001(3)	0.006(3)
C(44)	4a		−0.8318(3)	−1.0072(3)	−0.1875(6)	0.030(4)	0.034(4)	0.036(4)	−0.001(3)	0.004(3)	−0.009(3)
C(45)	4a		−0.9683(3)	−0.9774(3)	−0.2449(6)	0.031(4)	0.045(4)	0.042(4)	−0.003(3)	−0.008(3)	−0.007(3)
C(46)	4a		−0.9934(3)	−1.0264(3)	−0.2427(7)	0.030(4)	0.059(5)	0.051(4)	−0.005(3)	−0.009(3)	−0.008(4)
C(47)	4a		−0.9653(3)	−1.0729(3)	−0.2211(6)	0.043(4)	0.046(4)	0.036(4)	−0.005(3)	−0.002(3)	−0.004(3)
C(48)	4a		−0.9131(3)	−1.0722(3)	−0.2012(6)	0.044(4)	0.039(4)	0.040(4)	−0.007(3)	0.005(3)	−0.003(3)
C(49)	4a		−0.7427(3)	−1.0324(3)	−0.1706(6)	0.038(4)	0.038(4)	0.036(4)	0.017(3)	0.001(3)	0.006(3)
C(50)	4a		−0.7011(3)	−1.0730(3)	−0.1775(6)	0.041(4)	0.059(5)	0.035(4)	0.019(4)	0.004(3)	0.002(3)
C(51)	4a		−0.6530(3)	−1.0462(3)	−0.1787(6)	0.032(4)	0.054(4)	0.034(3)	0.012(3)	0.009(3)	0.010(3)
C(52)	4a		−0.6662(3)	−0.9895(3)	−0.1746(6)	0.030(4)	0.051(4)	0.030(3)	0.005(3)	0.008(3)	0.000(3)
C(53)	4a		−0.7029(3)	−1.1285(3)	−0.1846(8)	0.045(5)	0.051(5)	0.060(5)	0.010(4)	−0.011(4)	0.010(4)
C(54)	4a		−0.6542(4)	−1.1549(4)	−0.1963(9)	0.063(6)	0.048(5)	0.077(6)	0.018(4)	−0.005(5)	−0.001(4)
C(55)	4a		−0.6069(4)	−1.1273(3)	−0.1961(8)	0.052(5)	0.051(5)	0.072(6)	0.017(4)	0.007(4)	0.008(4)
C(56)	4a		−0.6049(3)	−1.0731(4)	−0.1846(7)	0.034(4)	0.075(6)	0.048(5)	0.011(4)	0.008(3)	0.011(4)
C(57)	4a		−0.6400(3)	−0.8987(3)	−0.1972(7)	0.026(4)	0.057(5)	0.021(4)	0.001(3)	0.001(3)	0.007(3)
C(58)	4a		−0.5998(3)	−0.8606(3)	−0.2173(6)	0.036(4)	0.056(4)	0.027(3)	−0.002(3)	0.005(3)	−0.006(3)
C(59)	4a		−0.6266(3)	−0.8143(3)	−0.2426(6)	0.028(4)	0.057(5)	0.032(4)	−0.004(3)	0.001(3)	−0.002(3)
C(60)	4a		−0.6824(3)	−0.8248(3)	−0.2357(6)	0.018(3)	0.047(4)	0.028(3)	−0.004(3)	−0.001(3)	−0.003(3)
C(61)	4a		−0.5443(3)	−0.8624(3)	−0.2149(7)	0.029(4)	0.064(5)	0.049(4)	−0.005(4)	0.010(3)	0.009(4)
C(62)	4a		−0.5177(3)	−0.8164(4)	−0.2417(8)	0.021(4)	0.089(7)	0.070(6)	−0.005(4)	0.005(4)	0.004(5)
C(63)	4a		−0.5443(3)	−0.7686(4)	−0.2709(8)	0.039(4)	0.060(5)	0.065(5)	−0.008(4)	0.005(4)	0.007(4)
C(64)	4a		−0.5989(3)	−0.7667(3)	−0.2726(7)	0.034(4)	0.052(4)	0.050(4)	−0.008(3)	0.005(3)	0.003(3)
N(1)	4a		−0.7434(2)	−0.8202(3)	0.0129(6)	0.031(3)	0.068(4)	0.040(3)	−0.023(3)	0.009(3)	−0.022(3)
N(2)	4a		−0.8291(3)	−0.7773(3)	0.0001(6)	0.036(3)	0.062(4)	0.054(4)	−0.012(3)	0.019(3)	−0.025(3)
N(3)	4a		−0.8407(2)	−0.8733(2)	0.0164(5)	0.019(3)	0.047(3)	0.041(3)	−0.004(2)	0.009(2)	−0.017(3)
N(4)	4a		−0.8846(2)	−0.9561(2)	0.0637(6)	0.021(3)	0.033(3)	0.047(3)	−0.004(3)	0.004(2)	−0.006(3)
N(5)	4a		−0.7892(2)	−0.9704(2)	0.0656(5)	0.030(3)	0.052(3)	0.024(3)	−0.002(3)	0.001(2)	−0.004(2)
N(6)	4a		−0.7040(2)	−1.0093(3)	0.1144(5)	0.022(3)	0.082(5)	0.032(3)	0.006(3)	−0.001(2)	0.001(3)
N(7)	4a		−0.6918(2)	−0.9167(3)	0.0625(5)	0.022(3)	0.088(5)	0.020(3)	−0.013(3)	−0.005(2)	0.005(3)
N(8)	4a		−0.6504(3)	−0.8281(4)	0.0551(5)	0.027(4)	0.104(6)	0.027(3)	−0.032(4)	−0.003(3)	0.000(4)
N(9)	4a		−0.7959(2)	−0.8490(2)	−0.2372(5)	0.025(3)	0.033(3)	0.036(3)	0.000(2)	−0.005(2)	−0.008(2)
N(10)	4a		−0.8850(2)	−0.8825(2)	−0.2587(5)	0.030(3)	0.037(3)	0.036(3)	0.002(3)	−0.007(2)	−0.011(3)
N(11)	4a		−0.8265(2)	−0.9540(2)	−0.1956(4)	0.019(3)	0.046(3)	0.025(3)	−0.002(2)	−0.007(2)	−0.008(2)
N(12)	4a		−0.7931(2)	−1.0447(2)	−0.1729(5)	0.027(3)	0.041(3)	0.035(3)	−0.004(2)	−0.004(2)	0.004(2)
N(13)	4a		−0.7192(2)	−0.9829(2)	−0.1664(5)	0.028(3)	0.038(3)	0.028(3)	0.006(2)	0.003(2)	0.000(2)
N(14)	4a		−0.6288(2)	−0.9523(3)	−0.1833(5)	0.026(3)	0.062(4)	0.036(3)	0.000(3)	0.004(2)	0.005(3)
N(15)	4a		−0.6885(2)	−0.8786(3)	−0.2048(5)	0.029(3)	0.051(4)	0.027(3)	−0.003(3)	0.009(2)	0.004(3)
N(16)	4a		−0.7191(2)	−0.7908(2)	−0.2628(6)	0.028(3)	0.036(3)	0.053(4)	−0.003(3)	0.006(3)	−0.009(3)
Tb(1)	4a		−0.761814(9)	−0.90525(1)	−0.08085(5)	0.0199(2)	0.0492(2)	0.0250(1)	−0.0033(1)	0.0005(2)	−0.0082(2)
N(17)	4a		−0.7598(4)	−0.8768(3)	−0.6002(8)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(65)	4a		−0.7328(6)	−0.8303(5)	−0.5423(9)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(66)	4a		−0.7016(6)	−0.7898(4)	−0.6163(8)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(67)	4a		−0.6754(6)	−0.7514(4)	−0.5328(9)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(68)	4a		−0.6531(5)	−0.7037(4)	−0.591(1)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(69)	4a		−0.7259(6)	−0.9224(5)	−0.6405(9)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(70)	4a		−0.7100(6)	−0.9612(5)	−0.5467(8)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(71)	4a	0.5	−0.686(1)	−1.0100(7)	−0.605(2)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(72)	4a	0.5	−0.655(1)	−1.0502(9)	−0.532(2)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(71A)	4a	0.5	−0.6661(8)	−0.931(1)	−0.488(2)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(72A)	4a	0.5	−0.624(1)	−0.9156(9)	−0.575(2)	0.147(4)	0.083(3)	0.062(2)	0.004(3)	0.004(2)	−0.003(2)
C(73)	4a		−0.7874(6)	−0.8568(6)	−0.709(1)	0.131(6)	0.104(5)	0.087(4)	0.009(4)	0.006(4)	0.019(4)
C(74)	4a		−0.8261(5)	−0.8109(5)	−0.692(1)	0.131(6)	0.104(5)	0.087(4)	0.009(4)	0.006(4)	0.019(4)
C(75)	4a		−0.8836(5)	−0.8335(5)	−0.694(1)	0.131(6)	0.104(5)	0.087(4)	0.009(4)	0.006(4)	0.019(4)
C(76)	4a		−0.9267(6)	−0.7900(5)	−0.695(1)	0.131(6)	0.104(5)	0.087(4)	0.009(4)	0.006(4)	0.019(4)
C(77)	4a		−0.8002(5)	−0.9034(4)	−0.526(1)	0.119(5)	0.085(4)	0.077(4)	−0.006(3)	−0.014(4)	0.004(3)
C(78)	4a		−0.8238(5)	−0.9521(4)	−0.591(1)	0.119(5)	0.085(4)	0.077(4)	−0.006(3)	−0.014(4)	0.004(3)
C(79)	4a		−0.8578(5)	−0.9776(5)	−0.501(1)	0.119(5)	0.085(4)	0.077(4)	−0.006(3)	−0.014(4)	0.004(3)
C(80)	4a		−0.8990(5)	−1.0186(5)	−0.534(1)	0.119(5)	0.085(4)	0.077(4)	−0.006(3)	−0.014(4)	0.004(3)
C(81)	4a		−0.9936(4)	−0.8735(5)	−0.4536(9)	0.065(6)	0.094(8)	0.068(6)	−0.002(6)	−0.020(5)	−0.006(6)
O(1)	4a		−0.9944(2)	−0.8578(3)	−0.3325(6)	0.044(3)	0.066(4)	0.074(4)	0.007(3)	−0.015(3)	−0.005(3)

2. Tetrabutylammonium bis(phthalocyaninato)dysprosium(III) methanol solvate hydrate (1:1:1), $[N(C_4H_9)_4][Dy(C_8H_4N_2)_2]\cdot CH_3OH\cdot H_2O$

Table 4. Data collection and handling.

Crystal:	red block, size 0.20 × 0.25 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	10.91 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS I, φ
$2\theta_{max}$:	58.56°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	45876, 16326
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 6870
$N(param)_{refined}$:	786
Programs:	PLATON [2], SHELXS-97 [5], SHELXL-97 [6]

Table 5. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{iso}
H(5A)	4a		−0.3808	−0.2809	−0.0941	0.091
H(6A)	4a		−0.3576	−0.3698	−0.1046	0.094
H(7A)	4a		−0.2696	−0.3958	−0.0775	0.136
H(8A)	4a		−0.2053	−0.3343	−0.0262	0.113
H(13A)	4a		−0.0590	−0.2546	0.0314	0.077
H(14A)	4a		0.0303	−0.2316	0.0324	0.072
H(15A)	4a		0.0577	−0.1444	0.0105	0.073
H(16A)	4a		−0.0035	−0.0750	−0.0214	0.056
H(21A)	4a		−0.0793	0.0621	−0.1561	0.049
H(22A)	4a		−0.0993	0.1418	−0.2477	0.066
H(23A)	4a		−0.1874	0.1681	−0.2855	0.070
H(24A)	4a		−0.2575	0.1115	−0.2222	0.059
H(29A)	4a		−0.4080	0.0459	−0.1446	0.099
H(30A)	4a		−0.4993	0.0195	−0.1599	0.127
H(31A)	4a		−0.5246	−0.0679	−0.1313	0.150
H(32A)	4a		−0.4637	−0.1320	−0.0833	0.095
H(37A)	4a		−0.2315	−0.3014	0.3582	0.066
H(38A)	4a		−0.1570	−0.3422	0.4427	0.067
H(39A)	4a		−0.0756	−0.3022	0.4284	0.069
H(40A)	4a		−0.0660	−0.2144	0.3637	0.055
H(45A)	4a		−0.0121	−0.0542	0.2623	0.055
H(46A)	4a		0.0310	0.0275	0.2578	0.053
H(47A)	4a		−0.0144	0.1056	0.2209	0.066
H(48A)	4a		−0.1059	0.1054	0.1828	0.051
H(53A)	4a		−0.2649	0.1501	0.1927	0.070
H(54A)	4a		−0.3457	0.1954	0.1998	0.093
H(55A)	4a		−0.4252	0.1503	0.1979	0.089
H(56A)	4a		−0.4280	0.0580	0.1865	0.069
H(61A)	4a		−0.4769	−0.1024	0.2012	0.058
H(62A)	4a		−0.5217	−0.1815	0.2381	0.067
H(63A)	4a		−0.4787	−0.2586	0.2846	0.077
H(64A)	4a		−0.3857	−0.2623	0.2859	0.061
H(65A)	4a	0.523	0.3452	0.0541	−0.0871	0.124
H(65B)	4a	0.523	0.3179	0.1083	−0.0421	0.124
H(65C)	4a	0.477	0.2414	0.1910	0.0218	0.124
H(65D)	4a	0.477	0.2871	0.1552	−0.0318	0.124
H(66A)	4a	0.523	0.3655	0.0982	0.1422	0.124
H(66B)	4a	0.523	0.3955	0.0472	0.0885	0.124
H(66C)	4a	0.477	0.3033	0.2201	0.1783	0.124
H(66D)	4a	0.477	0.3495	0.1863	0.1163	0.124
H(67A)	4a	0.523	0.4198	0.1066	−0.0670	0.124
H(67B)	4a	0.523	0.4030	0.1534	0.0196	0.124
H(67C)	4a	0.477	0.3521	0.2409	−0.0391	0.124
H(67D)	4a	0.477	0.2936	0.2634	−0.0156	0.124
H(68A)	4a	0.523	0.4679	0.0926	0.1285	0.155
H(68B)	4a	0.523	0.4755	0.1531	0.0868	0.155
H(68C)	4a	0.523	0.4919	0.1050	0.0023	0.155
H(68D)	4a	0.477	0.3211	0.3071	0.1354	0.155
H(68E)	4a	0.477	0.3571	0.3217	0.0251	0.155
H(68F)	4a	0.477	0.3791	0.2817	0.1226	0.155
H(69A)	4a	0.523	0.2369	0.0583	−0.0884	0.086
H(69B)	4a	0.523	0.2654	0.0020	−0.1061	0.086
H(69C)	4a	0.477	0.2247	0.0790	−0.0470	0.086
H(69D)	4a	0.477	0.1808	0.1196	−0.0007	0.086
H(70A)	4a	0.523	0.2077	−0.0255	0.0591	0.086
H(70B)	4a	0.523	0.1883	−0.0289	−0.0718	0.086
H(70C)	4a	0.477	0.2010	0.0177	0.1161	0.086
H(70D)	4a	0.477	0.1527	0.0571	0.1468	0.086
H(71A)	4a	0.523	0.1463	0.0430	0.1011	0.086
H(71B)	4a	0.523	0.1304	0.0479	−0.0349	0.086
H(71C)	4a	0.477	0.1679	−0.0042	−0.0527	0.086
H(71D)	4a	0.477	0.1330	0.0486	−0.0612	0.086
H(72A)	4a	0.523	0.1011	−0.0389	−0.0404	0.107
H(72B)	4a	0.523	0.0763	−0.0156	0.0774	0.107
H(72C)	4a	0.523	0.1282	−0.0524	0.0822	0.107
H(72D)	4a	0.477	0.1073	−0.0426	0.0672	0.107
H(72E)	4a	0.477	0.0786	−0.0219	−0.0485	0.107
H(72F)	4a	0.477	0.0732	0.0113	0.0699	0.107
H(73A)	4a	0.523	0.2274	0.0508	0.1725	0.116
H(73B)	4a	0.523	0.2810	0.0805	0.2079	0.116
H(73C)	4a	0.477	0.2235	0.1213	0.2681	0.116
H(73D)	4a	0.477	0.2559	0.1730	0.2325	0.116
H(74A)	4a	0.523	0.2606	0.1525	0.0795	0.116
H(74B)	4a	0.523	0.2074	0.1219	0.0378	0.116
H(74C)	4a	0.477	0.1823	0.2106	0.1567	0.116
H(74D)	4a	0.477	0.1779	0.1980	0.2915	0.116
H(75A)	4a	0.523	0.1771	0.1175	0.2379	0.116
H(75B)	4a	0.523	0.2307	0.1474	0.2804	0.116
H(75C)	4a	0.477	0.1171	0.1435	0.1171	0.116
H(75D)	4a	0.477	0.1118	0.1327	0.2542	0.116
H(76A)	4a	0.523	0.1751	0.1920	0.0906	0.145
H(76B)	4a	0.523	0.2102	0.2228	0.1853	0.145
H(76C)	4a	0.523	0.1515	0.2034	0.2176	0.145
H(76D)	4a	0.477	0.0762	0.2164	0.2867	0.145
H(76E)	4a	0.477	0.0457	0.1947	0.1740	0.145
H(76F)	4a	0.477	0.0930	0.2369	0.1599	0.145
H(77A)	4a	0.523	0.2762	−0.0347	0.1065	0.122
H(77B)	4a	0.523	0.3207	−0.0028	0.1764	0.122
H(77C)	4a	0.477	0.2694	0.0487	0.1591	0.122
H(77D)	4a	0.477	0.3112	0.0946	0.1856	0.122
H(78A)	4a	0.523	0.3426	−0.0507	−0.0546	0.122
H(78B)	4a	0.523	0.3873	−0.0236	0.0270	0.122
H(78C)	4a	0.477	0.3530	0.0844	0.0097	0.122
H(78D)	4a	0.477	0.3038	0.0540	−0.0467	0.122
H(79A)	4a	0.523	0.3687	−0.0863	0.1776	0.122
H(79B)	4a	0.523	0.3219	−0.1119	0.1017	0.122
H(79C)	4a	0.477	0.3598	−0.0143	−0.0313	0.122
H(79D)	4a	0.477	0.3900	0.0104	0.0771	0.122
H(80A)	4a	0.523	0.3834	−0.1438	−0.0313	0.153
H(80B)	4a	0.523	0.3969	−0.1655	0.0964	0.153
H(80C)	4a	0.523	0.4304	−0.1173	0.0422	0.153
H(80D)	4a	0.477	0.3456	−0.0399	0.2055	0.153
H(80E)	4a	0.477	0.3455	−0.0792	0.0956	0.153
H(80F)	4a	0.477	0.2940	−0.0445	0.1251	0.153
H(81A)	4a		0.0183	0.0914	−0.0292	0.186
H(81B)	4a		−0.0273	0.1346	−0.0066	0.186
H(81C)	4a		0.0337	0.1519	0.0004	0.186
H(1)	4a		0.0383	0.1401	−0.1896	0.098

Table 6. 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}
C(1)	4a		−0.3079(4)	−0.1957(6)	−0.0375(9)	0.042(5)	0.10(1)	0.023(6)	−0.022(6)	0.001(4)	0.010(7)
C(2)	4a		−0.3069(4)	−0.2531(5)	−0.048(1)	0.077(7)	0.064(9)	0.070(9)	−0.048(6)	0.033(6)	−0.039(7)
C(3)	4a		−0.2542(3)	−0.2695(4)	−0.0302(8)	0.045(6)	0.080(8)	0.060(6)	−0.027(5)	0.025(4)	−0.032(6)
C(4)	4a		−0.2245(3)	−0.2200(4)	−0.0074(8)	0.037(4)	0.057(7)	0.033(6)	−0.014(4)	0.006(4)	−0.020(5)
C(5)	4a		−0.3454(4)	−0.2915(5)	−0.0789(9)	0.090(7)	0.09(1)	0.046(7)	−0.057(7)	0.017(5)	−0.009(8)
C(6)	4a		−0.3315(5)	−0.3437(6)	−0.087(1)	0.078(9)	0.08(1)	0.07(1)	−0.053(9)	0.010(7)	−0.03(1)
C(7)	4a		−0.2790(5)	−0.3592(5)	−0.069(1)	0.106(9)	0.09(1)	0.14(1)	−0.065(8)	0.062(8)	−0.08(1)
C(8)	4a		−0.2407(4)	−0.3230(4)	−0.040(1)	0.070(6)	0.071(8)	0.14(1)	−0.008(7)	0.043(7)	−0.052(8)
C(9)	4a		−0.1430(3)	−0.1766(4)	0.0014(8)	0.032(4)	0.056(7)	0.052(7)	−0.021(4)	0.019(4)	−0.010(6)
C(10)	4a		−0.0846(3)	−0.1774(4)	0.0034(9)	0.041(4)	0.042(6)	0.058(7)	0.003(4)	0.017(4)	−0.001(5)
C(11)	4a		−0.0686(3)	−0.1258(4)	−0.0130(8)	0.026(4)	0.044(6)	0.047(6)	0.006(4)	0.010(4)	−0.001(5)
C(12)	4a		−0.1166(3)	−0.0907(5)	−0.0292(8)	0.027(4)	0.058(7)	0.027(6)	0.005(5)	−0.004(3)	−0.005(7)
C(13)	4a		−0.0480(3)	−0.2186(4)	0.0208(9)	0.043(4)	0.045(6)	0.10(1)	−0.002(4)	0.020(4)	−0.003(6)
C(14)	4a		0.0043(3)	−0.2046(4)	0.0217(9)	0.038(4)	0.061(7)	0.082(8)	0.011(4)	0.016(4)	0.015(6)
C(15)	4a		0.0208(3)	−0.1522(4)	0.0075(9)	0.023(4)	0.070(8)	0.089(8)	0.006(4)	0.006(4)	0.026(6)
C(16)	4a		−0.0147(2)	−0.1109(3)	−0.0109(8)	0.025(3)	0.047(7)	0.067(7)	0.008(3)	−0.001(3)	0.005(5)
C(17)	4a		−0.1595(3)	−0.0131(4)	−0.0844(9)	0.014(4)	0.059(7)	0.044(6)	0.019(4)	0.005(4)	−0.018(6)
C(18)	4a		−0.1566(3)	0.0396(4)	−0.1372(8)	0.040(4)	0.035(6)	0.039(6)	0.005(4)	0.008(4)	0.001(5)
C(19)	4a		−0.2096(3)	0.0556(4)	−0.1549(8)	0.034(4)	0.039(6)	0.038(6)	0.007(4)	−0.001(4)	0.004(5)
C(20)	4a		−0.2427(3)	0.0118(4)	−0.1073(7)	0.037(4)	0.068(6)	0.021(4)	0.012(4)	0.001(4)	−0.007(4)
C(21)	4a		−0.1151(3)	0.0721(4)	−0.1702(8)	0.040(4)	0.039(6)	0.044(6)	−0.002(4)	0.008(4)	−0.009(5)
C(22)	4a		−0.1274(3)	0.1190(4)	−0.224(1)	0.055(5)	0.049(7)	0.060(8)	0.001(5)	0.008(5)	−0.002(6)
C(23)	4a		−0.1802(4)	0.1355(5)	−0.247(1)	0.049(6)	0.037(7)	0.09(1)	−0.002(5)	0.007(6)	−0.006(7)
C(24)	4a		−0.2216(3)	0.1018(4)	−0.2092(8)	0.041(4)	0.069(8)	0.038(5)	0.001(5)	0.000(3)	−0.010(6)
C(25)	4a		−0.3261(3)	−0.0307(5)	−0.0921(9)	0.017(4)	0.089(9)	0.039(6)	0.001(5)	0.000(4)	0.014(6)
C(26)	4a		−0.3837(3)	−0.0320(5)	−0.1085(9)	0.023(4)	0.10(1)	0.041(7)	−0.003(5)	−0.006(4)	0.026(7)
C(27)	4a		−0.3982(3)	−0.0811(6)	−0.0936(8)	0.028(4)	0.14(1)	0.021(5)	−0.013(6)	−0.006(3)	0.015(7)
C(28)	4a		−0.3533(4)	−0.1159(6)	−0.0688(9)	0.055(6)	0.09(1)	0.012(6)	−0.034(6)	−0.013(4)	0.007(6)
C(29)	4a		−0.4191(3)	0.0100(5)	−0.134(1)	0.031(4)	0.15(1)	0.065(8)	−0.002(6)	−0.001(4)	0.046(8)
C(30)	4a		−0.4730(4)	−0.0064(7)	−0.142(1)	0.043(6)	0.20(2)	0.07(1)	0.020(8)	−0.011(6)	0.06(1)
C(31)	4a		−0.4882(4)	−0.0586(8)	−0.125(1)	0.032(5)	0.26(2)	0.08(1)	−0.011(8)	−0.026(5)	0.05(1)
C(32)	4a		−0.4530(3)	−0.0963(7)	−0.0983(9)	0.041(5)	0.14(1)	0.056(7)	−0.016(7)	−0.020(4)	0.020(9)
C(33)	4a		−0.2308(2)	−0.1946(3)	0.2708(8)	0.006(4)	0.042(6)	0.056(6)	0.000(3)	0.000(3)	0.000(5)
C(34)	4a		−0.1928(3)	−0.2318(4)	0.3182(7)	0.036(4)	0.042(6)	0.027(5)	0.000(4)	−0.004(3)	−0.006(5)
C(35)	4a		−0.1449(3)	−0.2058(4)	0.3196(8)	0.029(4)	0.041(6)	0.044(6)	0.010(4)	−0.002(3)	−0.008(5)
C(36)	4a		−0.1529(3)	−0.1538(3)	0.2698(8)	0.026(4)	0.026(5)	0.039(6)	−0.010(3)	−0.002(3)	−0.018(5)
C(37)	4a		−0.1983(3)	−0.2835(4)	0.361(1)	0.038(4)	0.047(7)	0.080(9)	−0.002(5)	0.003(5)	−0.013(6)
C(38)	4a		−0.1540(3)	−0.3080(4)	0.407(1)	0.046(5)	0.036(7)	0.085(9)	−0.003(5)	−0.003(5)	0.027(6)
C(39)	4a		−0.1060(3)	−0.2832(4)	0.4028(9)	0.052(5)	0.057(8)	0.065(8)	0.025(5)	−0.009(5)	0.024(7)
C(40)	4a		−0.0996(3)	−0.2316(4)	0.3625(9)	0.040(4)	0.047(7)	0.051(7)	0.001(4)	0.001(4)	0.010(6)
C(41)	4a		−0.1262(3)	−0.0661(5)	0.2256(8)	0.024(4)	0.061(8)	0.017(5)	−0.001(4)	−0.004(3)	−0.013(6)
C(42)	4a		−0.0854(3)	−0.0227(4)	0.2263(8)	0.039(4)	0.031(5)	0.038(6)	−0.008(4)	−0.007(4)	−0.010(5)
C(43)	4a		−0.1135(3)	0.0240(3)	0.2043(7)	0.034(4)	0.034(5)	0.029(5)	0.001(4)	−0.011(3)	−0.002(4)
C(44)	4a		−0.1689(3)	0.0086(3)	0.1884(8)	0.020(4)	0.028(5)	0.044(6)	0.005(3)	−0.005(3)	0.015(5)
C(45)	4a		−0.0310(3)	−0.0222(4)	0.2469(8)	0.041(4)	0.053(7)	0.043(6)	0.002(4)	−0.010(4)	−0.008(5)
C(46)	4a		−0.0062(3)	0.0260(4)	0.2440(8)	0.028(4)	0.049(7)	0.055(7)	−0.007(4)	−0.010(4)	−0.009(5)
C(47)	4a		−0.0333(3)	0.0728(4)	0.2215(8)	0.046(4)	0.051(7)	0.069(8)	−0.024(4)	−0.009(4)	0.013(5)
C(48)	4a		−0.0875(3)	0.0732(3)	0.1998(8)	0.050(4)	0.037(6)	0.040(6)	−0.011(4)	−0.006(4)	−0.016(5)
C(49)	4a		−0.2581(3)	0.0341(3)	0.1715(6)	0.049(4)	0.042(5)	0.030(5)	0.011(4)	0.017(4)	−0.002(4)
C(50)	4a		−0.2998(3)	0.0765(4)	0.1776(9)	0.048(4)	0.030(6)	0.050(7)	0.013(4)	0.011(4)	0.003(5)
C(51)	4a		−0.3471(3)	0.0489(4)	0.1779(8)	0.050(5)	0.068(8)	0.027(6)	0.012(5)	0.008(4)	0.008(5)
C(52)	4a		−0.3355(3)	−0.0061(4)	0.1725(8)	0.026(4)	0.060(8)	0.036(6)	0.006(4)	0.004(4)	0.012(5)
C(53)	4a		−0.2977(3)	0.1314(4)	0.1890(9)	0.055(5)	0.072(9)	0.049(7)	0.010(5)	0.001(5)	0.004(6)
C(54)	4a		−0.3455(4)	0.1575(5)	0.195(1)	0.065(7)	0.051(8)	0.12(1)	0.032(6)	−0.002(7)	0.003(8)
C(55)	4a		−0.3931(4)	0.1306(5)	0.194(1)	0.072(7)	0.09(1)	0.065(9)	0.042(7)	0.015(6)	0.015(8)
C(56)	4a		−0.3951(3)	0.0765(4)	0.186(1)	0.042(5)	0.057(8)	0.074(8)	0.011(4)	0.014(4)	0.020(6)
C(57)	4a		−0.3600(3)	−0.0972(5)	0.1979(9)	0.035(4)	0.046(7)	0.031(6)	−0.014(5)	0.015(4)	0.011(6)
C(58)	4a		−0.4021(3)	−0.1353(5)	0.2205(8)	0.031(4)	0.078(9)	0.023(5)	−0.013(5)	0.008(3)	0.001(6)
C(59)	4a		−0.3765(3)	−0.1834(4)	0.2438(8)	0.019(3)	0.056(7)	0.042(6)	−0.007(4)	0.005(4)	−0.010(5)
C(60)	4a		−0.3192(3)	−0.1727(4)	0.2366(8)	0.025(4)	0.020(5)	0.021(5)	0.003(3)	0.009(3)	−0.008(4)
C(61)	4a		−0.4580(3)	−0.1343(4)	0.2180(9)	0.019(4)	0.073(8)	0.052(7)	0.001(4)	0.010(4)	0.007(6)
C(62)	4a		−0.4841(3)	−0.1813(5)	0.2408(8)	0.027(4)	0.11(1)	0.028(6)	−0.009(5)	0.012(4)	0.012(6)
C(63)	4a		−0.4586(3)	−0.2275(4)	0.267(1)	0.033(4)	0.071(8)	0.089(9)	−0.010(5)	−0.024(5)	0.013(7)
C(64)	4a		−0.4039(3)	−0.2300(4)	0.2686(8)	0.035(4)	0.059(7)	0.057(7)	0.005(4)	0.013(4)	−0.001(6)
C(65A)	4a	0.523(5)	0.3324(8)	0.073(1)	−0.017(2)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)
C(65B)	4a	0.477	0.2715(8)	0.1676(9)	0.043(2)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)

Table 6. Continued.

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(66A)	4*a*	0.523	0.3789(5)	0.0819(9)	0.069(2)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)
C(66B)	4*a*	0.477	0.3164(8)	0.207(1)	0.102(2)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)
C(67A)	4*a*	0.523	0.4170(7)	0.117(1)	0.016(2)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)
C(67B)	4*a*	0.477	0.327(1)	0.252(1)	0.022(2)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)
C(68A)	4*a*	0.523	0.4665(6)	0.1168(8)	0.062(2)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)
C(68B)	4*a*	0.477	0.3474(7)	0.2934(9)	0.080(4)	0.102(5)	0.153(9)	0.056(7)	−0.044(5)	−0.009(5)	0.035(7)
C(69A)	4*a*	0.523	0.2475(6)	0.0250(8)	−0.048(2)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(69B)	4*a*	0.477	0.2071(7)	0.093(1)	0.024(2)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(70A)	4*a*	0.523	0.1972(6)	−0.0035(9)	−0.009(2)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(70B)	4*a*	0.477	0.1758(6)	0.0440(7)	0.083(3)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(71A)	4*a*	0.523	0.1434(8)	0.023(1)	0.026(2)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(71B)	4*a*	0.477	0.144(1)	0.020(1)	−0.008(2)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(72A)	4*a*	0.523	0.1093(8)	−0.0250(9)	0.037(3)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(72B)	4*a*	0.477	0.0969(8)	−0.011(1)	0.023(3)	0.079(5)	0.077(6)	0.059(6)	−0.006(4)	−0.007(4)	0.002(5)
C(73A)	4*a*	0.523	0.257(1)	0.0733(9)	0.142(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(73B)	4*a*	0.477	0.227(1)	0.149(1)	0.207(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(74A)	4*a*	0.523	0.2329(9)	0.1266(9)	0.103(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(74B)	4*a*	0.477	0.178(1)	0.181(1)	0.213(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(75A)	4*a*	0.523	0.205(1)	0.143(1)	0.215(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(75B)	4*a*	0.477	0.1200(9)	0.160(1)	0.195(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(76A)	4*a*	0.523	0.184(1)	0.195(1)	0.174(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(76B)	4*a*	0.477	0.0801(9)	0.206(1)	0.205(2)	0.144(8)	0.118(9)	0.028(5)	−0.004(6)	0.020(6)	−0.015(6)
C(77A)	4*a*	0.523	0.3071(7)	−0.0107(8)	0.097(3)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(77B)	4*a*	0.477	0.2880(9)	0.080(1)	0.124(2)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(78A)	4*a*	0.523	0.3533(8)	−0.043(1)	0.027(2)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(78B)	4*a*	0.477	0.325(1)	0.057(1)	0.025(2)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(79A)	4*a*	0.523	0.3574(6)	−0.0951(9)	0.097(2)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(79B)	4*a*	0.477	0.354(1)	0.002(1)	0.047(2)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(80A)	4*a*	0.523	0.3952(6)	−0.1337(8)	0.047(2)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(80B)	4*a*	0.477	0.3328(9)	−0.045(1)	0.126(2)	0.106(6)	0.121(8)	0.078(8)	0.056(6)	−0.031(5)	−0.002(7)
C(81)	4*a*		0.0080(5)	0.1289(7)	−0.040(1)	0.097(9)	0.15(2)	0.12(2)	0.005(8)	0.055(9)	0.06(1)
N(1)	4*a*		−0.2580(2)	−0.1769(3)	−0.0086(5)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(2)	4*a*		−0.1719(2)	−0.2207(3)	0.0035(6)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(3)	4*a*		−0.1604(2)	−0.1254(3)	−0.0118(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(4)	4*a*		−0.1148(3)	−0.0419(4)	−0.0622(8)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(5)	4*a*		−0.2111(2)	−0.0288(3)	−0.0637(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(6)	4*a*		−0.2963(2)	0.0114(3)	−0.1154(6)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(7)	4*a*		−0.3084(2)	−0.0797(3)	−0.0608(6)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(8)	4*a*		−0.3512(3)	−0.1674(4)	−0.0574(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(9)	4*a*		−0.2071(2)	−0.1483(3)	0.2368(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(10)	4*a*		−0.1164(2)	−0.1159(3)	0.2603(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(11)	4*a*		−0.1756(2)	−0.0447(3)	0.1971(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(12)	4*a*		−0.2054(2)	0.0465(3)	0.1765(6)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(13)	4*a*		−0.2812(2)	−0.0150(3)	0.1651(6)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(14)	4*a*		−0.3725(2)	−0.0447(3)	0.1838(6)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(15)	4*a*		−0.3126(2)	−0.1200(3)	0.2051(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(16)	4*a*		−0.2818(2)	−0.2082(3)	0.2631(7)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(17A)	4*a*	0.523	0.2881(4)	0.0397(5)	0.046(1)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
N(17B)	4*a*	0.477	0.2480(3)	0.1198(5)	0.098(2)	0.0282(7)	0.051(1)	0.035(1)	−0.0004(8)	0.0029(7)	−0.003(1)
O(1)	4*a*		0.0073(2)	0.1418(3)	−0.1629(8)	0.058(4)	0.081(6)	0.105(7)	0.005(4)	0.020(4)	−0.010(6)
Dy(1)	4*a*		−0.239155(9)	−0.09234(1)	0.08139(6)	0.02116(9)	0.0499(2)	0.0238(1)	−0.0035(2)	0.0020(4)	−0.0104(4)

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