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Crystal structure of *catena*-[(μ_4-bromo)-tetrakis(μ_3-bromo)-octakis(μ_3-isonicotinato)-tris(μ_2-bromo)-hexakis(μ_2-isonicotinato)-deca-aqua-deca-copper(I)-tetra-terbium(III) dihydrate], $C_{42}H_{40}Br_4Cu_5N_7O_{20}Tb_2$

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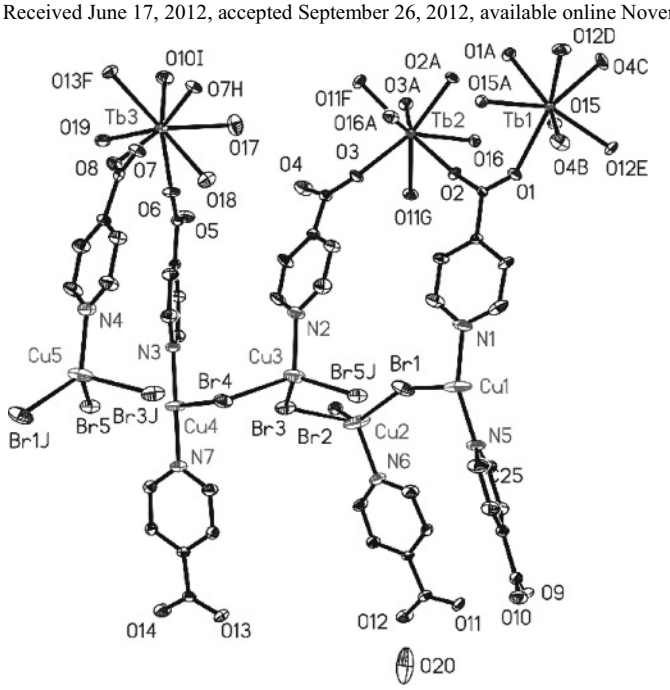

Abstract

$C_{42}H_{40}Br_4Cu_5N_7O_{20}Tb_2$, monoclinic, *P*2/*c* (no. 13), a = 17.677(5) Å, b = 9.812(2) Å, c = 32.145(8) Å, β = 103.625(4)°, V = 5418.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.0483, $wR_{ref}(F^2)$ = 0.1355, T = 293 K.

Table 1. Data collection and handling.

Crystal:	orange prisms, size 0.05×0.2×0.3 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	75.30 cm^{-1}
Diffractometer, scan mode:	Rigaku Mercury CCD diffractometer, ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	33287, 9514
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 8122
$N(param)_{refined}$:	724
Programs:	PLATON [4], SHELX [5]

Source of material

A mixture of Tb_4O_7 (0.187 g, 0.25 mmol), $CuBr_2$ (0.223 g, 1 mmol), isonicotinic acid (0.246 g, 2 mmol), and H_2O (10 mL) was stirred at room temperature until a homogeneous mixture was obtained. The mixture was transferred into a Teflon-lined steel autoclave (23 mL) and heated at 453 K for 5 days and then cooled at rate of 2 K·h^{-1} to room temperature. The orange crystals obtained were washed with water and dried in air (yield 36% based on Tb).

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Experimental details

All non-hydrogen atoms were refined anisotropically. The H atoms were positioned geometrically and refined as riding atoms with d(C–H) = 0.93 Å, d(O–H) = 0.85 Å, and U_{iso}(H) = 1.2U_{eq}(C or O).

Discussion

There has been growing interest in recent years in the design and synthesis of 3*d*-4*f* heterometallic coordination polymers not only for their fascinating structural topology, but also for their potential applications in magnetism, luminescence, molecular adsorption, and bimetallic catalysis. Isonicotinic acid (HIN) which is a linear and potentially bridging ligand with O and N donors on opposite sides of the molecule bearing diverse coordination modes was chosen to construct lots of heterometallic coordination polymers [1-3]. The asymmetric unit of the title crystal structure contains one Tb^{3+} ion in general position and two Tb^{3+} ions: on special sites with *i*- and *2*-site symmetry, three Br^- ions in general position and two half Br^- ions: on special sites with *i*- and *2*-site symmetry, five Cu^+ ions, seven IN^- ligands, five coordinated water molecules and one uncoordinated water molecule, all in general position. The Tb1, Tb2, and Tb3 centers all are eight-coordinated and display bicapped trigonal prismatic coordination environment (six oxygen atoms from six IN^- ligands, two oxygen atoms from two coordinated water molecules for the Tb1 and Tb2 centers; five oxygen atoms from five IN^- ligands, three oxygen atoms from three coordinated water molecules for the Tb3 center with the distances d(Tb–O) = 2.295(5)-2.630(6) Å). Both Cu1 and Cu4 centers exhibit trigonal conformation, being coordinated by two nitrogen atoms from two different IN^- ligands and one Br^- ion. However, all of the Cu2, Cu3 and Cu5 centers present tetrahedral geometry, being coordinated by one nitrogen atom from IN^- ligand and three Br^- ions with the distances d(Cu–N) = 1.945(7)-2.038(7) Å and d(Cu–Br) = 2.3873(18)-2.909(2) Å. In this structure, the IN^- ligands have two evidently different coordination modes: one behaves as a bridging ligand to coordinate two Tb^{3+} ions and one Cu^+ ion, another also behaves as a bridging ligand, but it coordinates one Tb^{3+} ion and one Cu^+ ion. The Tb1 and Tb2 centers are alternately bridged by two and four μ-carboxylate groups of IN^- ligands in a 4–2–4–2 (the number indicates the number of the bridges) mode to construct a one-dimensional linear Tb-carboxylate chain along *b* axis with the distance d(Tb···Tb) = 4.541(2) and 5.271(2) Å, respectively, and the Tb···Tb···Tb angles of 180°. Tb3 and its symmetry related center are linked by two μ-carboxylate groups of IN^- ligands to form a zero-dimensional $Tb_2(IN)_8$ dimer with the distance d(Tb···Tb) = 5.170(2) Å. The [Cu2Br_3N], [Cu3Br_3N] and [Cu5Br_3N] tetrahedra are connected with each other by common edges (Br1–Br3,

Br3–Br5) to form trimers with the distance *d*(Cu3–Cu5) = 2.683(2) Å, which is much shorter than the double van der Waals radius of the Cu^+ ion (1.4 Å), implying a strong Cu–Cu interactions. The trimer links two triangles ($Cu1BrN_2$, $Cu4BrN_2$) through common vertices (Br1, Br4) to generate a pentanuclear Cu cluster. And then the pentanuclear Cu cluster is connected with its symmetry-related structure by sharing vertex (Br4) to produce a octanuclear Cu cluster. Neighboring octanuclear Cu clusters further link each other by common vertex (Br2) to give rise to one-dimensional zigzag $[Cu_5Br_4]_n$ inorganic chains extending along *c*-axis. The one-dimensional zigzag $[Cu_5Br_4]_n$ inorganic chains parallel each other extending along *bc*-plane. As a consequence of the connectivity of $[CuBr_3N]$ tetrahedra and $[CuBrN_2]$ triangles, the Br^- ions act as μ_2 (Br2, Br5), μ_3 (Br1, Br3) and μ_4 (Br4) ligands. The linkages of one-dimensional linear Tb-carboxylate chains, zero-dimensional $Tb_2(IN)_8$ dimers and $[Cu_5Br_4]_n$ inorganic chains by IN^- pillars construct a three-dimensional framework. In this three-dimensional structure, it is noticed that the one-dimensional Tb-carboxylate chains and $Tb_2(IN)_8$ dimers are joined by weak O–H···O hydrogen bondings to produce two-dimensional Tb-carboxylate layers extending along *bc*-plane. And the two-dimensional Tb-carboxylate layer is further stabilized by the uncoordinated water molecules situating between one-dimensional Tb-carboxylate chains and $Tb_2(IN)_8$ dimers through O–H···O hydrogen bondings.

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(15A)	4*g*	0.0410	1.2192	0.1895	0.034
H(15B)	4*g*	–0.0377	1.2386	0.1687	0.034
H(16B)	4*g*	0.0403	1.0056	0.1797	0.041
H(16C)	4*g*	–0.0389	0.9621	0.1593	0.041
H(17B)	4*g*	0.0053	0.4402	0.3623	0.066
H(17C)	4*g*	–0.0475	0.5258	0.3693	0.066
H(18A)	4*g*	0.1137	0.5636	0.4441	0.052
H(18B)	4*g*	0.0844	0.5465	0.4757	0.052
H(19B)	4*g*	0.0254	0.0416	0.4694	0.047
H(19C)	4*g*	–0.0531	0.0370	0.4535	0.047
H(20B)	4*g*	1.0171	0.7620	0.3680	0.143
H(20C)	4*g*	0.9854	0.6633	0.3819	0.143
H(1A)	4*g*	0.3881	1.2504	0.3104	0.061
H(2A)	4*g*	0.2556	1.2985	0.2867	0.043
H(4A)	4*g*	0.2146	0.8986	0.2899	0.039
H(5A)	4*g*	0.3449	0.8623	0.3154	0.060
H(7A)	4*g*	0.3186	0.8050	0.4123	0.051
H(8A)	4*g*	0.1938	0.8154	0.3704	0.040
H(10A)	4*g*	0.2091	0.4174	0.3457	0.050
H(11A)	4*g*	0.3333	0.4189	0.3875	0.057
H(13A)	4*g*	0.3934	0.0960	0.4083	0.044
H(14A)	4*g*	0.2634	0.0748	0.3778	0.037
H(16A)	4*g*	0.2193	0.3123	0.4708	0.038
H(17A)	4*g*	0.3504	0.3254	0.4993	0.042
H(19A)	4*g*	0.3266	0.5077	0.6186	0.052
H(20A)	4*g*	0.1953	0.5363	0.5880	0.044
H(22A)	4*g*	0.1871	0.1498	0.5481	0.048
H(23A)	4*g*	0.3165	0.1284	0.5817	0.060
H(25A)	4*g*	0.6130	0.9955	0.2863	0.052
H(26A)	4*g*	0.7432	1.0450	0.2959	0.038
H(28A)	4*g*	0.7392	1.2172	0.4079	0.051
H(29A)	4*g*	0.6112	1.1629	0.3954	0.060
H(31A)	4*g*	0.6439	0.7504	0.2977	0.057
H(32A)	4*g*	0.7690	0.7980	0.2924	0.048
H(34A)	4*g*	0.8046	0.3944	0.2897	0.043
H(35A)	4*g*	0.6780	0.3616	0.2913	0.048
H(37A)	4*g*	0.6341	0.4110	0.4792	0.045
H(38A)	4*g*	0.7661	0.3909	0.4884	0.040
H(40A)	4*g*	0.7456	–0.0100	0.5040	0.040
H(41A)	4*g*	0.6143	0.0195	0.4960	0.042

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}
Tb(1)	2*e*	0	1.38889(5)	¼	0.0141(2)	0.0146(2)	0.0257(2)	0	0.0035(2)	0
Tb(2)	2*e*	0	0.85171(5)	¼	0.0141(2)	0.0157(2)	0.0295(3)	0	0.0019(2)	0
Tb(3)	4*g*	–0.01254(2)	0.31250(4)	0.44229(1)	0.0174(2)	0.0271(2)	0.0291(2)	0.0026(1)	0.0050(2)	–0.0051(2)
Cu(1)	4*g*	0.49021(7)	1.0204(2)	0.33021(5)	0.0195(6)	0.146(2)	0.090(1)	0.0029(8)	0.0072(6)	–0.017(1)
Cu(2)	4*g*	0.53612(8)	0.5154(2)	0.29780(7)	0.0326(7)	0.067(1)	0.165(2)	–0.0103(7)	0.0379(9)	–0.048(1)
Cu(3)	4*g*	0.45659(7)	0.6099(1)	0.42477(5)	0.0287(6)	0.0655(9)	0.0780(9)	0.0022(6)	–0.0055(6)	–0.0090(7)
Cu(4)	4*g*	0.49799(6)	0.2389(1)	0.47962(4)	0.0168(5)	0.0510(7)	0.0866(9)	–0.0009(5)	0.0053(5)	–0.0131(7)
Cu(5)	4*g*	0.45054(7)	0.3057(2)	0.62515(5)	0.0291(6)	0.099(1)	0.0647(8)	0.0150(7)	–0.0042(6)	–0.0138(8)
Br(1)	4*g*	0.48008(6)	0.7465(1)	0.30352(3)	0.0457(6)	0.0729(7)	0.0578(6)	0.0298(5)	0.0016(5)	–0.0141(6)
Br(2)	2*f*	½	0.3181(1)	¼	0.0334(7)	0.0369(7)	0.0536(7)	0	0.0115(6)	0
Br(3)	4*g*	0.50614(5)	0.4296(1)	0.37904(4)	0.0322(5)	0.0464(6)	0.0765(7)	–0.0019(4)	0.0100(5)	–0.0204(5)
Br(4)	2*b*	½	½	½	0.0286(6)	0.0326(7)	0.0671(8)	0.0063(5)	0.0051(6)	–0.0082(6)
Br(5)	4*g*	0.49715(5)	0.1473(1)	0.57157(3)	0.0289(5)	0.0432(5)	0.0567(5)	0.0011(4)	0.0060(4)	–0.0163(4)
O(1)	4*g*	0.1112(3)	1.2475(5)	0.2650(2)	0.024(3)	0.029(3)	0.037(3)	0.009(2)	0.004(2)	0.004(2)
O(2)	4*g*	0.0913(3)	1.0224(5)	0.2641(2)	0.022(3)	0.024(3)	0.042(3)	–0.009(2)	0.005(2)	–0.001(2)
O(3)	4*g*	0.0813(3)	0.7310(6)	0.3074(2)	0.026(3)	0.031(3)	0.041(3)	0.010(2)	–0.001(2)	0.006(3)
O(4)	4*g*	0.0849(3)	0.5038(6)	0.3057(2)	0.037(3)	0.034(3)	0.057(4)	–0.002(3)	–0.013(3)	–0.020(3)
O(5)	4*g*	0.1208(3)	0.1208(7)	0.3643(2)	0.027(3)	0.063(4)	0.038(3)	0.006(3)	0.002(3)	–0.018(3)
O(6)	4*g*	0.0928(3)	0.2341(6)	0.4188(2)	0.020(3)	0.048(4)	0.042(3)	0.007(3)	0.011(2)	–0.011(3)
O(7)	4*g*	0.0644(3)	0.4826(6)	0.5440(2)	0.027(3)	0.033(3)	0.035(3)	0.013(2)	0.002(2)	–0.004(2)
O(8)	4*g*	0.0643(3)	0.2820(6)	0.5114(2)	0.032(3)	0.034(3)	0.033(3)	0.003(3)	–0.002(2)	–0.005(3)
O(9)	4*g*	0.8755(3)	1.1322(6)	0.3315(2)	0.023(3)	0.054(4)	0.054(4)	–0.008(3)	0.018(3)	–0.004(3)
O(10)	4*g*	0.8745(3)	1.2350(7)	0.3934(2)	0.028(3)	0.048(4)	0.047(4)	–0.003(3)	–0.004(3)	–0.007(3)
O(11)	4*g*	0.9001(3)	0.7463(6)	0.2770(2)	0.030(3)	0.033(3)	0.050(3)	–0.011(3)	0.015(3)	0.004(3)
O(12)	4*g*	0.9223(3)	0.5225(6)	0.2822(2)	0.029(3)	0.036(3)	0.068(4)	0.006(3)	0.024(3)	–0.014(3)
O(13)	4*g*	0.8927(3)	0.2678(6)	0.4858(2)	0.026(3)	0.031(3)	0.048(3)	–0.007(2)	0.016(3)	–0.006(3)
O(14)	4*g*	0.8801(3)	0.0467(6)	0.4977(2)	0.031(3)	0.032(4)	0.099(5)	0.012(3)	0.022(3)	0.008(4)
O(15)	4*g*	0.0034(3)	1.2753(5)	0.1836(2)	0.023(3)	0.031(3)	0.028(3)	0.000(2)	0.003(2)	–0.007(2)

Table 3. continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(16)	4*g*	0.0047(3)	0.9454(5)	0.1763(2)	0.028(3)	0.026(3)	0.045(3)	–0.002(2)	0.002(2)	0.008(3)
O(17)	4*g*	–0.0203(4)	0.4585(7)	0.3809(2)	0.086(5)	0.048(4)	0.035(3)	0.012(4)	0.023(3)	0.002(3)
O(18)	4*g*	0.0986(3)	0.4969(6)	0.4570(2)	0.041(4)	0.042(4)	0.050(3)	–0.007(3)	0.019(3)	–0.010(3)
O(19)	4*g*	–0.0109(3)	0.0663(6)	0.4484(2)	0.027(3)	0.041(3)	0.050(3)	0.003(3)	0.011(3)	0.000(3)
O(20)	4*g*	1.0012(7)	0.743(1)	0.3903(3)	0.24(2)	0.063(6)	0.079(6)	–0.016(7)	0.077(8)	0.006(5)
N(1)	4*g*	0.3784(4)	1.0508(9)	0.3148(3)	0.023(4)	0.069(6)	0.056(5)	0.016(4)	0.007(3)	0.003(4)
N(2)	4*g*	0.3396(4)	0.6118(8)	0.4029(2)	0.025(4)	0.043(5)	0.051(4)	0.003(3)	–0.006(3)	0.000(4)
N(3)	4*g*	0.3857(4)	0.2126(7)	0.4568(2)	0.018(3)	0.032(4)	0.052(4)	0.002(3)	0.006(3)	0.003(3)
N(4)	4*g*	0.3352(4)	0.3166(8)	0.6022(3)	0.027(4)	0.047(5)	0.055(5)	0.002(3)	0.009(3)	–0.003(4)
N(5)	4*g*	0.5995(4)	1.0706(9)	0.3404(2)	0.018(3)	0.065(5)	0.055(5)	0.006(4)	0.009(3)	0.002(4)
N(6)	4*g*	0.6486(4)	0.5514(8)	0.2955(3)	0.025(4)	0.037(4)	0.069(5)	–0.005(3)	0.018(3)	–0.008(4)
N(7)	4*g*	0.6099(4)	0.2171(7)	0.4863(2)	0.021(3)	0.039(4)	0.046(4)	0.001(3)	0.007(3)	–0.009(3)
C(1)	4*g*	0.3524(6)	1.179(1)	0.3064(3)	0.033(5)	0.070(7)	0.050(6)	–0.022(5)	0.015(4)	–0.009(5)
C(2)	4*g*	0.2726(5)	1.2090(9)	0.2919(3)	0.021(4)	0.042(5)	0.044(5)	–0.012(4)	0.010(4)	–0.003(4)
C(3)	4*g*	0.2205(4)	1.1032(7)	0.2856(2)	0.018(4)	0.025(4)	0.027(4)	0.001(3)	0.008(3)	–0.003(3)
C(4)	4*g*	0.2487(5)	0.9721(8)	0.2942(3)	0.024(4)	0.031(4)	0.042(4)	0.006(3)	0.005(3)	–0.006(4)
C(5)	4*g*	0.3272(5)	0.951(1)	0.3091(3)	0.035(5)	0.050(6)	0.058(6)	0.012(5)	0.000(4)	–0.005(5)
C(6)	4*g*	0.1339(4)	1.1259(7)	0.2702(2)	0.017(4)	0.018(4)	0.024(3)	0.002(3)	0.002(3)	0.003(3)
C(7)	4*g*	0.2966(5)	0.727(1)	0.3980(3)	0.037(5)	0.043(5)	0.042(5)	–0.007(4)	0.001(4)	–0.014(4)
C(8)	4*g*	0.2215(5)	0.7340(9)	0.3730(3)	0.026(4)	0.028(4)	0.041(4)	0.003(3)	0.000(3)	–0.011(4)
C(9)	4*g*	0.1880(4)	0.6174(8)	0.3517(2)	0.019(4)	0.026(4)	0.032(4)	0.001(3)	0.002(3)	–0.001(3)
C(10)	4*g*	0.2306(5)	0.4983(8)	0.3583(3)	0.032(5)	0.020(4)	0.061(6)	0.003(4)	–0.014(4)	–0.003(4)
C(11)	4*g*	0.3053(5)	0.5000(9)	0.3836(3)	0.031(5)	0.032(5)	0.068(6)	0.010(4)	–0.008(4)	0.007(5)
C(12)	4*g*	0.1107(4)	0.6192(8)	0.3190(2)	0.019(4)	0.027(4)	0.029(4)	–0.004(3)	–0.001(3)	–0.002(3)
C(13)	4*g*	0.3580(5)	0.1397(9)	0.4211(3)	0.029(5)	0.037(5)	0.044(5)	0.004(4)	0.010(4)	–0.003(4)
C(14)	4*g*	0.2797(5)	0.1267(8)	0.4025(3)	0.024(4)	0.034(5)	0.034(4)	0.002(3)	0.004(3)	–0.006(3)
C(15)	4*g*	0.2253(4)	0.1906(8)	0.4205(2)	0.018(4)	0.028(4)	0.024(4)	0.000(3)	0.005(3)	0.001(3)
C(16)	4*g*	0.2536(5)	0.2670(9)	0.4576(2)	0.027(4)	0.036(5)	0.035(4)	0.003(4)	0.010(3)	–0.011(4)
C(17)	4*g*	0.3326(5)	0.2748(8)	0.4745(3)	0.029(4)	0.030(4)	0.043(5)	–0.007(4)	0.004(4)	–0.011(4)
C(18)	4*g*	0.1394(4)	0.1807(8)	0.3996(3)	0.017(4)	0.025(4)	0.039(4)	0.002(3)	0.005(3)	0.004(3)
C(19)	4*g*	0.2983(5)	0.435(1)	0.6042(3)	0.029(5)	0.043(5)	0.051(5)	0.003(4)	–0.004(4)	–0.004(4)
C(20)	4*g*	0.2192(5)	0.4533(9)	0.5857(3)	0.026(4)	0.038(5)	0.044(5)	0.005(4)	0.004(4)	–0.006(4)
C(21)	4*g*	0.1774(4)	0.3467(8)	0.5639(2)	0.022(4)	0.029(4)	0.026(4)	0.009(3)	0.005(3)	–0.002(3)
C(22)	4*g*	0.2143(5)	0.2239(9)	0.5623(3)	0.029(5)	0.032(5)	0.054(5)	–0.004(4)	–0.001(4)	–0.007(4)
C(23)	4*g*	0.2924(6)	0.212(1)	0.5822(3)	0.037(5)	0.044(6)	0.063(6)	0.017(4)	0.000(5)	0.002(5)
C(24)	4*g*	0.0957(4)	0.3721(8)	0.5385(2)	0.025(4)	0.026(4)	0.026(4)	–0.002(3)	0.010(3)	0.004(3)
C(25)	4*g*	0.6389(5)	1.039(1)	0.3112(3)	0.029(5)	0.052(6)	0.043(5)	–0.009(4)	–0.002(4)	–0.008(4)
C(26)	4*g*	0.7173(5)	1.0697(9)	0.3168(2)	0.029(4)	0.036(5)	0.032(4)	0.002(4)	0.009(3)	–0.008(4)
C(27)	4*g*	0.7570(4)	1.1363(8)	0.3532(3)	0.020(4)	0.023(4)	0.040(4)	0.002(3)	0.009(3)	0.000(3)
C(28)	4*g*	0.7152(5)	1.171(1)	0.3830(3)	0.032(5)	0.055(6)	0.038(5)	0.001(4)	0.003(4)	–0.005(4)
C(29)	4*g*	0.6385(5)	1.138(1)	0.3752(3)	0.031(5)	0.080(8)	0.042(5)	0.006(5)	0.014(4)	–0.003(5)
C(30)	4*g*	0.8432(5)	1.1696(8)	0.3601(3)	0.025(4)	0.026(4)	0.038(4)	0.002(3)	0.009(3)	0.002(4)
C(31)	4*g*	0.6767(5)	0.678(1)	0.2955(3)	0.032(5)	0.040(5)	0.076(7)	0.014(4)	0.026(5)	–0.003(5)
C(32)	4*g*	0.7521(5)	0.7082(8)	0.2923(3)	0.026(4)	0.020(4)	0.078(6)	0.007(3)	0.020(4)	0.013(4)
C(33)	4*g*	0.8010(4)	0.6013(8)	0.2890(2)	0.015(4)	0.028(4)	0.037(4)	–0.003(3)	0.004(3)	0.000(3)
C(34)	4*g*	0.7724(5)	0.4690(8)	0.2902(3)	0.027(4)	0.028(4)	0.053(5)	0.003(3)	0.012(4)	–0.002(4)
C(35)	4*g*	0.6968(5)	0.4503(9)	0.2922(3)	0.030(5)	0.028(5)	0.062(6)	–0.012(4)	0.013(4)	–0.008(4)
C(36)	4*g*	0.8819(4)	0.6254(8)	0.2826(2)	0.024(4)	0.033(5)	0.025(4)	–0.007(3)	0.008(3)	–0.007(3)
C(37)	4*g*	0.6566(5)	0.3251(9)	0.4842(3)	0.023(4)	0.028(4)	0.062(6)	0.002(3)	0.009(4)	–0.002(4)
C(38)	4*g*	0.7360(5)	0.3136(8)	0.4890(3)	0.028(4)	0.030(4)	0.044(5)	0.003(3)	0.012(4)	0.007(4)
C(39)	4*g*	0.7703(4)	0.1867(8)	0.4949(2)	0.018(4)	0.032(4)	0.026(4)	0.000(3)	0.004(3)	–0.001(3)
C(40)	4*g*	0.7239(5)	0.0764(8)	0.4985(3)	0.031(4)	0.022(4)	0.048(5)	0.001(3)	0.010(4)	0.008(4)
C(41)	4*g*	0.6448(5)	0.0951(9)	0.4939(3)	0.030(4)	0.034(5)	0.041(5)	–0.004(4)	0.008(4)	0.002(4)
C(42)	4*g*	0.8548(4)	0.1659(8)	0.4933(3)	0.020(4)	0.030(4)	0.037(4)	0.002(3)	0.004(3)	0.001(3)

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