Supporting information for the manuscript:

1D and 2D coordination polymers based on ring-reduced free-base and copper-containing *meso*-tetra(4-pyridyl)porphyrins and $M^{III}(TMHD)_3$ units (M = Dy, Tb and Gd; TMHD: 2,2,6,6-tetramethyl-3,5-heptanedionate).

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Table S1. IR-spectra (cm^{-1}) of starting macrocycle and polymers **1**-**4** measured in KBr pellets.

Compo-nents	H_2TPyP	$Ln(TMHD)_3$	crypt	CuTPyP	**1** H_2TPyP	**2** CuTPyP	**3** H_2TPyP	**4** H_2TPyP
H_2TPyP	413w			443w	428w	-	-	-
	-			532w	454w	-	-	-
	531m			574w	-	-	-	-
	555m			667m	-	-	-	-
	565m			682m	669w	669w	666w	667w
	659s			717m		717w		
	723s			795s	792m*	794m*	792m*	791m*
	785s			854w		869m	848w	847w
	800s			873w	-	887w	881w	880w
	842m			891w	889w	1003m	-	-
	882s			1001s	971w	1025w*	-	-
	971s			1026w	-	1069m*	1012w	1012w
	980m			1068m	1047m	-	-	-
	1004m			1080w	1072w*	-	1068m*	1068m*
	1069m			1213w	1261w	1224m*	--	-
	1082w			1261w	1358s*	1261w	1357s*	1357s*
	1258w			1346m	1413s	1357s*	1413s	1414s
	1351m			1404m	-	1411s*	-	-
	1401s			1425m	1538m*	1538m*	1537m*	1537m*
	1469m			1543m	-	1538m*	-	-
	1542m			1593s	1590s	1591s	1589s	1589s
	1557w						-	-
	1594s				-			
					472m*		-	-
					604w		474m*	473m*
Ln		409m			736w*	-	603w	603w
$(TMHD)_3$		474s			755w	474m*	737w*	735w*
		601m			792m*	605w	753w	751w
		737m			869m	737w*	792m*	791m*
		763m			-	757w	868m	868m
		794m			-	794m*	-	-
		867s			1020w	869m	944m*	944m*
		935w			1139m*	-	-	-
		950m			1179m	942w*	1139m*	1138m*
		1025w			1226m	1025w*	1180m	1180m
		1130s			1245w	1140m*	1226w	1225w
		1181m			1287w*	1178m	1245w	1245w
		1224m			1358s*	1224m*	1282w	1283w
		1247w			1388w	1245w	1357s*	1357s*
		1279m			-	1284w	1387w	1387w
		1353s			1452m*	1357s*	-	-
		1382s			1505s	1388w	1451m*	1451m*
		1399m			1538m*	1411s*	1505s	1505s
		1452m			-	1451m*	1538m*	1537m*
		1504s			1575s	1506s	-	-
		1541m			-	1538m*	1575s	1575s
		1551m			2873m*	-	-	-
		1574vs			2902w	1574s	2869m	2865m
		1580vs			2962m	-	2900w	2900w
		2865w				2865m	2952m	2952m
		2906w			472m*	2902w		
		2952m			736w*	2957m	474m*	473m*
crypt					-		737w*	735w*
			476w		-	474m*	-	-
			735m*		-	737w*	944m*	944m*
			922m		1072w*	-	990w	990w
			948w		1105m	942w*	1068m*	1068m*
			982m		1139m*	-	1109m	1108m
			1071m		1287w*	1069m*	1139m*	1138m*
			1100s		-	1106m	-	-
			1127s		1358s*	1140m*	1298w	-
			1295m		1452m*	-	1357s*	1357s*
			1329m		-	-	1451m*	1451m*
			1360s		2873m*	1357s*	-	-
			1446m			1451m*	-	
			1462m			-		
			2877w			-		

* - bands are coincided; w – weak, m –middle and s – strong intensity

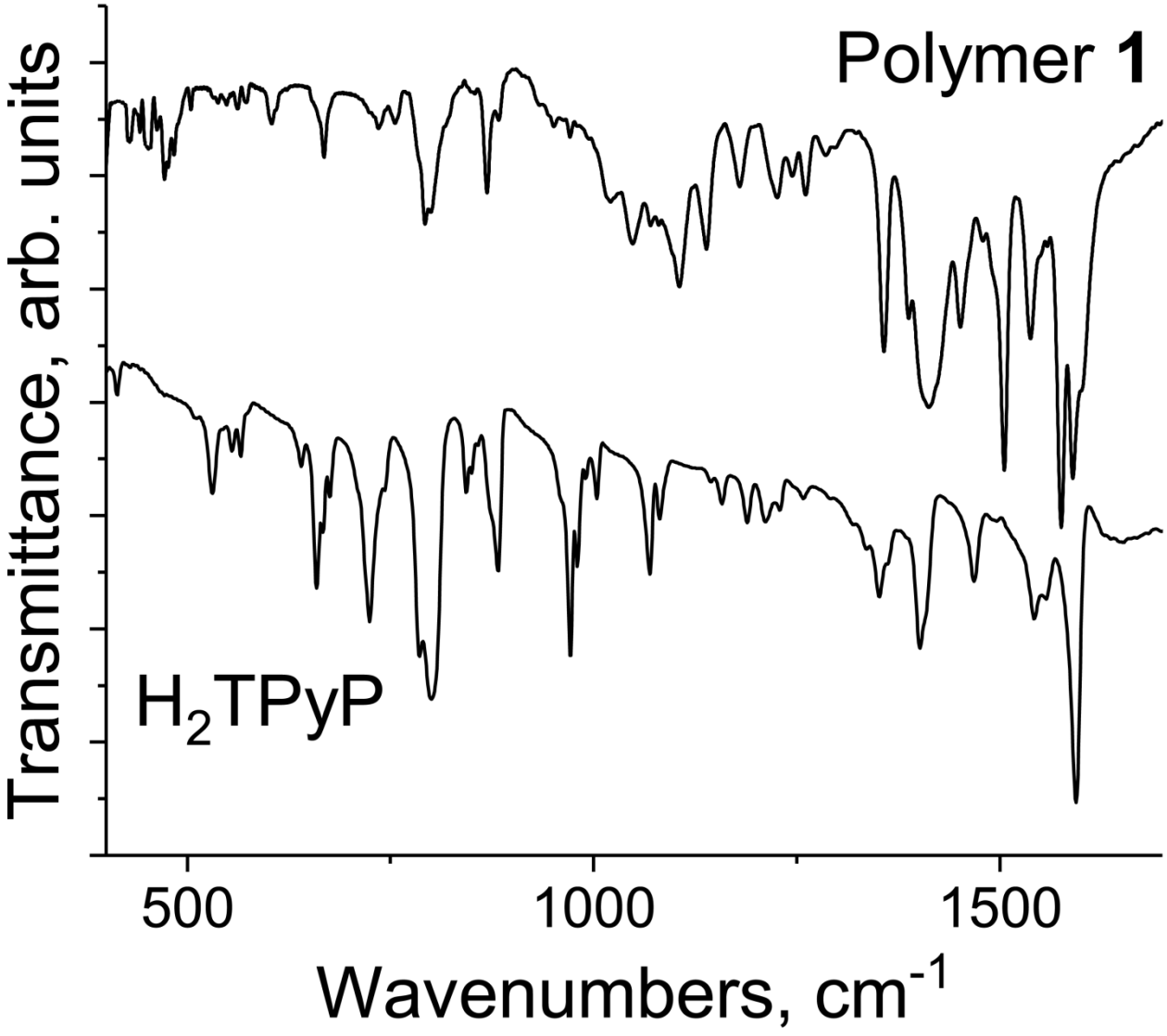

Figure S1. IR spectra of starting H_2TPyP porphyrin and salt **1** in KBr pellets. Pellet for **1** was prepared in anaerobic condition.

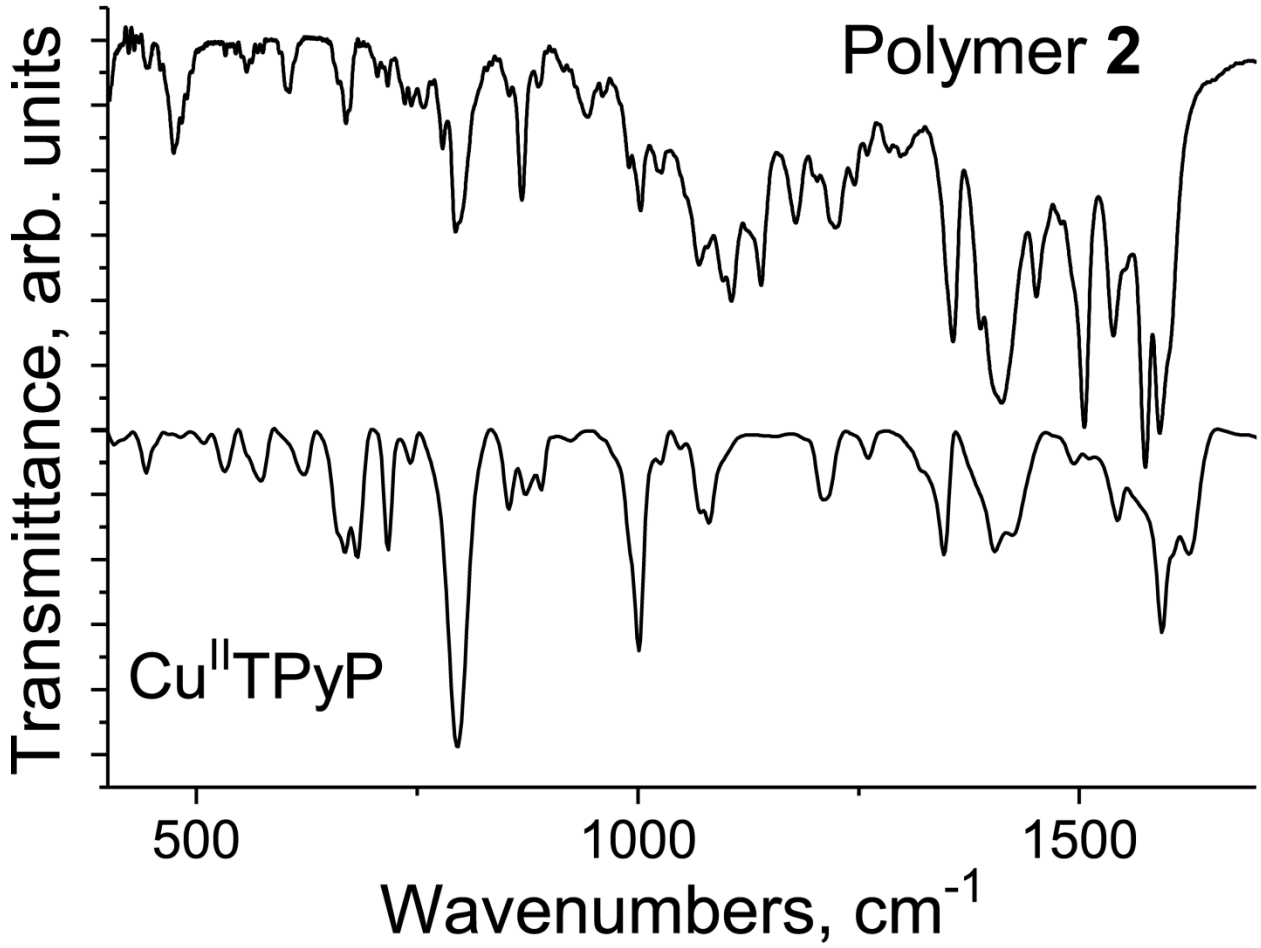

Figure S2. IR spectra of starting Cu^{II}TPyP porphyrin and salt **2** in KBr pellets. Pellet for **2** was prepared in anaerobic condition.

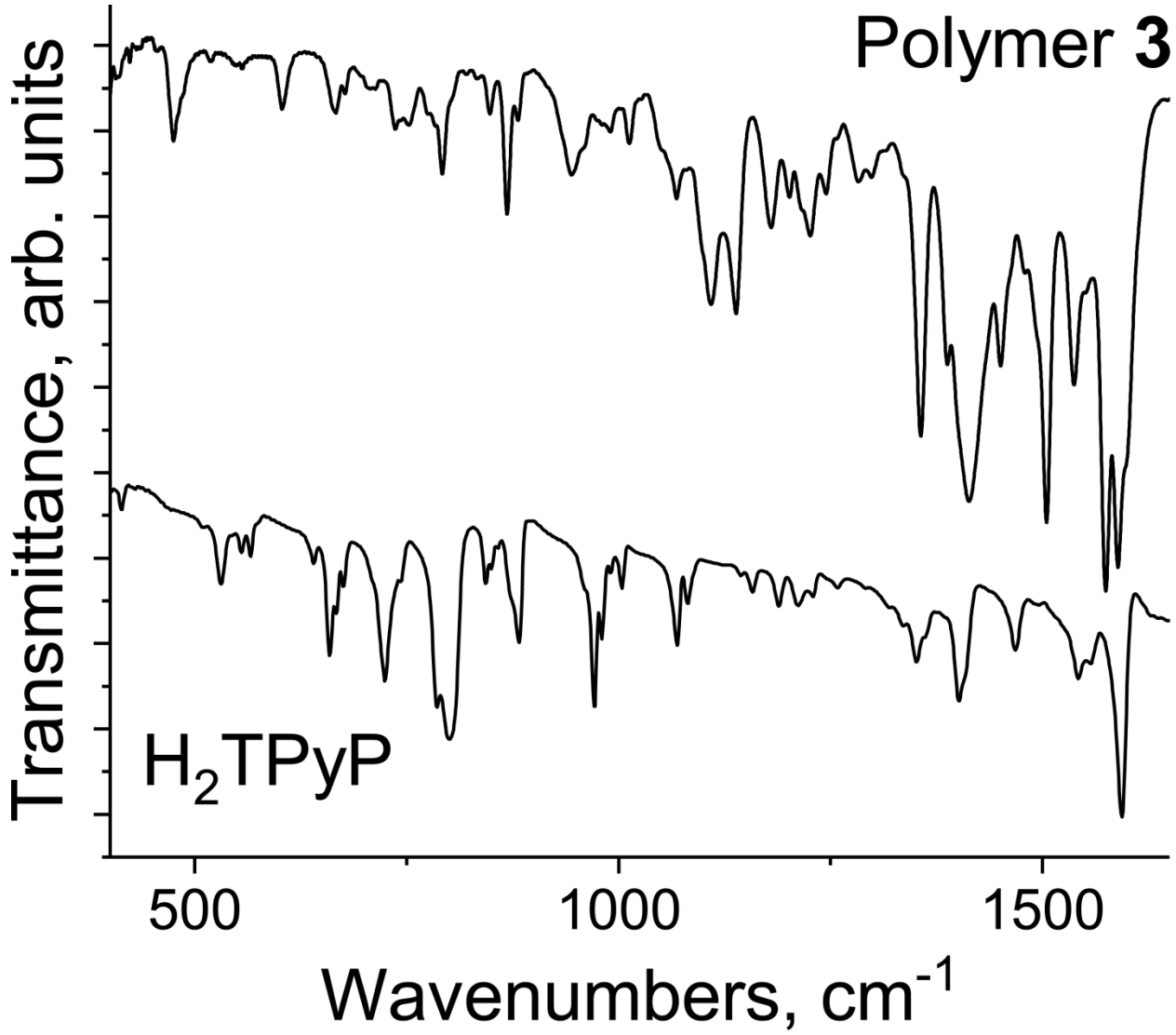

Figure S3. IR spectra of starting H_2TPyP porphyrin and salt **3** in KBr pellets. Pellet for **3** was prepared in anaerobic condition.

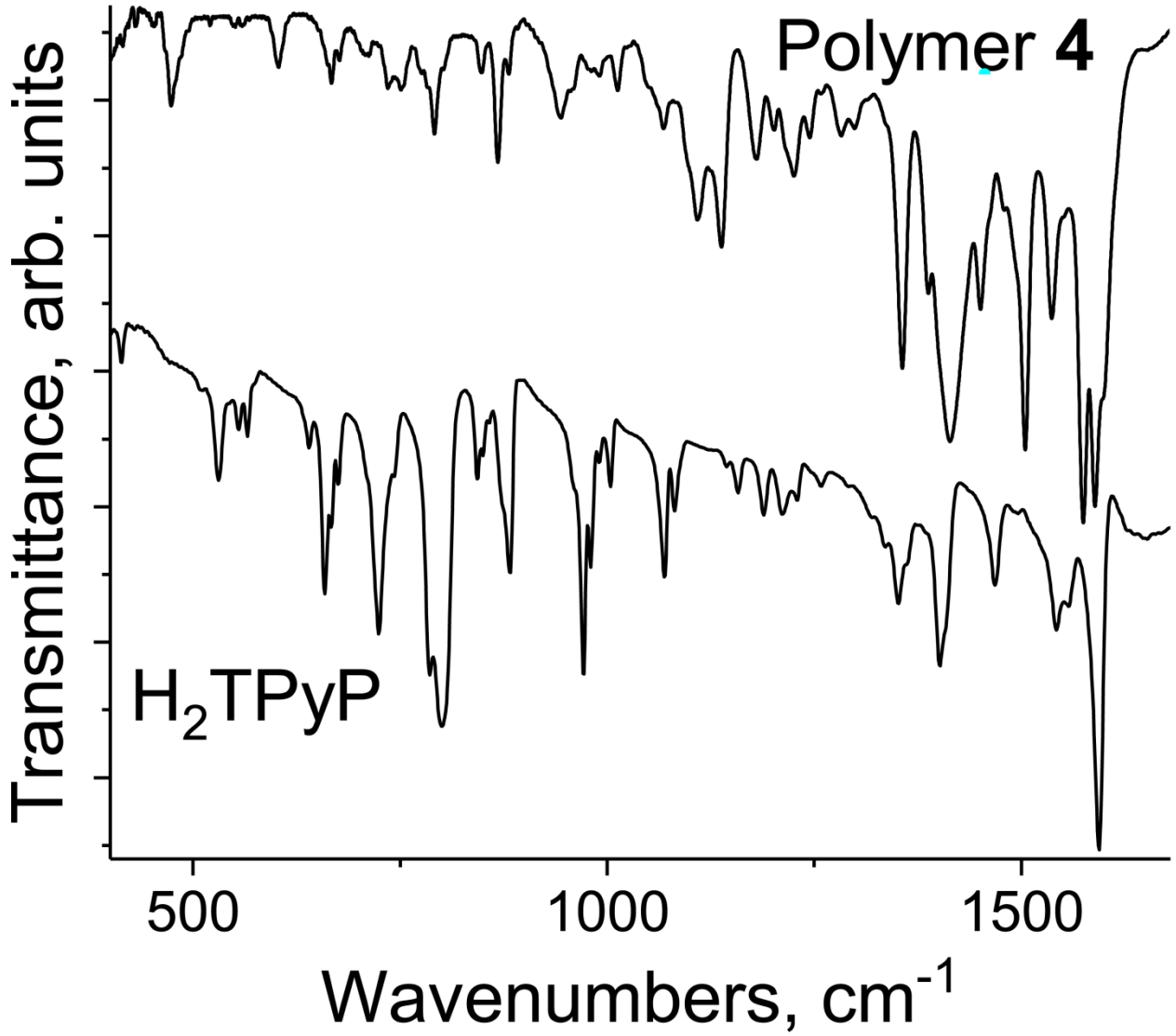

Figure S4. IR spectra of starting H_2TPyP porphyrin and salt **4** in KBr pellets. Pellet for **4** was prepared in anaerobic condition.

Crystal structure

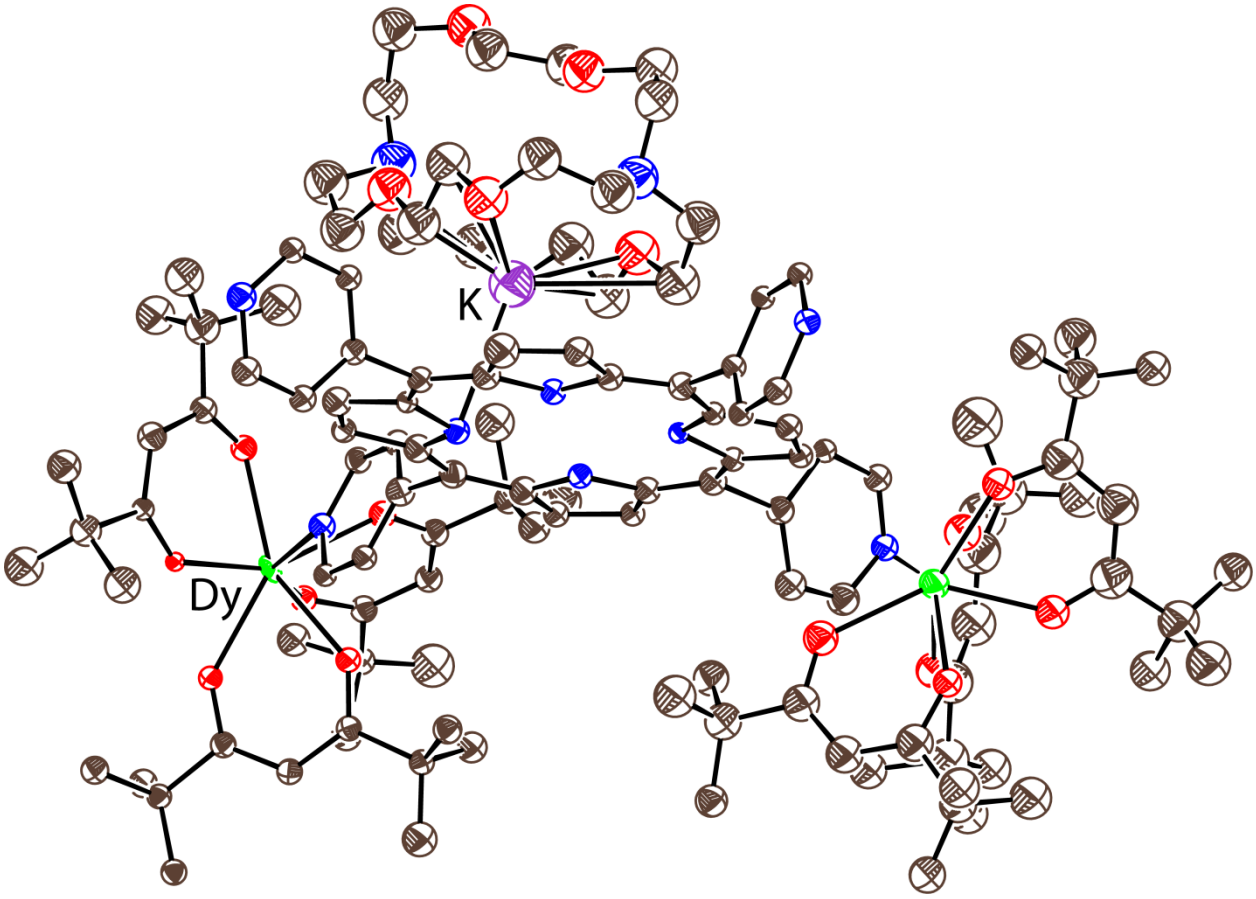

Figure S5. Crystallographically independent part and repeating unit of polymer **1**. Solvent *n*-hexane molecules (4 molecules per one crystallographically independent part) are strongly disordered and are squeezed from the crystal structure of **1**. Thermal ellipsoid plot with the 30% probability is shown. All fragments are shown in major orientations.

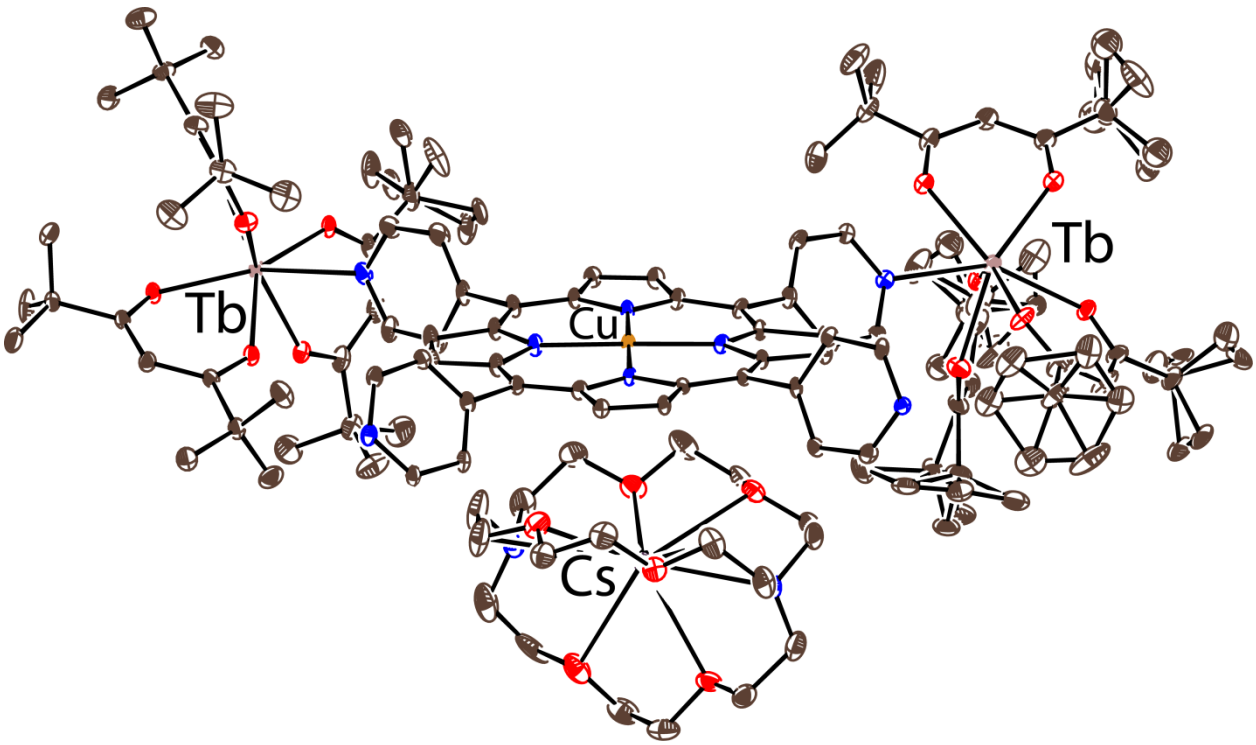

Figure S6. Crystallographically independent part and repeating unit of polymer **2**. Solvent *n*-hexane molecules (4 molecules per one crystallographically independent part) are strongly disordered and are squeezed from the crystal structure of **2**. Thermal ellipsoid plot with the 30% probability is shown. Some of *tert*-Bu groups of TMHD are disordered between two orientations.

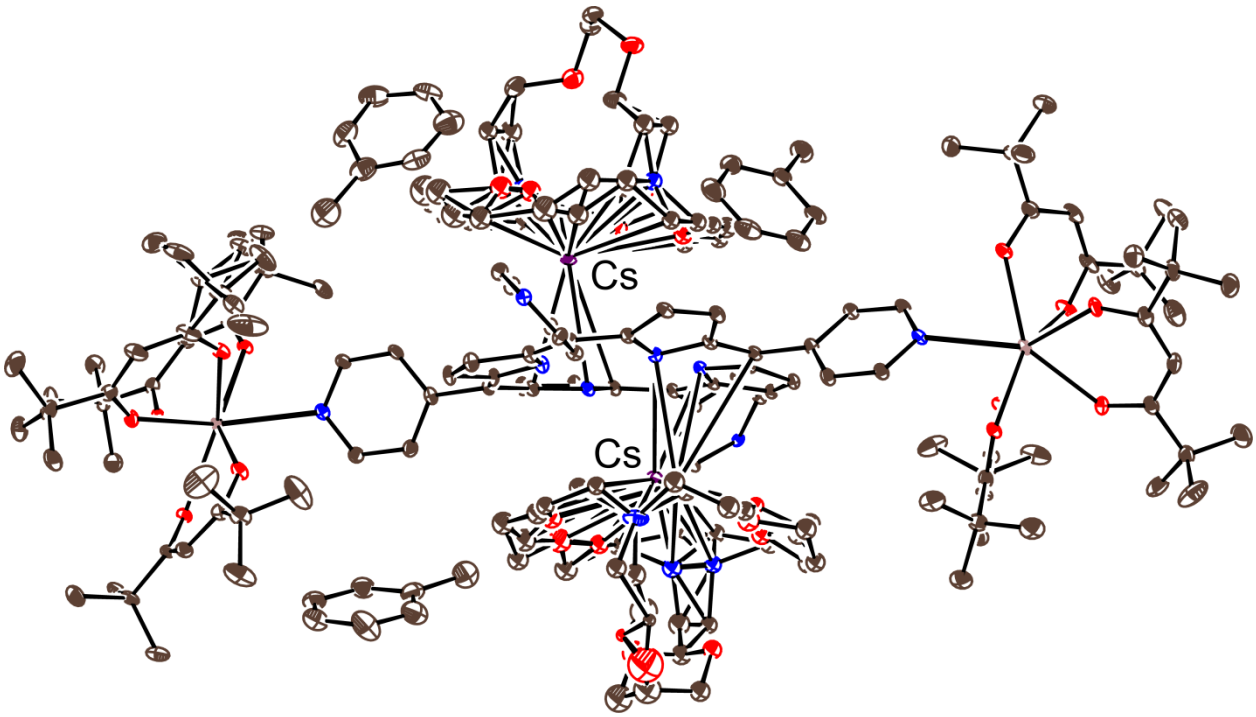

Figure S7. Crystallographically independent part and repeating unit of polymer **3**. Thermal ellipsoid plot with the 30% probability is shown. Some of *tert*-Bu groups of TMHD are disordered between two orientations with the 0.59(6)/0.41(6) occupancies. One of three toluene molecules is disordered between two orientations with the 0.503(9)/0.497(9) occupancies. One of two {Crypt(Cs^+)} cations has two different positions relative to the porphyrin with the 0.701(2)/0.299(2) occupancies. Another {Crypt(Cs^+)} cation has disordered between two positions -CH_2-CH_2-O- fragments (upper cation in figure) with the 0.523(7)/0.477(7) occupancies. .

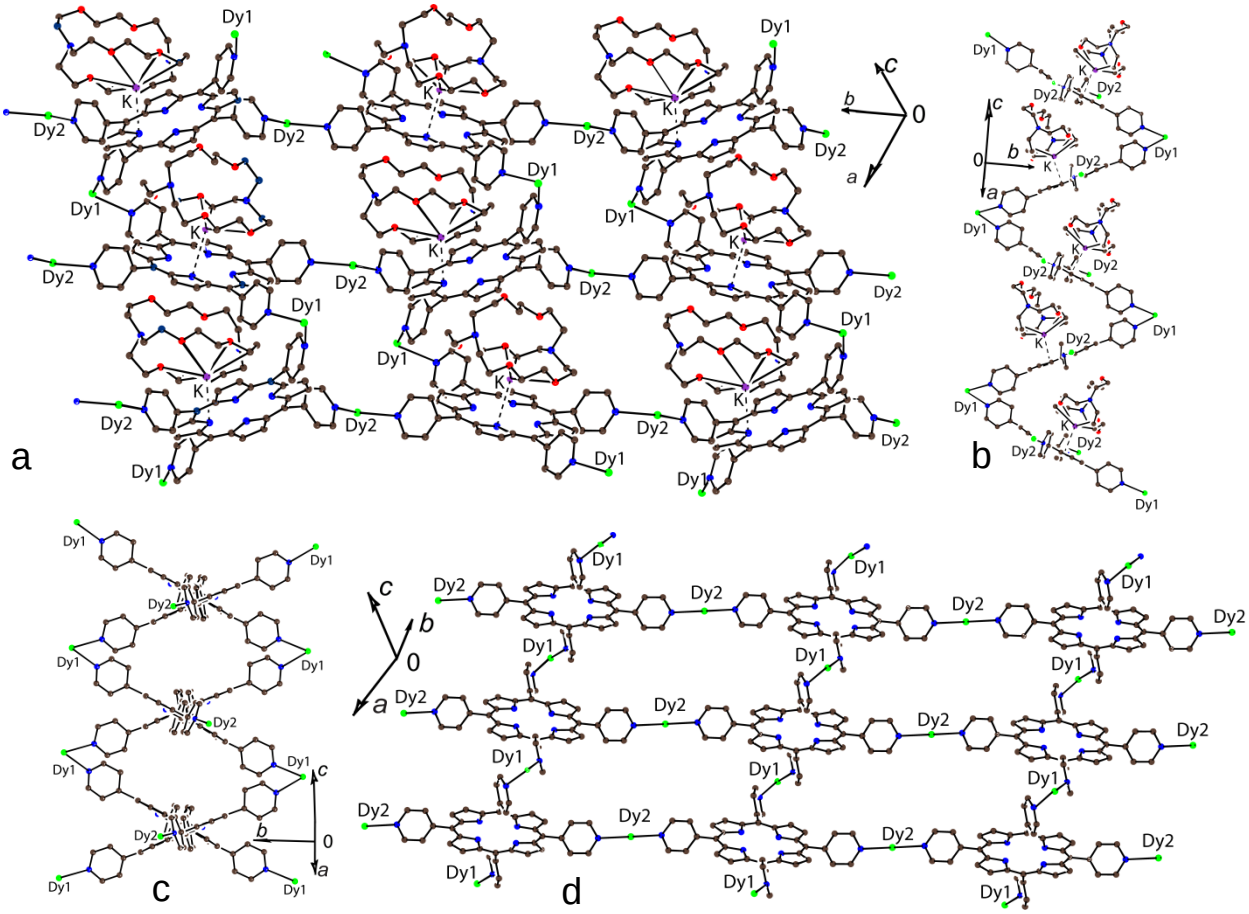

Fig. S8. View on the 2D zig-zag polymer formed in **1**: (a) view on the folded 2D polymer and (b) along a zig-zag polymer (only one H_2TPyP molecule depth is shown); view with the {Crypt(K^+)} cations whereas bulky TMHD ligands at Dy^{III} are not shown. View on the same polymer but without {Crypt(K^+)} cations: (c) view along a zig-zag polymer (two H_2TPyP molecules depth is shown); (d) view on the folded 2D polymer.

Table S2. Shape analysis of the metal polymer **1** using SHAPE 2.1 software.[1] The smaller value is the closer geometry of the coordination polyhedron of a metal center gets to the perfect one.

Dy1

			Symmetry	**100 K**
1	OP-8	Octagon	D_{8h}	29.447
2	HPY-8	Heptagonal pyramid	C_{7v}	23.229
3	HBPY-8	Hexagonal bipyramid	D_{6h}	16.404
4	CU-8	Cube	O_h	10.540
5	SAPR-8	Square antiprism	D_{4d}	0.717
6	TDD-8	Triangular dodecahedron	D_{2d}	1.966
7	JGBF-8	Johnson - Gyrobifastigium (J26)	D_{2d}	13.862
8	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	D_{3h}	26.088
9	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	C_{2v}	2.078
10	BTPR-8	Biaugmented trigonal prism	C_{2v}	2.068
11	JSD-8	Snub disphenoid (J84)	D_{2d}	3.354
12	TT-8	Triakis tetrahedron	T_d	11.298
13	ETBPY-8	Elongated trigonal bipyramid	D_{3h}	23.288

Dy2

			Symmetry	**100 K**
1	OP-8	Octagon	D_{8h}	28.941
2	HPY-8	Heptagonal pyramid	C_{7v}	23.189
3	HBPY-8	Hexagonal bipyramid	D_{6h}	16.455
4	CU-8	Cube	O_h	9.697
5	SAPR-8	Square antiprism	D_{4d}	0.546
6	TDD-8	Triangular dodecahedron	D_{2d}	2.689
7	JGBF-8	Johnson - Gyrobifastigium (J26)	D_{2d}	15.914
8	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	D_{3h}	27.095
9	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	C_{2v}	2.528
10	BTPR-8	Biaugmented trigonal prism	C_{2v}	2.649
11	JSD-8	Snub disphenoid (J84)	D_{2d}	4.807
12	TT-8	Triakis tetrahedron	T_d	10.475
13	ETBPY-8	Elongated trigonal bipyramid	D_{3h}	24.132

Table S3. Shape analysis of the metal polymer **2** using SHAPE 2.1 software.[1] The smaller value is the closer geometry of the coordination polyhedron of a metal center gets to the perfect one.

Tb1

			Symmetry	**100 K**
1	OP-8	Octagon	D_{8h}	29.090
2	HPY-8	Heptagonal pyramid	C_{7v}	22.890
3	HBPY-8	Hexagonal bipyramid	D_{6h}	16.653
4	CU-8	Cube	O_h	9.946
5	SAPR-8	Square antiprism	D_{4d}	0.607
6	TDD-8	Triangular dodecahedron	D_{2d}	1.950
7	JGBF-8	Johnson - Gyrobifastigium (J26)	D_{2d}	15.101
8	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	D_{3h}	25.911
9	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	C_{2v}	1.987
10	BTPR-8	Biaugmented trigonal prism	C_{2v}	1.793
11	JSD-8	Snub disphenoid (J84)	D_{2d}	4.339
12	TT-8	Triakis tetrahedron	T_d	10.782
13	ETBPY-8	Elongated trigonal bipyramid	D_{3h}	23.516

Tb2

			Symmetry	**100 K**
1	OP-8	Octagon	D_{8h}	28.536
2	HPY-8	Heptagonal pyramid	C_{7v}	23.580
3	HBPY-8	Hexagonal bipyramid	D_{6h}	16.451
4	CU-8	Cube	O_h	9.552
5	SAPR-8	Square antiprism	D_{4d}	0.394
6	TDD-8	Triangular dodecahedron	D_{2d}	2.396
7	JGBF-8	Johnson - Gyrobifastigium (J26)	D_{2d}	16.417
8	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	D_{3h}	27.086
9	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	C_{2v}	2.062
10	BTPR-8	Biaugmented trigonal prism	C_{2v}	5.154
11	JSD-8	Snub disphenoid (J84)	D_{2d}	3.789
12	TT-8	Triakis tetrahedron	T_d	10.363
13	ETBPY-8	Elongated trigonal bipyramid	D_{3h}	23.421

Table S3. Shape analysis of the metal polymer **3** using SHAPE 2.1 software.[1] The smaller value is the closer geometry of the coordination polyhedron of a metal center gets to the perfect one.

Tb1

			Symmetry	**100 K**
1	OP-8	Octagon	D_{8h}	28.834
2	HPY-8	Heptagonal pyramid	C_{7v}	23.646
3	HBPY-8	Hexagonal bipyramid	D_{6h}	16.465
4	CU-8	Cube	O_h	9.846
5	SAPR-8	Square antiprism	D_{4d}	0.367
6	TDD-8	Triangular dodecahedron	D_{2d}	2.176
7	JGBF-8	Johnson - Gyrobifastigium (J26)	D_{2d}	16.055
8	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	D_{3h}	28.216
9	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	C_{2v}	2.677
10	BTPR-8	Biaugmented trigonal prism	C_{2v}	2.291
11	JSD-8	Snub disphenoid (J84)	D_{2d}	5.017
12	TT-8	Triakis tetrahedron	T_d	10.694
13	ETBPY-8	Elongated trigonal bipyramid	D_{3h}	24.225

Tb2

			Symmetry	**100 K**
1	OP-8	Octagon	D_{8h}	30.325
2	HPY-8	Heptagonal pyramid	C_{7v}	23.461
3	HBPY-8	Hexagonal bipyramid	D_{6h}	16.099
4	CU-8	Cube	O_h	9.401
5	SAPR-8	Square antiprism	D_{4d}	0.662
6	TDD-8	Triangular dodecahedron	D_{2d}	1.500
7	JGBF-8	Johnson - Gyrobifastigium (J26)	D_{2d}	15.873
8	JETBPY-8	Johnson - Elongated triangular bipyramid (J14)	D_{3h}	28.518
9	JBTP-8	Johnson - Biaugmented trigonal prism (J50)	C_{2v}	2.635
10	BTPR-8	Biaugmented trigonal prism	C_{2v}	1.660
11	JSD-8	Snub disphenoid (J84)	D_{2d}	4.230
12	TT-8	Triakis tetrahedron	T_d	10.192
13	ETBPY-8	Elongated trigonal bipyramid	D_{3h}	24.506

Magnetic data.

Table S4. Magnetic data obtained by using SQUID magnetometer and EPR spectroscopy for **1**-**4.**

Compound	SQUID	EPR
1	$\chi_M T$ value is 28.75 emu K/mol at 300 K Magnetization is 11.23 $\mu_B N_A$ at 2 K and 50 kOe.	EPR signal from Dy(III) is observed below 20 K. 13 K, g_1 = 9.2766 (ΔH = 41.5 mT), g_2 = 5.9359 (ΔH = 68.6 mT), g_3 = 3.5946 (ΔH = 160.0 mT) EPR signal from $H_2TPyP^{\bullet-}$ 207 K, g_1 = 2.0030 (ΔH = 0.73 mT) 24K, g_1 = 2.0017 (ΔH = 0.72 mT), g_2 = 1.9966 (ΔH = 0.53 mT) 4.2 K, g_1 = 2.0020 (ΔH = 0.79 mT), g_2 = 1.9966 (ΔH = 0.51 mT)
2	$\chi_M T$ value is 24.35 emu K/mol at 300 K Magnetization is 12.38 $\mu_B N_A$ at 2 K and 50 kOe.	EPR signal from Cu^{II} 100 K, g_1 = 2.210, A_1 = 20.695 mT, g_2 = 1.9916. 4.2 K, g_1 = 2.1963, A_1 = 20.750 mT,g_2 = 2.0437. Signal from Tb(III) is not observed
3	$\chi_M T$ value is 23.60 emu K/mol at 300 K Magnetization is 10.30 $\mu_B N_A$ at 2 K and 50 kOe	**3** is EPR silent in whole studied temperature range
4	$\chi_M T$ value is 15.48 emu K/mol at 300 K Magnetization is 13.86 $\mu_B N_A$ at 2 K and 50 kOe Theoretical values are $\chi_M T$ = 15.55 emu K/mol at 300 K and magnetization is 13.80$\mu_B N_A$ at 2 K and 50 kOe. D = –0.017 cm^{-1} from EPR.	EPR signal from Gd(III) g_1 = 2.424, g_2 = 1.750, g_3 = 0.709, D = –0.017 cm^{-1}, E = –0,011 cm^{-1} H_2TPyP^{2-} dianion is EPR silent

Compound {Cryptand(K^+)}{H_2TPyP·[Dy^{III}(TMHD)$_3$]$_2$}$^-$·3C_6H_{14} (1)

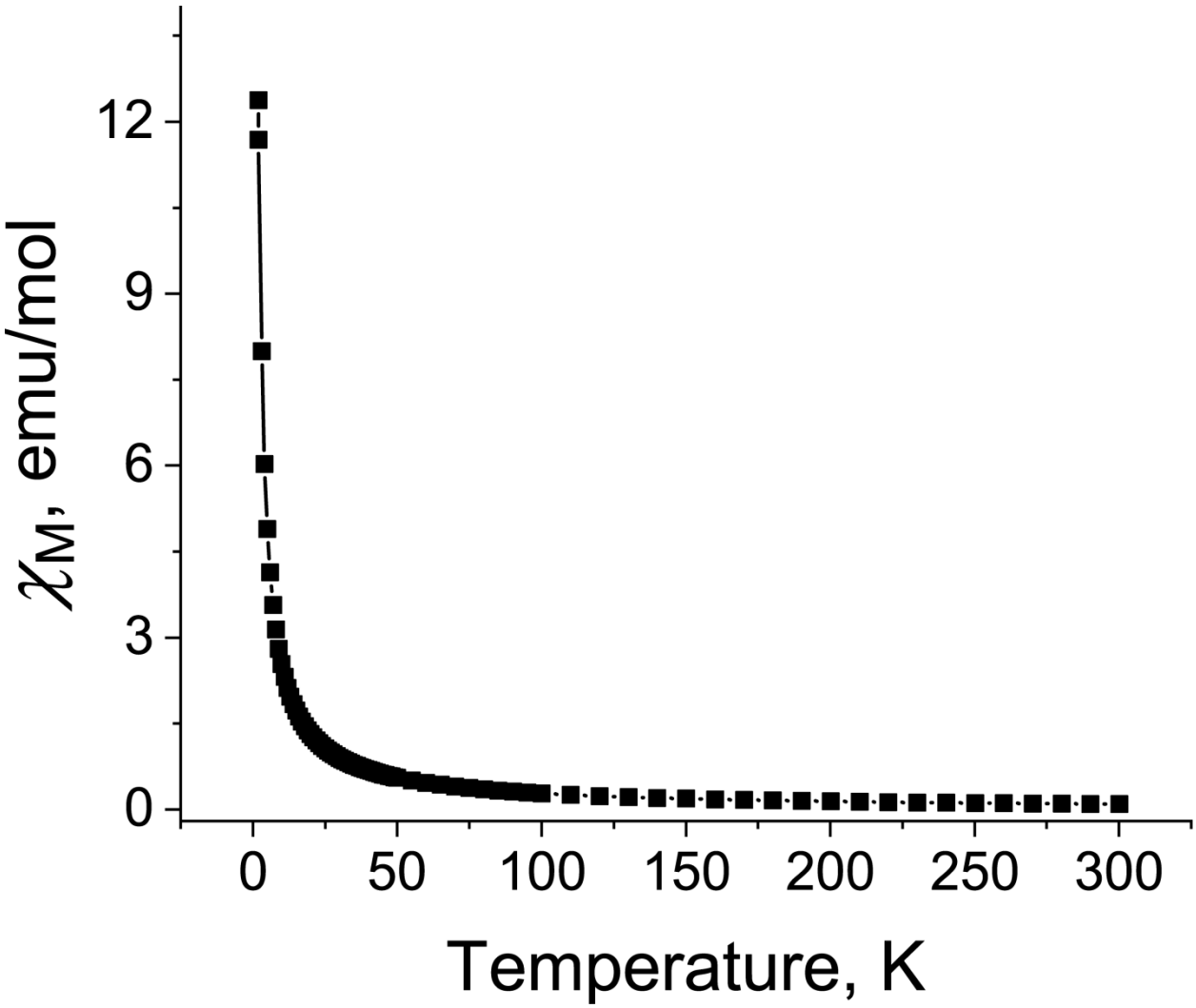

Figure S9. Temperature dependence for molar magnetic susceptibility of polycrystalline **1** in the 1.9-300 K range after the subtraction of temperature independent contribution.

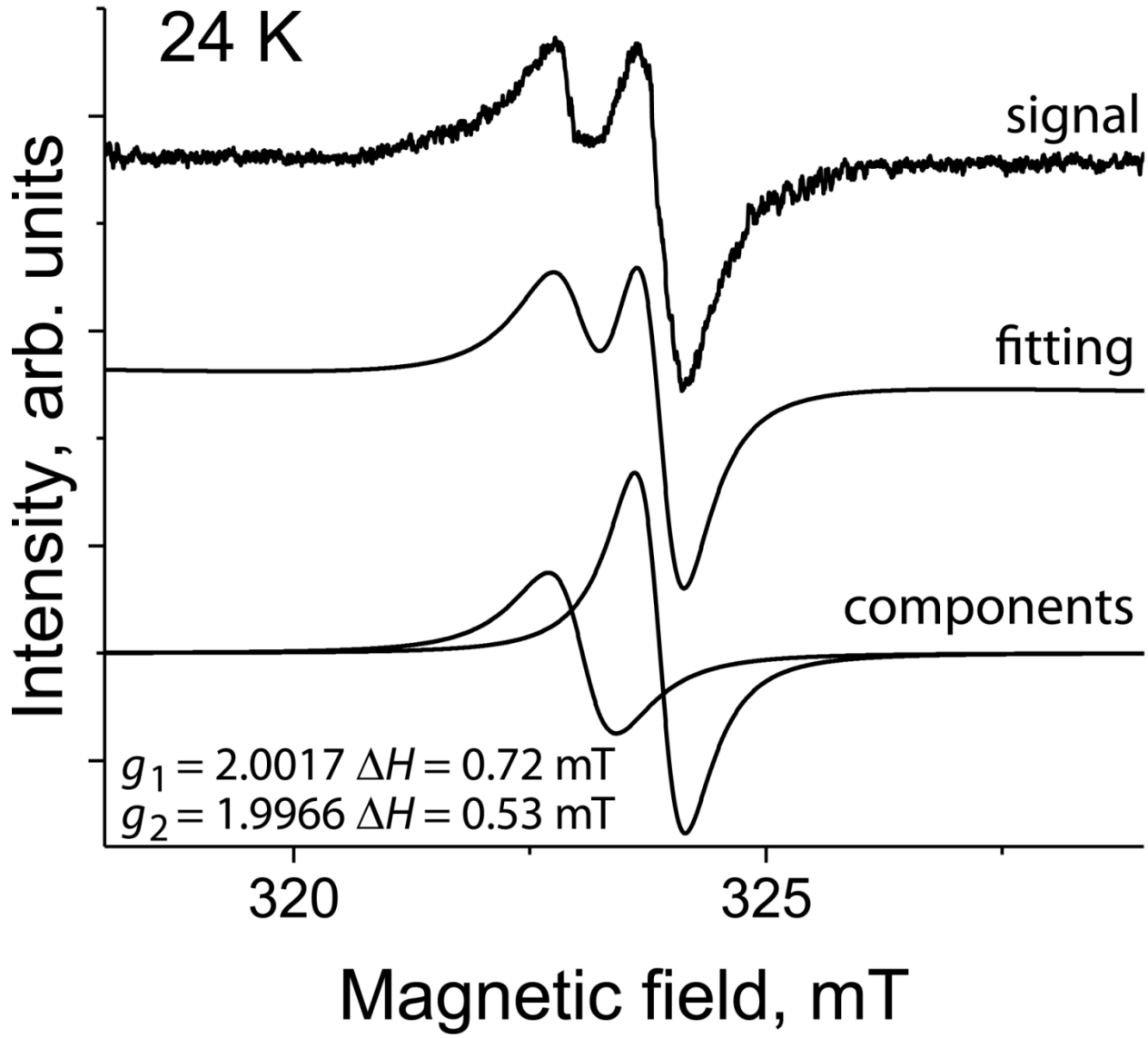

Fig. S10. EPR spectrum of polycrystalline **1** at 24 K Below fitting of the signal by two Lorentzian components is shown (parameters of components are given)

Compound {Cryptand(Cs^{+})}{CuTPyP·[$Tb^{III}(TMHD)_3]_2$}$^{2-}$·$3C_6H_{14}$ (2).

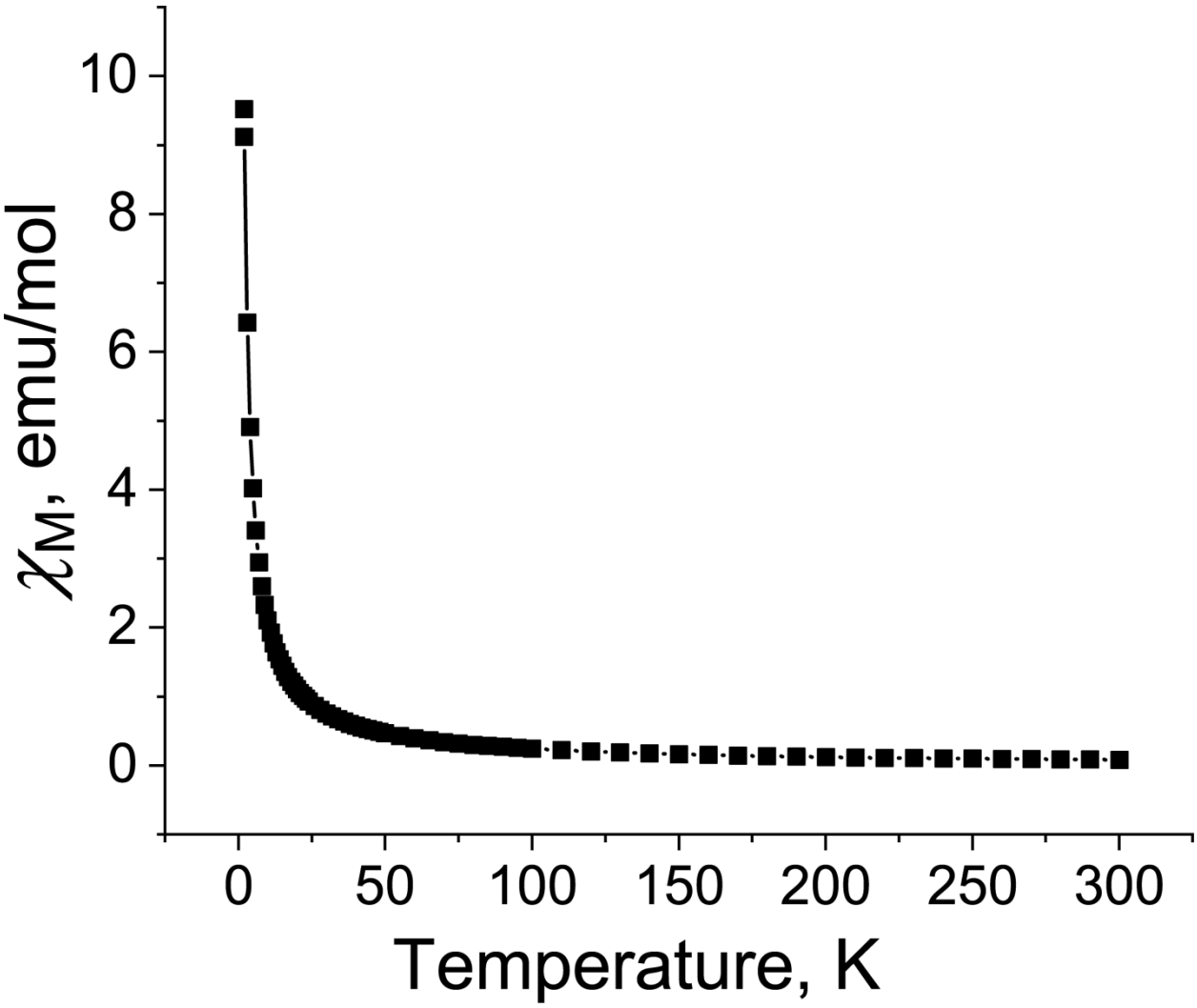

Figure S11. Temperature dependence for molar magnetic susceptibility of polycrystalline **2** in the 1.9-300 K range after the subtraction of temperature independent contribution.

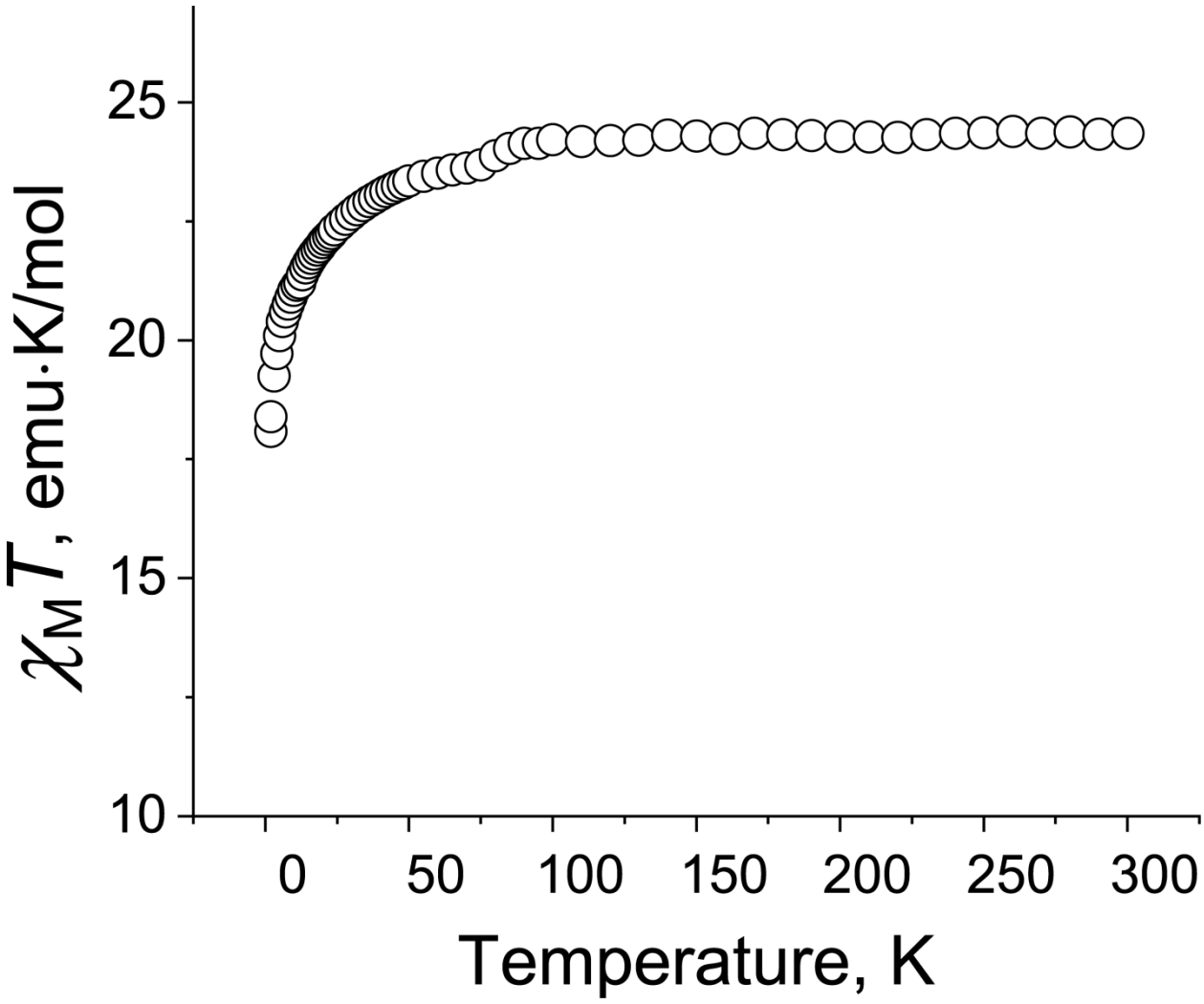

Fig. S12. Temperature dependence of the $\chi_M T$ values for polycrystalline **2** in the 1.9-300 K range.

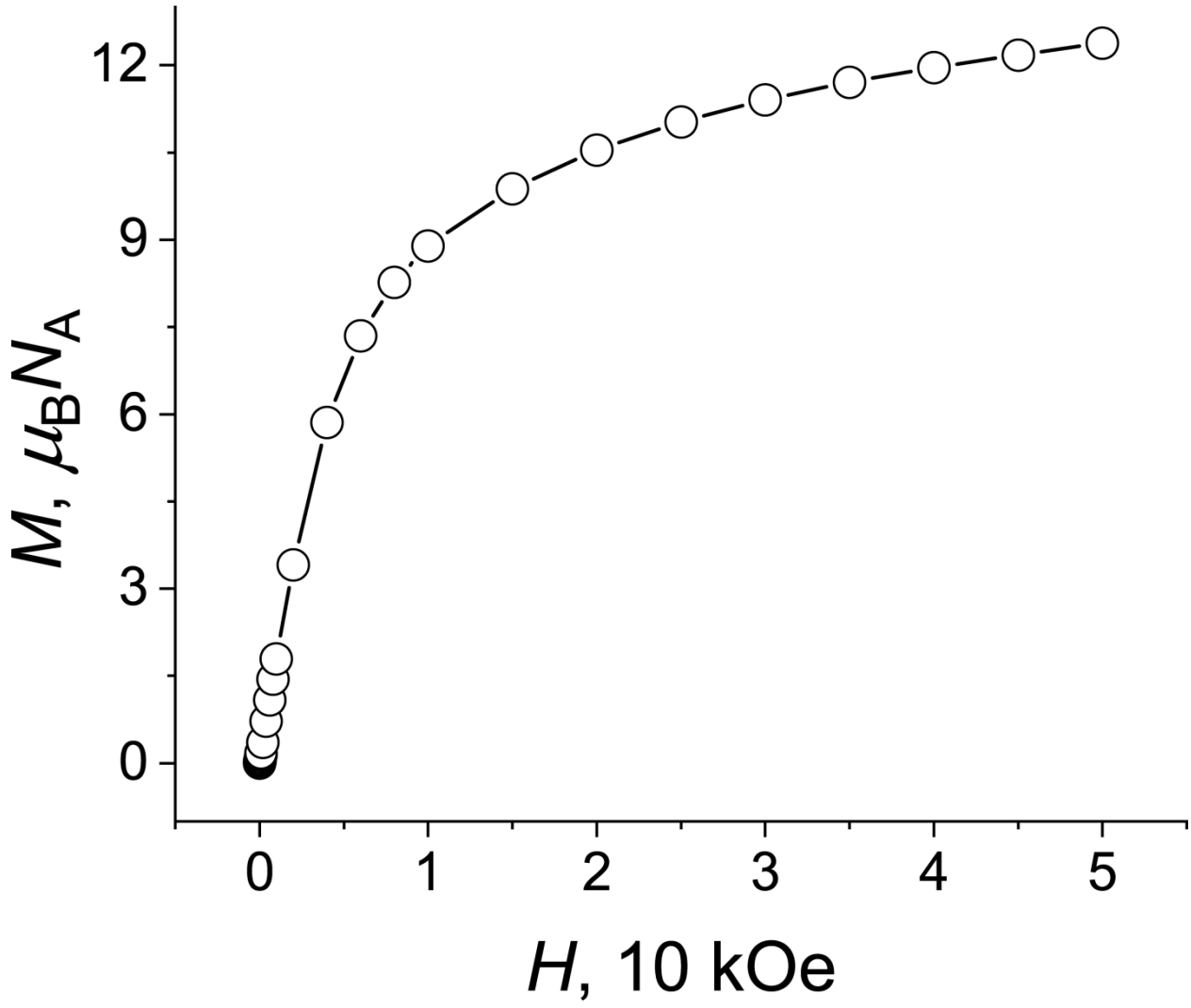

Figure S13. Dependence of magnetization of polycrystalline **2** *vs* magnetic field up to 50 kOe at 2 K (black line is a guide to the eye).

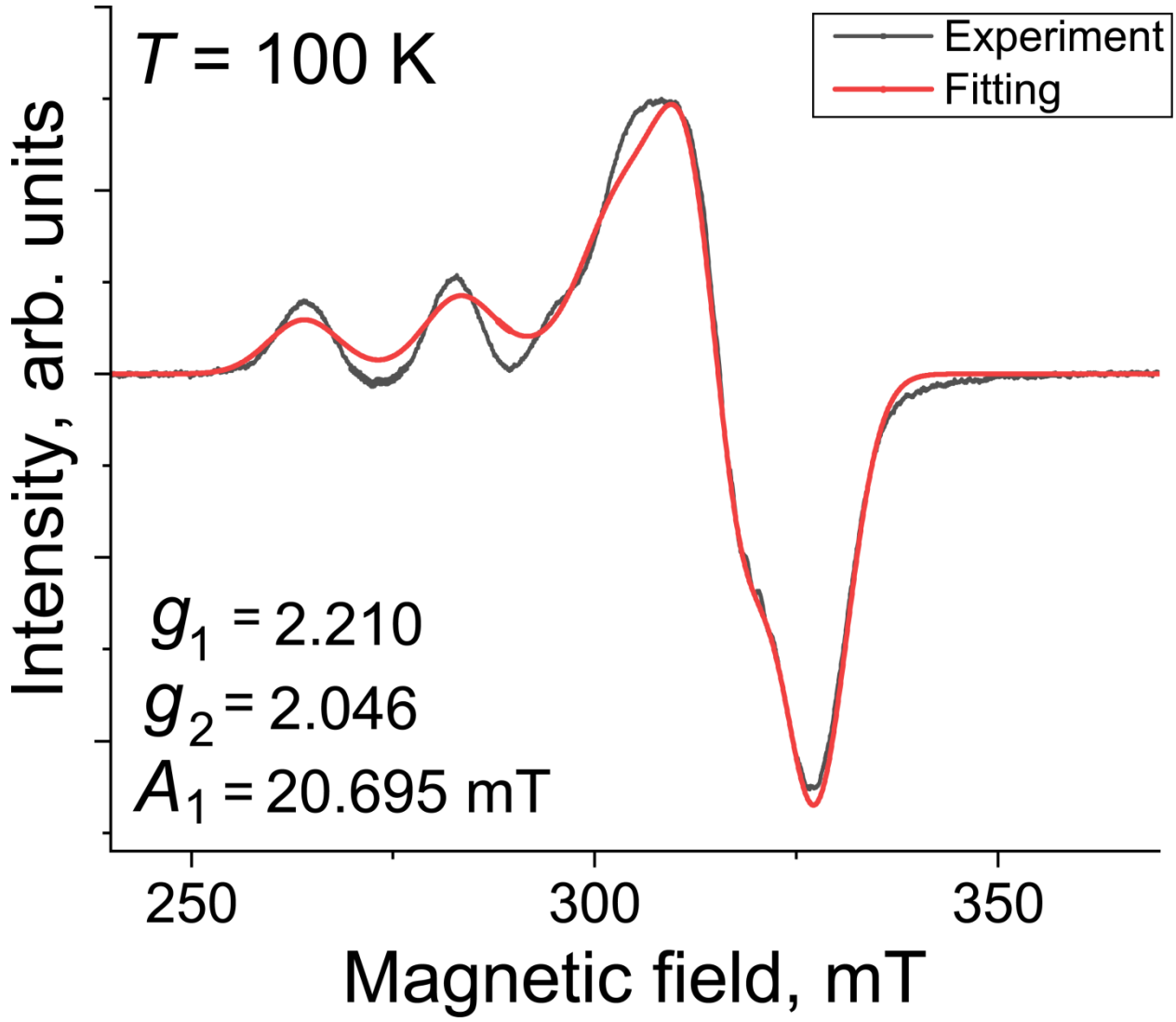

Fig. S14. EPR spectrum of polycrystalline **2** at 100 K. Determination of splitting parameter *A* as well as parallel and perpendicular *g*-factors by Easyspin programm[2] is shown.

Compound {Cryptand(Cs^+)}$_2${H_2TPyP·[Tb^{III}(TMHD)$_3$]$_2$}$^{2-}$·3$C_6H_5CH_3$ (3)

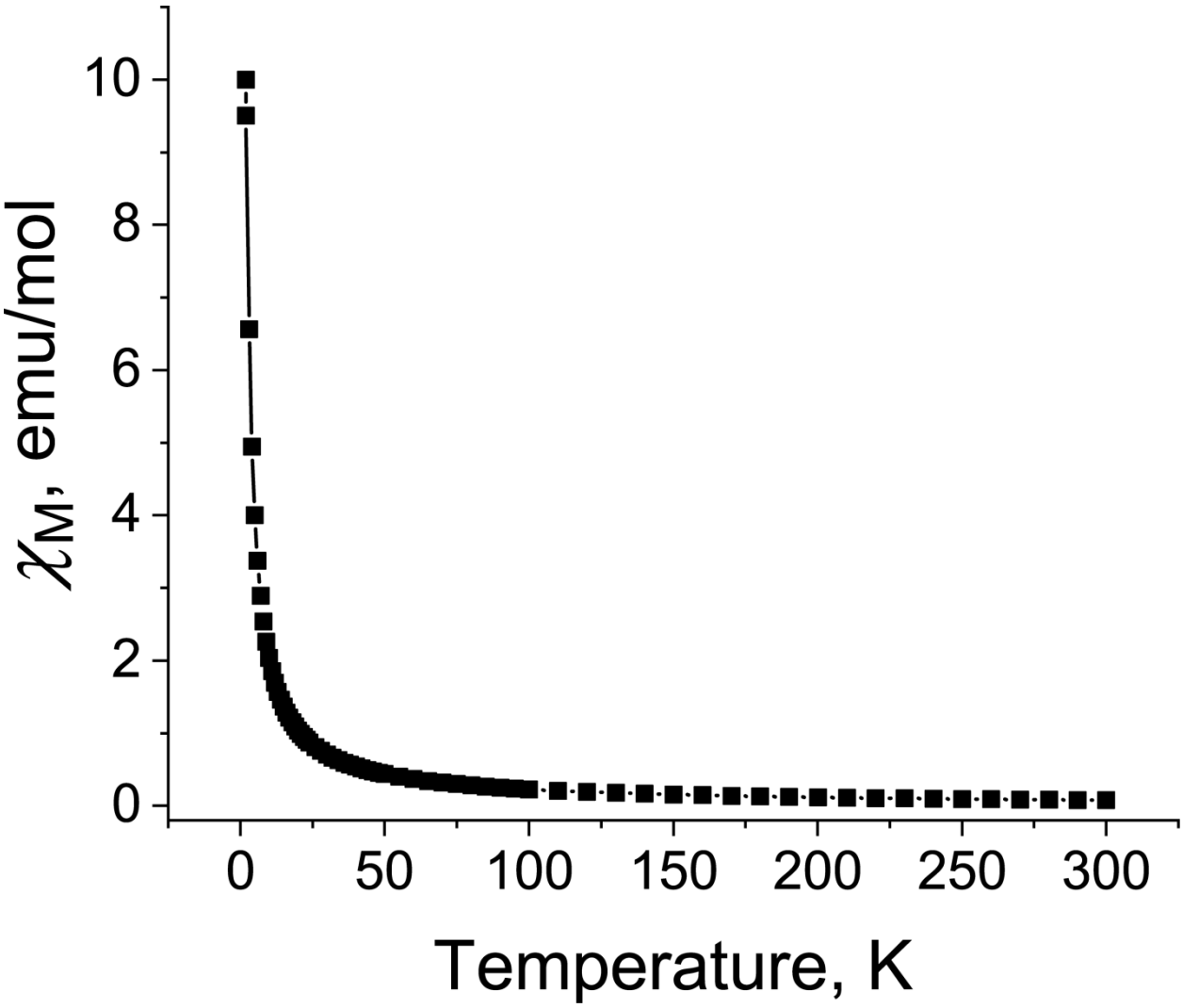

Figure S15. Temperature dependence for molar magnetic susceptibility of polycrystalline **3** in the 1.9-300 K range after the subtraction of temperature independent contribution.

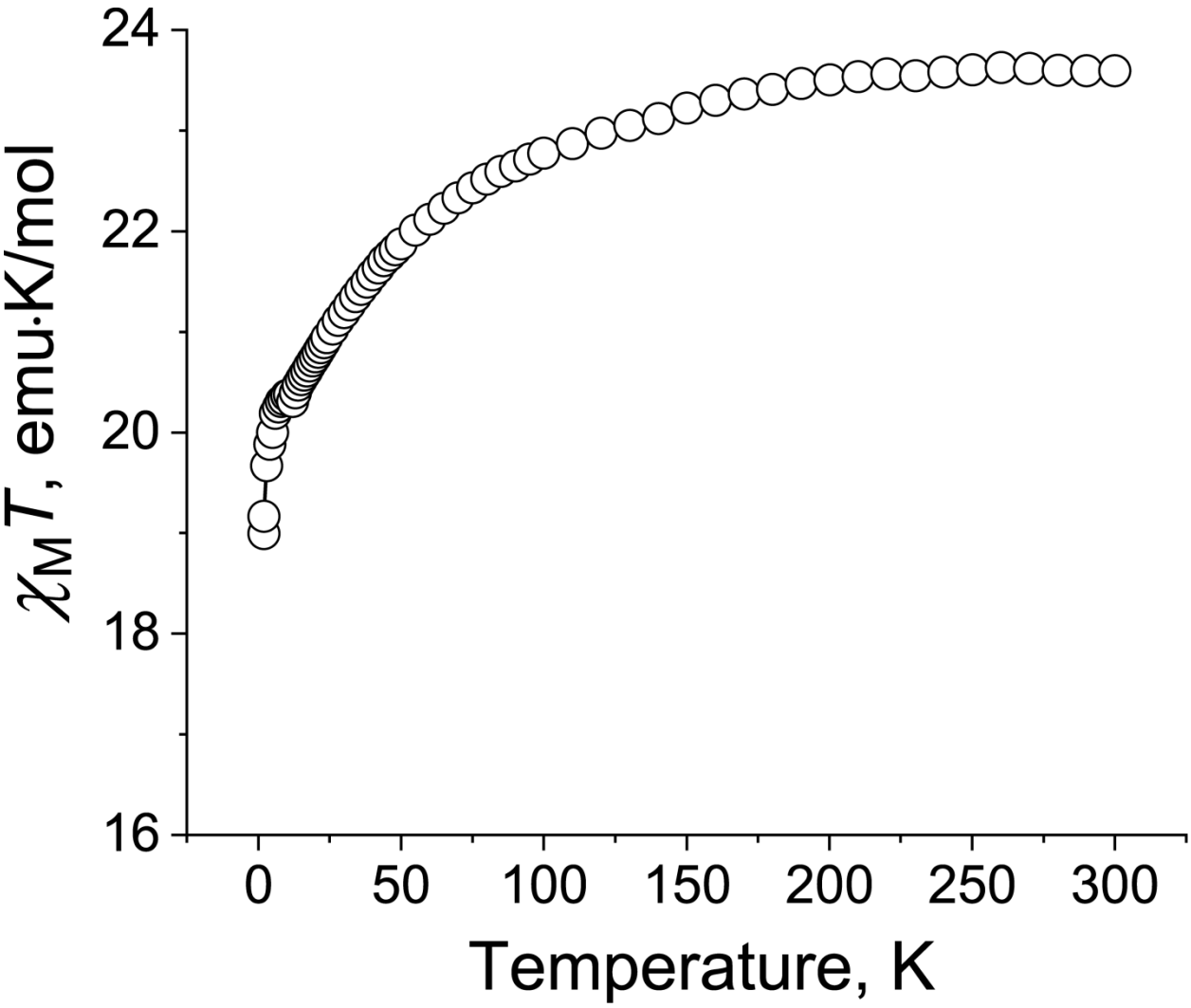

Fig. S16. Temperature dependence of the $\chi_M T$ values for polycrystalline **3** in the 1.9-300 K range.

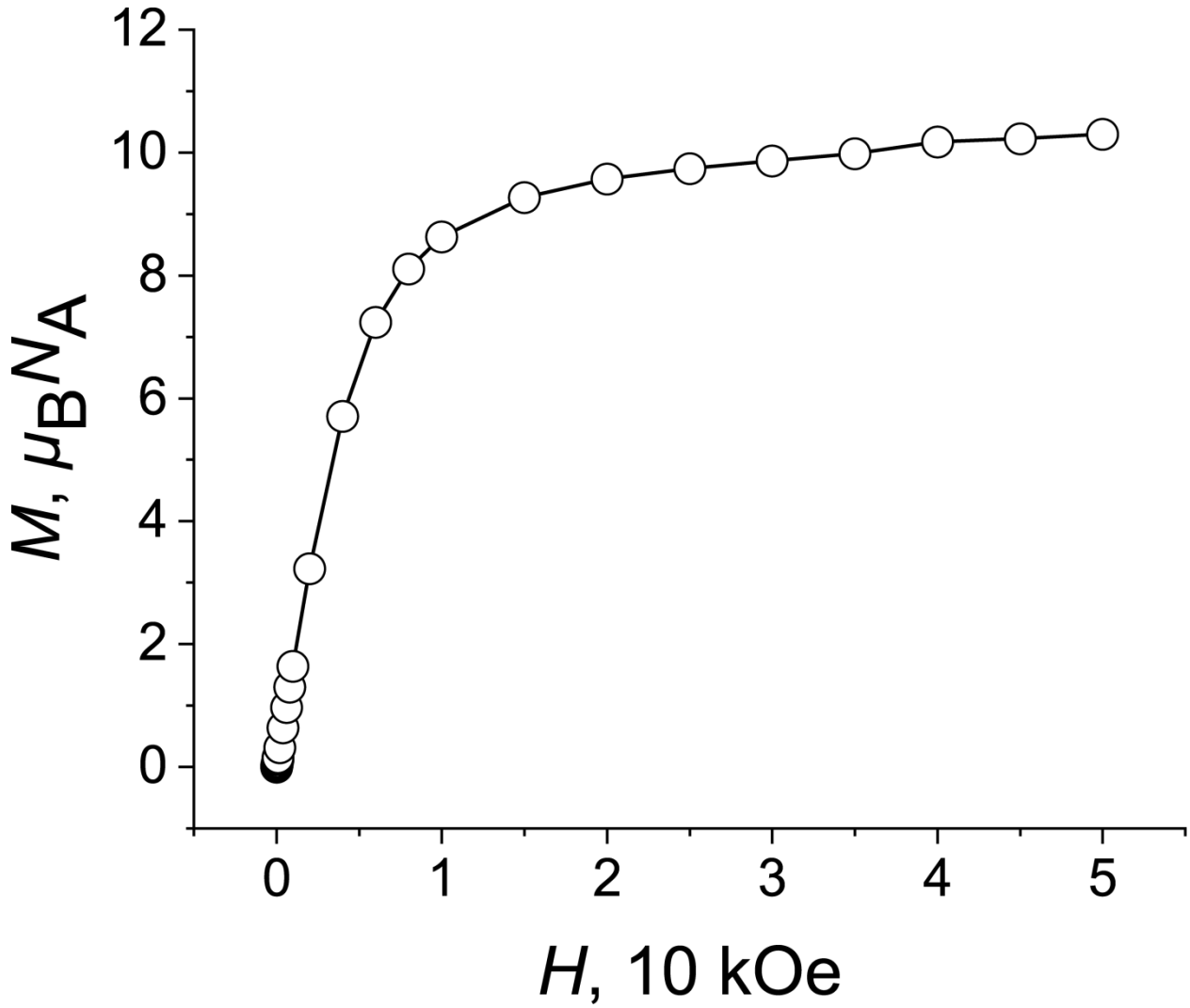

Figure S17. Dependence of magnetization of polycrystalline **3** *vs* magnetic field up to 50 kOe at 2 K (black line is a guide to the eye).

Compound {Cryptand(Cs^+)}$_2${H_2TPyP·[Gd^{III}(TMHD)$_3$]$_2$}$^{2-}$·3$C_6H_5CH_3$ (4)

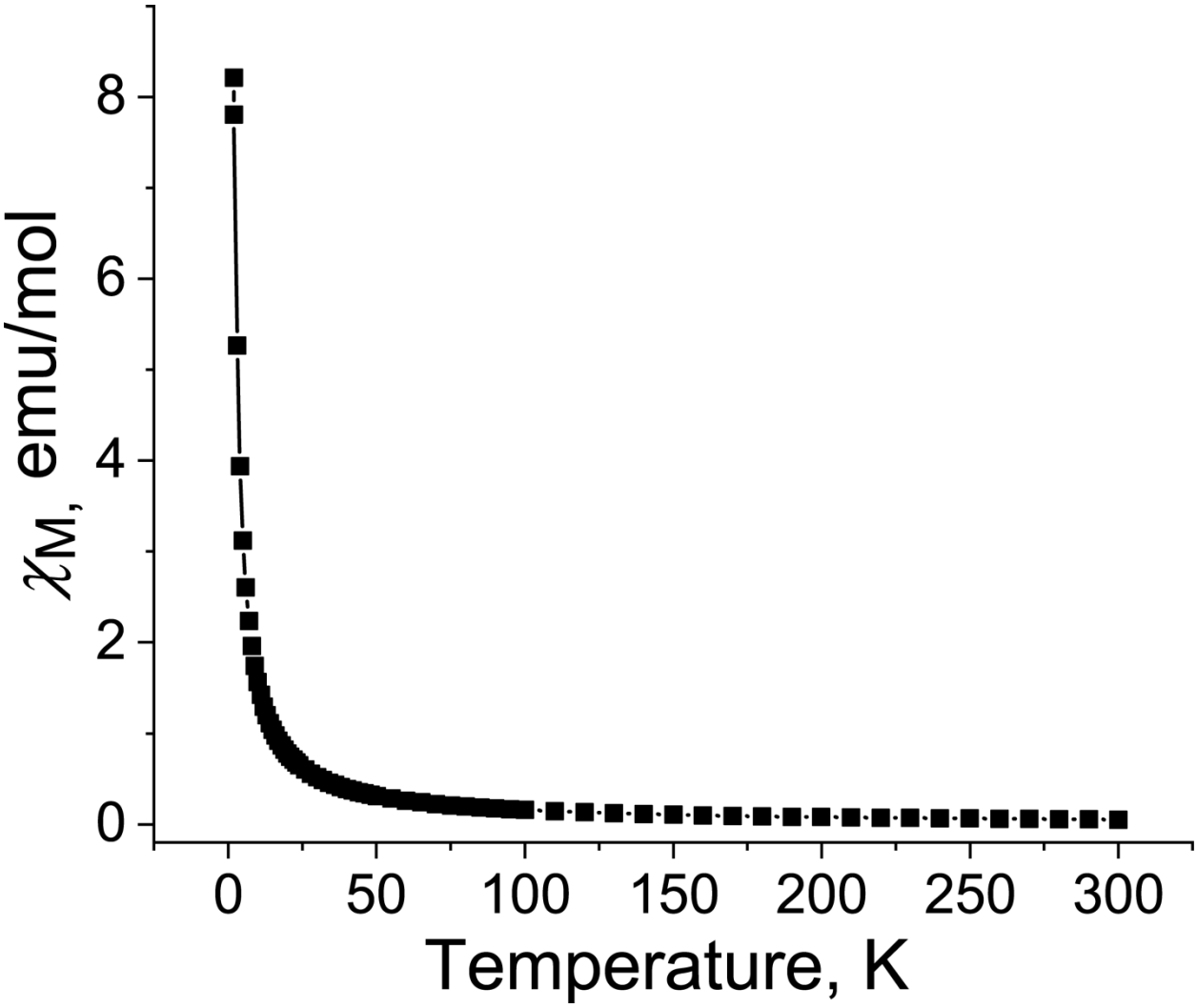

Figure S18. Temperature dependence for molar magnetic susceptibility of polycrystalline **4** in the 1.9-300 K range after the subtraction of temperature independent contribution.

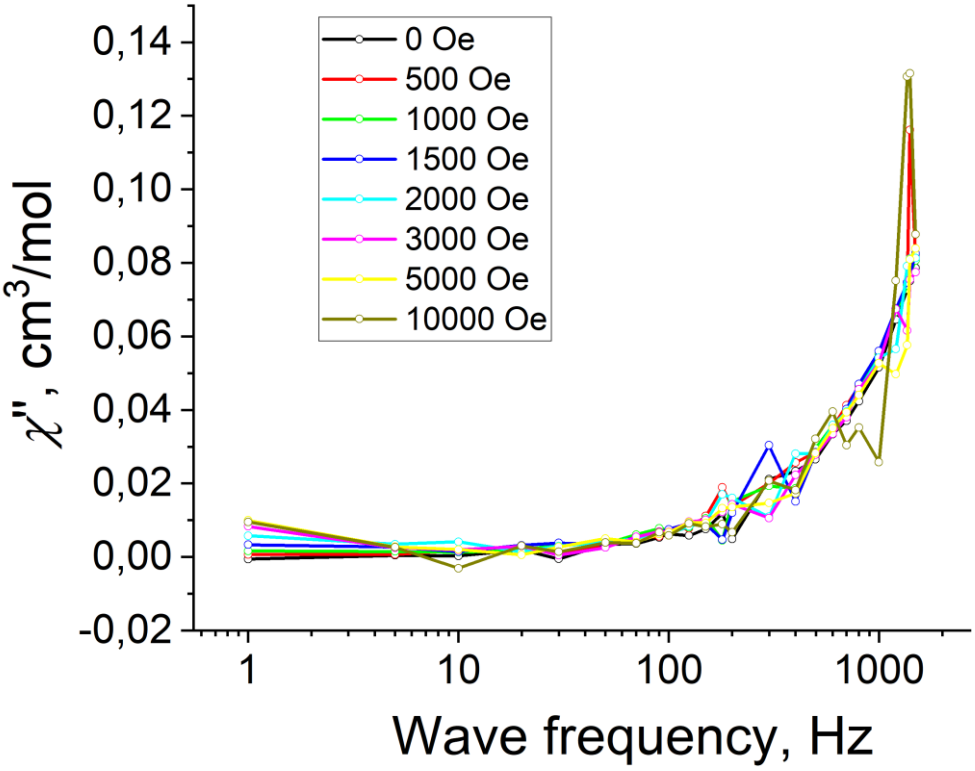

Figure S19. Frequency dependences of out-of-phase (χ'') AC susceptibility for **1** at different applied static magnetic fields HDC and T = 2 K.

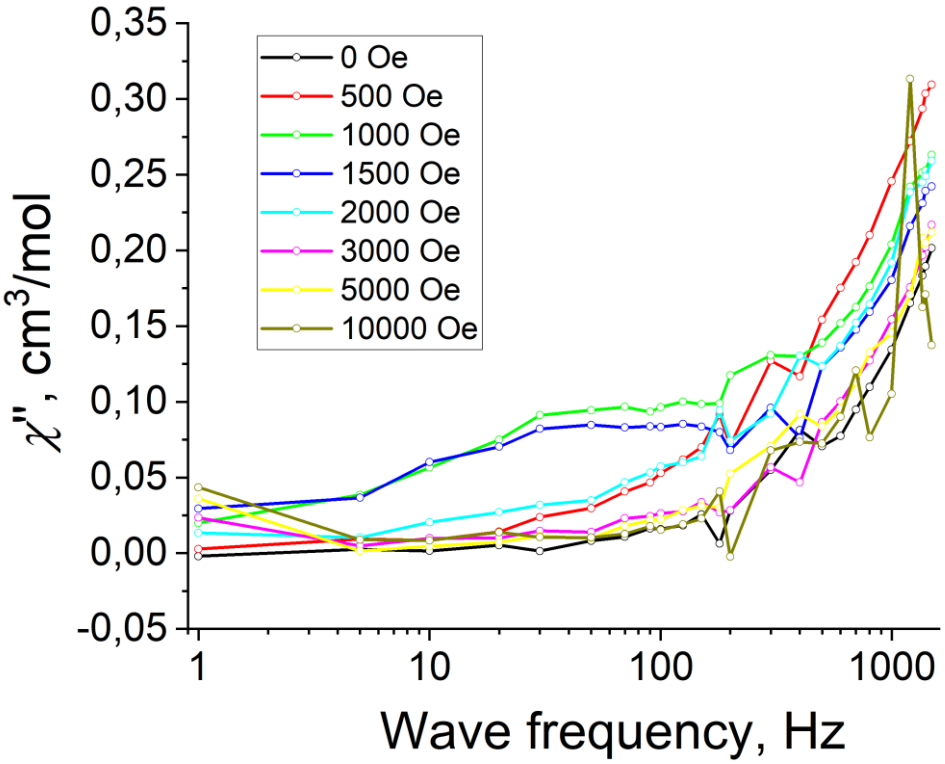

Figure S20. Frequency dependences of out-of-phase (χ'') AC susceptibility for **2** at different applied static magnetic fields HDC and T = 2 K.

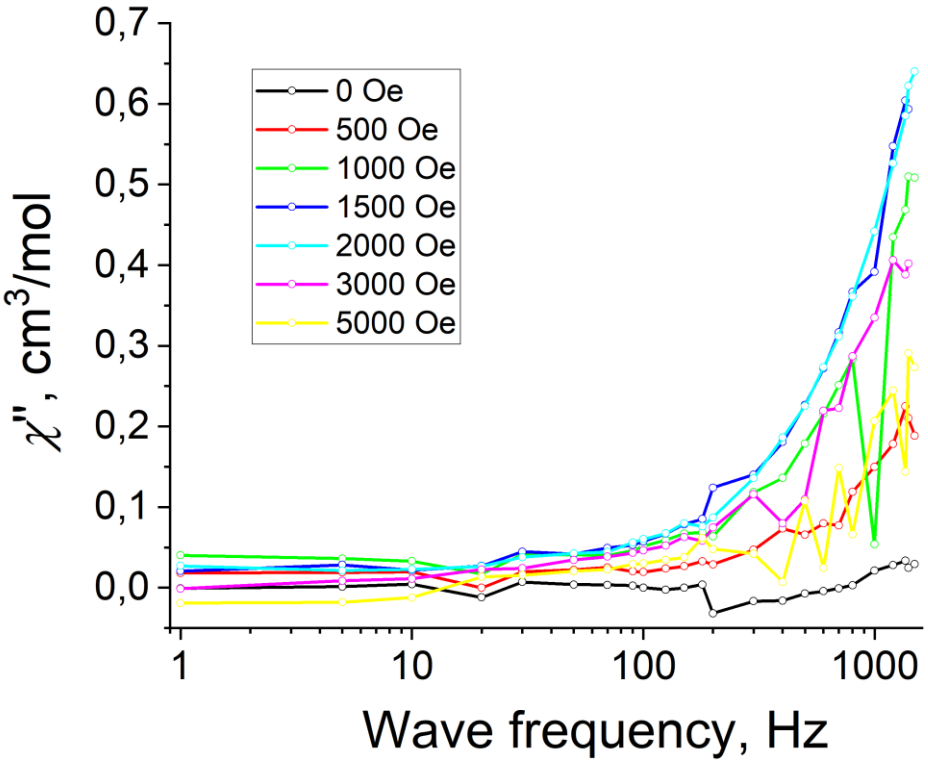

Figure S21. Frequency dependences of out-of-phase (χ'') AC susceptibility for **3** at different applied static magnetic fields HDC and T = 2 K.

Table S5. Bond lengths and angles for **1**

Atom–Atom	Length [Å]
O501–C502	1.431(14)
O501–C503	1.417(14)
N501–C501	1.468(15)
N501–C507	1.459(15)
N501–C513	1.468(15)
C501–H50A	0.9900
C501–H50B	0.9900
C501–C502	1.504(15)
O502–C504	1.428(14)
O502–C505	1.430(14)
N502–C506	1.464(15)
N502–C512	1.466(15)
N502–C518	1.473(15)
C502–H50C	0.9900
C502–H50D	0.9900
O503–C508	1.425(14)
O503–C509	1.420(14)
C503–H50E	0.9900
C503–H50F	0.9900
C503–C504	1.503(15)
O504–C510	1.427(14)
O504–C511	1.420(14)
C504–H50G	0.9900
C504–H50H	0.9900
O505–C514	1.428(14)
O505–C515	1.419(14)
C505–H50I	0.9900
C505–H50J	0.9900
C505–C506	1.505(15)
O506–C516	1.427(14)
O506–C517	1.424(14)
C506–H50K	0.9900
C506–H50L	0.9900
C507–H50M	0.9900
C507–H50N	0.9900
C507–C508	1.503(15)
C508–H50O	0.9900
C508–H50P	0.9900
C509–H50Q	0.9900
C509–H50R	0.9900
C509–C510	1.495(15)
C510–H51A	0.9900
C510–H51B	0.9900
C511–H51C	0.9900
C511–H51D	0.9900
C511–C512	1.495(14)
C512–H51E	0.9900
C512–H51F	0.9900
C513–H51G	0.9900
C513–H51H	0.9900
C513–C514	1.503(15)
C514–H51I	0.9900
C514–H51J	0.9900
C515–H51K	0.9900
C515–H51L	0.9900
C515–C516	1.501(15)

C516–H51M	0.9900
C516–H51N	0.9900
C517–H51O	0.9900
C517–H51P	0.9900
C517–C518	1.504(14)
C518–H51Q	0.9900
C518–H51R	0.9900
Dy11–O105	2.33(3)
Dy11–O106	2.28(3)
Dy11–O101	2.30(3)
Dy11–O102	2.24(3)
Dy11–O103	2.25(3)
Dy11–O104	2.26(4)
Dy11–N306	2.77(4)
Dy11–N308$^{\#1}$	2.60(10)
Dy21–O204	2.28(3)
Dy21–O206	2.31(3)
Dy21–O201	2.301(18)
Dy21–O203	2.35(3)
Dy21–O205	2.29(2)
Dy21–O202	2.294(19)
Dy21–N307	2.58(2)
Dy21–N305$^{\#2}$	2.61(2)
K51–N304	3.02(3)
K51–C315	3.54(4)
K51–C318	3.40(3)
O105–C127	1.27(2)
O204–C218	1.268(19)
O206–C229	1.261(19)
O201–C205	1.26(2)
C205–C204	1.58(3)
C205–C206	1.39(5)
C204–C201	1.46(3)
C204–C203	1.57(3)
C204–C202	1.52(3)
C201–H20A	0.9800
C201–H20B	0.9800
C201–H20C	0.9800
C203–H20D	0.9800
C203–H20E	0.9800
C203–H20F	0.9800
C202–H20G	0.9800
C202–H20H	0.9800
C202–H20I	0.9800
O106–C129	1.266(19)
O101–C105	1.28(2)
O203–C216	1.261(19)
O102–C107	1.27(2)
O205–C227	1.260(19)
O103–C116	1.27(2)
O104–C118	1.26(2)
O202–C207	1.26(2)
C207–C208	1.58(3)
C207–C206	1.42(5)
C208–C209	1.46(3)
C208–C210	1.57(3)
C208–C211	1.52(3)
C209–H20J	0.9800
C209–H20K	0.9800

C209–H20L	0.9800
C210–H21A	0.9800
C210–H21B	0.9800
C210–H21C	0.9800
C211–H21D	0.9800
C211–H21E	0.9800
C211–H21F	0.9800
N302–H302	0.8800
N302–C305	1.4200
N302–C308	1.4200
C305–C306	1.4200
C305–C304	1.365(18)
C306–H306	0.9500
C306–C307	1.4200
C307–H307	0.9500
C307–C308	1.4200
C308–C309	1.363(18)
N307–C334	1.3900
N307–C333	1.3900
C334–H334	0.9500
C334–C335	1.3900
C335–H335	0.9500
C335–C331	1.3900
C331–C332	1.3900
C331–C314	1.49(4)
C332–H332	0.9500
C332–C333	1.3900
C333–H333	0.9500
N301–H301	0.8800
N301–C320	1.4200
N301–C303	1.4200
C320–C301	1.4200
C320–C319	1.371(18)
C301–H30A	0.9500
C301–C302	1.4200
C302–H30B	0.9500
C302–C303	1.4200
C303–C304	1.365(18)
N304–H304	0.8800
N304–C315	1.4200
N304–C318	1.4200
C315–C316	1.4200
C315–C314	1.357(18)
C316–H316	0.9500
C316–C317	1.4200
C317–H317	0.9500
C317–C318	1.4200
C318–C319	1.368(17)
N305–C324	1.3900
N305–C323	1.3900
C324–H324	0.9500
C324–C325	1.3900
C325–H325	0.9500
C325–C321	1.3900
C321–C322	1.3900
C321–C304	1.49(4)
C322–H322	0.9500
C322–C323	1.3900
C323–H323	0.9500

N306–C328	1.33(5)
N306–C329	1.32(5)
C109–H10A	0.9800
C109–H10B	0.9800
C109–H10C	0.9800
C109–C108	1.48(2)
C108–C110	1.48(2)
C108–C111	1.51(2)
C108–C107	1.556(15)
C110–H11A	0.9800
C110–H11B	0.9800
C110–H11C	0.9800
C111–H11D	0.9800
C111–H11E	0.9800
C111–H11F	0.9800
C226–C224	1.50(2)
C226–C223	1.49(2)
C226–C225	1.48(2)
C226–C227	1.554(14)
C112–H11G	0.9800
C112–H11H	0.9800
C112–H11I	0.9800
C112–C115	1.425(15)
C113–H11J	0.9800
C113–H11K	0.9800
C113–H11L	0.9800
C113–C115	1.423(16)
C336–C337	1.3900
C336–C340	1.3900
C336–C319	1.54(4)
C337–H337	0.9500
C337–C338	1.3900
C338–H338	0.9500
C338–N308	1.3900
N308–C339	1.3900
C339–H339	0.9500
C339–C340	1.3900
C340–H340	0.9500
C114–H11M	0.9800
C114–H11N	0.9800
C114–H11O	0.9800
C114–C115	1.446(16)
C222–H22A	0.9800
C222–H22B	0.9800
C222–H22C	0.9800
C222–C219	1.50(2)
C115–C116	1.559(15)
C230–C232	1.431(15)
C230–C229	1.555(14)
C230–C231	1.441(15)
C230–C233	1.454(15)
C116–C117	1.390(6)
C117–H117	0.9500
C117–C118	1.390(6)
C118–C119	1.546(15)
C119–C120	1.51(2)
C119–C121	1.47(2)
C119–C122	1.48(2)
C120–H12A	0.9800

C120–H12B	0.9800
C120–H12C	0.9800
C220–H22D	0.9800
C220–H22E	0.9800
C220–H22F	0.9800
C220–C219	1.51(2)
C121–H12D	0.9800
C121–H12E	0.9800
C121–H12F	0.9800
C224–H22G	0.9800
C224–H22H	0.9800
C224–H22I	0.9800
C122–H12G	0.9800
C122–H12H	0.9800
C122–H12I	0.9800
C228–H228	0.9500
C228–C227	1.391(6)
C228–C229	1.391(6)
C123–H12J	0.9800
C123–H12K	0.9800
C123–H12L	0.9800
C123–C126	1.50(2)
C232–H23A	0.9800
C232–H23B	0.9800
C232–H23C	0.9800
C124–H12M	0.9800
C124–H12N	0.9800
C124–H12O	0.9800
C124–C126	1.52(2)
C104–C105	1.556(15)
C104–C101	1.432(15)
C104–C102	1.437(15)
C104–C103	1.448(16)
C125–H12P	0.9800
C125–H12Q	0.9800
C125–H12R	0.9800
C125–C126	1.48(2)
C105–C106	1.390(6)
C126–C127	1.552(15)
C127–C128	1.390(6)
C128–H128	0.9500
C128–C129	1.390(6)
C129–C130	1.556(15)
C130–C131	1.436(15)
C130–C132	1.446(15)
C130–C133	1.453(16)
C131–H13A	0.9800
C131–H13B	0.9800
C131–H13C	0.9800
C314–C313	1.360(18)
C132–H13D	0.9800
C132–H13E	0.9800
C132–H13F	0.9800
C219–C221	1.47(2)
C219–C218	1.552(15)
C133–H13G	0.9800
C133–H13H	0.9800
C133–H13I	0.9800
C221–H22J	0.9800

C221–H22K	0.9800
C221–H22L	0.9800
C223–H22M	0.9800
C223–H22N	0.9800
C223–H22O	0.9800
C225–H22P	0.9800
C225–H22Q	0.9800
C225–H22R	0.9800
C101–H10D	0.9800
C101–H10E	0.9800
C101–H10F	0.9800
C328–H328	0.9500
C328–C327	1.45(6)
C231–H23D	0.9800
C231–H23E	0.9800
C231–H23F	0.9800
C233–H23G	0.9800
C233–H23H	0.9800
C233–H23I	0.9800
C102–H10G	0.9800
C102–H10H	0.9800
C102–H10I	0.9800
C103–H10J	0.9800
C103–H10K	0.9800
C103–H10L	0.9800
C330–H330	0.9500
C330–C326	1.44(6)
C330–C329	1.34(6)
C213–H21G	0.9800
C213–H21H	0.9800
C213–H21I	0.9800
C213–C215	1.434(15)
C214–H21J	0.9800
C214–H21K	0.9800
C214–H21L	0.9800
C214–C215	1.422(16)
C215–C216	1.552(14)
C215–C212	1.442(16)
C106–H106	0.9500
C106–C107	1.390(6)
C216–C217	1.390(6)
C217–H217	0.9500
C217–C218	1.392(6)
C206–H206	0.9500
C311–H311	0.9500
C311–C310	1.4200
C311–C312	1.4200
C310–N303	1.4200
C310–C309	1.363(18)
N303–H303	0.8800
N303–C313	1.4200
C313–C312	1.4200
C312–H312	0.9500
C309–C326	1.60(6)
C326–C327	1.48(5)
C329–H329	0.9500
C212–H21M	0.9800
C212–H21N	0.9800
C212–H21O	0.9800

C327–H327	0.9500

Atom–Atom–Atom	Angle [°]
C503–O501–C502	120(3)
C507–N501–C501	97(4)
C507–N501–C513	117(5)
C513–N501–C501	115(5)
N501–C501–H50A	109.2
N501–C501–H50B	109.2
N501–C501–C502	112(2)
H50A–C501–H50B	107.9
C502–C501–H50A	109.2
C502–C501–H50B	109.2
C504–O502–C505	119(3)
C506–N502–C512	112(4)
C506–N502–C518	105(4)
C512–N502–C518	111(4)
O501–C502–C501	106(2)
O501–C502–H50C	110.5
O501–C502–H50D	110.5
C501–C502–H50C	110.5
C501–C502–H50D	110.5
H50C–C502–H50D	108.7
C509–O503–C508	119(3)
O501–C503–H50E	110.2
O501–C503–H50F	110.2
O501–C503–C504	107(2)
H50E–C503–H50F	108.5
C504–C503–H50E	110.2
C504–C503–H50F	110.2
C511–O504–C510	124(3)
O502–C504–C503	107(2)
O502–C504–H50G	110.4
O502–C504–H50H	110.4
C503–C504–H50G	110.4
C503–C504–H50H	110.4
H50G–C504–H50H	108.6
C515–O505–C514	119(3)
O502–C505–H50I	110.2
O502–C505–H50J	110.2
O502–C505–C506	107(2)
H50I–C505–H50J	108.5
C506–C505–H50I	110.2
C506–C505–H50J	110.2
C517–O506–C516	122(3)
N502–C506–C505	114(2)
N502–C506–H50K	108.8
N502–C506–H50L	108.8
C505–C506–H50K	108.8
C505–C506–H50L	108.8
H50K–C506–H50L	107.7
N501–C507–H50M	108.9
N501–C507–H50N	108.9
N501–C507–C508	113(2)
H50M–C507–H50N	107.7
C508–C507–H50M	108.9
C508–C507–H50N	108.9
O503–C508–C507	107(2)
O503–C508–H50O	110.3

O503–C508–H50P	110.3
C507–C508–H50O	110.3
C507–C508–H50P	110.3
H50O–C508–H50P	108.6
O503–C509–H50Q	110.1
O503–C509–H50R	110.1
O503–C509–C510	108(2)
H50Q–C509–H50R	108.4
C510–C509–H50Q	110.1
C510–C509–H50R	110.1
O504–C510–C509	106(2)
O504–C510–H51A	110.6
O504–C510–H51B	110.6
C509–C510–H51A	110.6
C509–C510–H51B	110.6
H51A–C510–H51B	108.7
O504–C511–H51C	110.0
O504–C511–H51D	110.0
O504–C511–C512	109(2)
H51C–C511–H51D	108.4
C512–C511–H51C	110.0
C512–C511–H51D	110.0
N502–C512–C511	115(2)
N502–C512–H51E	108.6
N502–C512–H51F	108.6
C511–C512–H51E	108.6
C511–C512–H51F	108.6
H51E–C512–H51F	107.6
N501–C513–H51G	109.0
N501–C513–H51H	109.0
N501–C513–C514	113(2)
H51G–C513–H51H	107.8
C514–C513–H51G	109.0
C514–C513–H51H	109.0
O505–C514–C513	107(2)
O505–C514–H51I	110.4
O505–C514–H51J	110.4
C513–C514–H51I	110.4
C513–C514–H51J	110.4
H51I–C514–H51J	108.6
O505–C515–H51K	110.1
O505–C515–H51L	110.1
O505–C515–C516	108(2)
H51K–C515–H51L	108.4
C516–C515–H51K	110.1
C516–C515–H51L	110.1
O506–C516–C515	104.7(19)
O506–C516–H51M	110.8
O506–C516–H51N	110.8
C515–C516–H51M	110.8
C515–C516–H51N	110.8
H51M–C516–H51N	108.9
O506–C517–H51O	110.5
O506–C517–H51P	110.5
O506–C517–C518	106(2)
H51O–C517–H51P	108.6
C518–C517–H51O	110.5
C518–C517–H51P	110.5
N502–C518–C517	113(2)

N502–C518–H51Q	109.0
N502–C518–H51R	109.0
C517–C518–H51Q	109.0
C517–C518–H51R	109.0
H51Q–C518–H51R	107.8
O105–Dy11–N306	75.8(10)
O105–Dy11–N308$^{\#1}$	74(6)
O106–Dy11–O105	73.6(11)
O106–Dy11–O101	113.9(9)
O106–Dy11–N306	72.1(11)
O106–Dy11–N308$^{\#1}$	137(6)
O101–Dy11–O105	142.2(11)
O101–Dy11–N306	72.3(11)
O101–Dy11–N308$^{\#1}$	78(6)
O102–Dy11–O105	141.1(11)
O102–Dy11–O106	75.0(10)
O102–Dy11–O101	72.7(12)
O102–Dy11–O103	79.9(10)
O102–Dy11–O104	78.5(11)
O102–Dy11–N306	115.2(9)
O102–Dy11–N308$^{\#1}$	145(6)
O103–Dy11–O105	116.3(10)
O103–Dy11–O106	146.0(11)
O103–Dy11–O101	79.1(10)
O103–Dy11–O104	70.8(12)
O103–Dy11–N306	140.7(13)
O103–Dy11–N308$^{\#1}$	75(5)
O104–Dy11–O105	74.8(10)
O104–Dy11–O106	81.9(10)
O104–Dy11–O101	141.4(11)
O104–Dy11–N306	145.1(12)
O104–Dy11–N308$^{\#1}$	115(5)
N308$^{\#1}$–Dy11–N306	73(5)
O204–Dy21–O206	86.0(8)
O204–Dy21–O201	145.1(8)
O204–Dy21–O203	71.0(9)
O204–Dy21–O205	82.2(8)
O204–Dy21–O202	108.6(8)
O204–Dy21–N307	142.2(9)
O204–Dy21–N305$^{\#2}$	73.1(9)
O206–Dy21–O203	79.8(8)
O206–Dy21–N307	74.6(9)
O206–Dy21–N305$^{\#2}$	142.3(9)
O201–Dy21–O206	109.4(7)
O201–Dy21–O203	141.0(8)
O201–Dy21–N307	72.7(8)
O201–Dy21–N305$^{\#2}$	76.3(9)
O203–Dy21–N307	73.8(9)
O203–Dy21–N305$^{\#2}$	120.0(9)
O205–Dy21–O206	71.7(9)
O205–Dy21–O201	73.9(8)
O205–Dy21–O203	142.0(9)
O205–Dy21–O202	138.6(9)
O205–Dy21–N307	120.1(9)
O205–Dy21–N305$^{\#2}$	74.6(9)
O202–Dy21–O206	146.4(9)
O202–Dy21–O201	76.0(8)
O202–Dy21–O203	77.0(8)
O202–Dy21–N307	75.8(9)

O202–Dy21–N305$^{\#2}$	71.1(9)
N307–Dy21–N305$^{\#2}$	139.0(9)
N304–K51–C315	23.4(3)
N304–K51–C318	24.6(3)
C318–K51–C315	38.6(3)
C127–O105–Dy11	132(2)
C218–O204–Dy21	135.9(18)
C229–O206–Dy21	137.5(19)
C205–O201–Dy21	133.0(15)
O201–C205–C204	114.3(17)
O201–C205–C206	128(3)
C206–C205–C204	118(3)
C201–C204–C205	109.6(19)
C201–C204–C203	115(2)
C201–C204–C202	109(2)
C203–C204–C205	112.9(18)
C202–C204–C205	107.4(17)
C202–C204–C203	103.1(18)
C204–C201–H20A	109.5
C204–C201–H20B	109.5
C204–C201–H20C	109.5
H20A–C201–H20B	109.5
H20A–C201–H20C	109.5
H20B–C201–H20C	109.5
C204–C203–H20D	109.5
C204–C203–H20E	109.5
C204–C203–H20F	109.5
H20D–C203–H20E	109.5
H20D–C203–H20F	109.5
H20E–C203–H20F	109.5
C204–C202–H20G	109.5
C204–C202–H20H	109.5
C204–C202–H20I	109.5
H20G–C202–H20H	109.5
H20G–C202–H20I	109.5
H20H–C202–H20I	109.5
C129–O106–Dy11	133(2)
C105–O101–Dy11	135(2)
C216–O203–Dy21	132.5(19)
C107–O102–Dy11	137(2)
C227–O205–Dy21	139.4(19)
C116–O103–Dy11	139(3)
C118–O104–Dy11	143(3)
C207–O202–Dy21	133.1(16)
O202–C207–C208	114.3(17)
O202–C207–C206	127(3)
C206–C207–C208	118(3)
C209–C208–C207	109.6(19)
C209–C208–C210	115(2)
C209–C208–C211	109(2)
C210–C208–C207	112.9(18)
C211–C208–C207	107.4(17)
C211–C208–C210	103.1(18)
C208–C209–H20J	109.5
C208–C209–H20K	109.5
C208–C209–H20L	109.5
H20J–C209–H20K	109.5
H20J–C209–H20L	109.5
H20K–C209–H20L	109.5

C208–C210–H21A	109.5
C208–C210–H21B	109.5
C208–C210–H21C	109.5
H21A–C210–H21B	109.5
H21A–C210–H21C	109.5
H21B–C210–H21C	109.5
C208–C211–H21D	109.5
C208–C211–H21E	109.5
C208–C211–H21F	109.5
H21D–C211–H21E	109.5
H21D–C211–H21F	109.5
H21E–C211–H21F	109.5
C305–N302–H302	126.0
C305–N302–C308	108.0
C308–N302–H302	126.0
C306–C305–N302	108.0
C304–C305–N302	128(2)
C304–C305–C306	124(2)
C305–C306–H306	126.0
C305–C306–C307	108.0
C307–C306–H306	126.0
C306–C307–H307	126.0
C306–C307–C308	108.0
C308–C307–H307	126.0
C307–C308–N302	108.0
C309–C308–N302	120(3)
C309–C308–C307	132(3)
C334–N307–Dy21	119.2(17)
C334–N307–C333	120.0
C333–N307–Dy21	119.8(17)
N307–C334–H334	120.0
N307–C334–C335	120.0
C335–C334–H334	120.0
C334–C335–H335	120.0
C331–C335–C334	120.0
C331–C335–H335	120.0
C335–C331–C332	120.0
C335–C331–C314	123(3)
C332–C331–C314	116(3)
C331–C332–H332	120.0
C333–C332–C331	120.0
C333–C332–H332	120.0
N307–C333–H333	120.0
C332–C333–N307	120.0
C332–C333–H333	120.0
C320–N301–H301	126.0
C320–N301–C303	108.0
C303–N301–H301	126.0
N301–C320–C301	108.0
C319–C320–N301	124(2)
C319–C320–C301	128(2)
C320–C301–H30A	126.0
C320–C301–C302	108.0
C302–C301–H30A	126.0
C301–C302–H30B	126.0
C303–C302–C301	108.0
C303–C302–H30B	126.0
C302–C303–N301	108.0
C304–C303–N301	125(2)

C304–C303–C302	127(2)
K51–N304–H304	79.7
C315–N304–K51	99.2(13)
C315–N304–H304	126.0
C318–N304–K51	92.9(15)
C318–N304–H304	126.0
C318–N304–C315	108.0
N304–C315–K51	57.5(11)
N304–C315–C316	108.0
C316–C315–K51	104.6(12)
C314–C315–K51	98(2)
C314–C315–N304	120(3)
C314–C315–C316	132(3)
C315–C316–H316	126.0
C317–C316–C315	108.0
C317–C316–H316	126.0
C316–C317–H317	126.0
C316–C317–C318	108.0
C318–C317–H317	126.0
N304–C318–K51	62.5(13)
N304–C318–C317	108.0
C317–C318–K51	107.3(11)
C319–C318–K51	101(2)
C319–C318–N304	128(2)
C319–C318–C317	124(2)
C324–N305–Dy21$^{\#3}$	119.9(16)
C324–N305–C323	120.0
C323–N305–Dy21$^{\#3}$	118.5(16)
N305–C324–H324	120.0
N305–C324–C325	120.0
C325–C324–H324	120.0
C324–C325–H325	120.0
C321–C325–C324	120.0
C321–C325–H325	120.0
C325–C321–C322	120.0
C325–C321–C304	120(3)
C322–C321–C304	119(3)
C321–C322–H322	120.0
C323–C322–C321	120.0
C323–C322–H322	120.0
N305–C323–H323	120.0
C322–C323–N305	120.0
C322–C323–H323	120.0
C328–N306–Dy11	121(3)
C329–N306–Dy11	110(4)
C329–N306–C328	123(5)
H10A–C109–H10B	109.5
H10A–C109–H10C	109.5
H10B–C109–H10C	109.5
C108–C109–H10A	109.5
C108–C109–H10B	109.5
C108–C109–H10C	109.5
C109–C108–C110	114(5)
C109–C108–C111	108(4)
C109–C108–C107	111(2)
C110–C108–C111	111(5)
C110–C108–C107	108(3)
C111–C108–C107	105(2)
C108–C110–H11A	109.5

C108–C110–H11B	109.5
C108–C110–H11C	109.5
H11A–C110–H11B	109.5
H11A–C110–H11C	109.5
H11B–C110–H11C	109.5
C108–C111–H11D	109.5
C108–C111–H11E	109.5
C108–C111–H11F	109.5
H11D–C111–H11E	109.5
H11D–C111–H11F	109.5
H11E–C111–H11F	109.5
C224–C226–C227	106(2)
C223–C226–C224	107(3)
C223–C226–C227	107(2)
C225–C226–C224	118(3)
C225–C226–C223	107(3)
C225–C226–C227	112(2)
H11G–C112–H11H	109.5
H11G–C112–H11I	109.5
H11H–C112–H11I	109.5
C115–C112–H11G	109.5
C115–C112–H11H	109.5
C115–C112–H11I	109.5
H11J–C113–H11K	109.5
H11J–C113–H11L	109.5
H11K–C113–H11L	109.5
C115–C113–H11J	109.5
C115–C113–H11K	109.5
C115–C113–H11L	109.5
C337–C336–C340	120.0
C337–C336–C319	122(3)
C340–C336–C319	118(3)
C336–C337–H337	120.0
C338–C337–C336	120.0
C338–C337–H337	120.0
C337–C338–H338	120.0
C337–C338–N308	120.0
N308–C338–H338	120.0
C338–N308–Dy11$^{\#4}$	126.7(17)
C339–N308–Dy11$^{\#4}$	109.1(17)
C339–N308–C338	120.0
N308–C339–H339	120.0
N308–C339–C340	120.0
C340–C339–H339	120.0
C336–C340–H340	120.0
C339–C340–C336	120.0
C339–C340–H340	120.0
H11M–C114–H11N	109.5
H11M–C114–H11O	109.5
H11N–C114–H11O	109.5
C115–C114–H11M	109.5
C115–C114–H11N	109.5
C115–C114–H11O	109.5
H22A–C222–H22B	109.5
H22A–C222–H22C	109.5
H22B–C222–H22C	109.5
C219–C222–H22A	109.5
C219–C222–H22B	109.5
C219–C222–H22C	109.5

C112–C115–C114	111.9(19)
C112–C115–C116	114(3)
C113–C115–C112	114(2)
C113–C115–C114	99(5)
C113–C115–C116	110(2)
C114–C115–C116	106(2)
C232–C230–C229	112(2)
C232–C230–C231	113.0(18)
C232–C230–C233	104(4)
C231–C230–C229	112(2)
C231–C230–C233	110.6(17)
C233–C230–C229	104(2)
O103–C116–C115	118(3)
O103–C116–C117	123(3)
C117–C116–C115	119.6(17)
C116–C117–H117	117.4
C118–C117–C116	125.3(17)
C118–C117–H117	117.4
O104–C118–C117	119(2)
O104–C118–C119	119(3)
C117–C118–C119	121.8(17)
C120–C119–C118	103(2)
C121–C119–C118	113(3)
C121–C119–C120	111(5)
C121–C119–C122	111(4)
C122–C119–C118	111(3)
C122–C119–C120	108(4)
C119–C120–H12A	109.5
C119–C120–H12B	109.5
C119–C120–H12C	109.5
H12A–C120–H12B	109.5
H12A–C120–H12C	109.5
H12B–C120–H12C	109.5
H22D–C220–H22E	109.5
H22D–C220–H22F	109.5
H22E–C220–H22F	109.5
C219–C220–H22D	109.5
C219–C220–H22E	109.5
C219–C220–H22F	109.5
C119–C121–H12D	109.5
C119–C121–H12E	109.5
C119–C121–H12F	109.5
H12D–C121–H12E	109.5
H12D–C121–H12F	109.5
H12E–C121–H12F	109.5
C226–C224–H22G	109.5
C226–C224–H22H	109.5
C226–C224–H22I	109.5
H22G–C224–H22H	109.5
H22G–C224–H22I	109.5
H22H–C224–H22I	109.5
C119–C122–H12G	109.5
C119–C122–H12H	109.5
C119–C122–H12I	109.5
H12G–C122–H12H	109.5
H12G–C122–H12I	109.5
H12H–C122–H12I	109.5
C227–C228–H228	118.0
C229–C228–H228	118.0

C229–C228–C227	124.0(15)
H12J–C123–H12K	109.5
H12J–C123–H12L	109.5
H12K–C123–H12L	109.5
C126–C123–H12J	109.5
C126–C123–H12K	109.5
C126–C123–H12L	109.5
C230–C232–H23A	109.5
C230–C232–H23B	109.5
C230–C232–H23C	109.5
H23A–C232–H23B	109.5
H23A–C232–H23C	109.5
H23B–C232–H23C	109.5
H12M–C124–H12N	109.5
H12M–C124–H12O	109.5
H12N–C124–H12O	109.5
C126–C124–H12M	109.5
C126–C124–H12N	109.5
C126–C124–H12O	109.5
C101–C104–C105	110(3)
C101–C104–C102	112.5(18)
C101–C104–C103	112.1(19)
C102–C104–C105	112(2)
C102–C104–C103	103(4)
C103–C104–C105	108(2)
H12P–C125–H12Q	109.5
H12P–C125–H12R	109.5
H12Q–C125–H12R	109.5
C126–C125–H12P	109.5
C126–C125–H12Q	109.5
C126–C125–H12R	109.5
O101–C105–C104	119(3)
O101–C105–C106	121(2)
C106–C105–C104	119.7(16)
C123–C126–C124	113(4)
C123–C126–C127	105(2)
C124–C126–C127	105(2)
C125–C126–C123	105(4)
C125–C126–C124	117(4)
C125–C126–C127	111(2)
O105–C127–C126	115(2)
O105–C127–C128	123(2)
C128–C127–C126	121.4(16)
C320–C319–C336	117(2)
C318–C319–C320	128(3)
C318–C319–C336	115(2)
C127–C128–H128	117.3
C127–C128–C129	125.4(17)
C129–C128–H128	117.3
O106–C129–C128	124(2)
O106–C129–C130	114(2)
C128–C129–C130	121.2(16)
C131–C130–C129	113(2)
C131–C130–C132	111.5(19)
C131–C130–C133	111(4)
C132–C130–C129	107(2)
C132–C130–C133	110.1(18)
C133–C130–C129	104(2)
C130–C131–H13A	109.5

C130–C131–H13B	109.5
C130–C131–H13C	109.5
H13A–C131–H13B	109.5
H13A–C131–H13C	109.5
H13B–C131–H13C	109.5
C315–C314–C331	110(2)
C315–C314–C313	132(3)
C313–C314–C331	117(3)
C130–C132–H13D	109.5
C130–C132–H13E	109.5
C130–C132–H13F	109.5
H13D–C132–H13E	109.5
H13D–C132–H13F	109.5
H13E–C132–H13F	109.5
C222–C219–C220	107(3)
C222–C219–C218	106(2)
C220–C219–C218	104(2)
C221–C219–C222	106(4)
C221–C219–C220	121(4)
C221–C219–C218	112(2)
C130–C133–H13G	109.5
C130–C133–H13H	109.5
C130–C133–H13I	109.5
H13G–C133–H13H	109.5
H13G–C133–H13I	109.5
H13H–C133–H13I	109.5
C219–C221–H22J	109.5
C219–C221–H22K	109.5
C219–C221–H22L	109.5
H22J–C221–H22K	109.5
H22J–C221–H22L	109.5
H22K–C221–H22L	109.5
C226–C223–H22M	109.5
C226–C223–H22N	109.5
C226–C223–H22O	109.5
H22M–C223–H22N	109.5
H22M–C223–H22O	109.5
H22N–C223–H22O	109.5
C226–C225–H22P	109.5
C226–C225–H22Q	109.5
C226–C225–H22R	109.5
H22P–C225–H22Q	109.5
H22P–C225–H22R	109.5
H22Q–C225–H22R	109.5
C104–C101–H10D	109.5
C104–C101–H10E	109.5
C104–C101–H10F	109.5
H10D–C101–H10E	109.5
H10D–C101–H10F	109.5
H10E–C101–H10F	109.5
O205–C227–C226	116(2)
O205–C227–C228	123(2)
C228–C227–C226	121.2(15)
O206–C229–C230	114(2)
O206–C229–C228	124(2)
C228–C229–C230	121.3(15)
N306–C328–H328	117.7
N306–C328–C327	125(4)
C327–C328–H328	117.7

C230–C231–H23D	109.5
C230–C231–H23E	109.5
C230–C231–H23F	109.5
H23D–C231–H23E	109.5
H23D–C231–H23F	109.5
H23E–C231–H23F	109.5
C230–C233–H23G	109.5
C230–C233–H23H	109.5
C230–C233–H23I	109.5
H23G–C233–H23H	109.5
H23G–C233–H23I	109.5
H23H–C233–H23I	109.5
C104–C102–H10G	109.5
C104–C102–H10H	109.5
C104–C102–H10I	109.5
H10G–C102–H10H	109.5
H10G–C102–H10I	109.5
H10H–C102–H10I	109.5
C104–C103–H10J	109.5
C104–C103–H10K	109.5
C104–C103–H10L	109.5
H10J–C103–H10K	109.5
H10J–C103–H10L	109.5
H10K–C103–H10L	109.5
C305–C304–C303	128(3)
C305–C304–C321	115(2)
C303–C304–C321	117(2)
C326–C330–H330	120.7
C329–C330–H330	120.7
C329–C330–C326	119(5)
H21G–C213–H21H	109.5
H21G–C213–H21I	109.5
H21H–C213–H21I	109.5
C215–C213–H21G	109.5
C215–C213–H21H	109.5
C215–C213–H21I	109.5
H21J–C214–H21K	109.5
H21J–C214–H21L	109.5
H21K–C214–H21L	109.5
C215–C214–H21J	109.5
C215–C214–H21K	109.5
C215–C214–H21L	109.5
C213–C215–C216	112(2)
C213–C215–C212	112.9(18)
C214–C215–C213	113.6(19)
C214–C215–C216	113(2)
C214–C215–C212	100(4)
C212–C215–C216	103(2)
C105–C106–H106	116.7
C105–C106–C107	126.6(17)
C107–C106–H106	116.7
O203–C216–C215	115(2)
O203–C216–C217	124(2)
C217–C216–C215	121.4(16)
O102–C107–C108	118(3)
O102–C107–C106	122(2)
C106–C107–C108	120.1(16)
C216–C217–H217	118.1
C216–C217–C218	123.8(16)

C218–C217–H217	118.1
O204–C218–C219	117(2)
O204–C218–C217	123(2)
C217–C218–C219	120.7(16)
C205–C206–C207	122(4)
C205–C206–H206	119.1
C207–C206–H206	119.1
C310–C311–H311	126.0
C312–C311–H311	126.0
C312–C311–C310	108.0
N303–C310–C311	108.0
C309–C310–C311	128(3)
C309–C310–N303	124(3)
C310–N303–H303	126.0
C310–N303–C313	108.0
C313–N303–H303	126.0
C314–C313–N303	123(3)
C314–C313–C312	128(3)
C312–C313–N303	108.0
C311–C312–C313	108.0
C311–C312–H312	126.0
C313–C312–H312	126.0
C308–C309–C310	132(3)
C308–C309–C326	113(2)
C310–C309–C326	115(2)
C330–C326–C309	126(4)
C330–C326–C327	122(4)
C327–C326–C309	111(4)
N306–C329–C330	122(6)
N306–C329–H329	119.1
C330–C329–H329	119.1
C215–C212–H21M	109.5
C215–C212–H21N	109.5
C215–C212–H21O	109.5
H21M–C212–H21N	109.5
H21M–C212–H21O	109.5
H21N–C212–H21O	109.5
C328–C327–C326	110(4)
C328–C327–H327	125.1
C326–C327–H327	125.1

Symmetry transformations used to generate equivalent atoms:
#1: +X, 0.5-Y, 0.5+Z; #2: 1+X, 0.5-Y, 0.5+Z; #3: -1+X, 0.5-Y, -0.5+Z; #4: +X, 0.5-Y, -0.5+Z;

Table S5. Bond lengths [E] and angles [°] for **2**.

Tb(1)-O(4)	2.293(5)
Tb(1)-O(1)	2.309(5)
Tb(1)-O(2)	2.326(6)
Tb(1)-O(3)	2.333(5)
Tb(1)-O(5)	2.335(6)
Tb(1)-O(6)	2.337(5)
Tb(1)-N(1)	2.579(6)
Tb(1)-N(6)#1	2.602(6)
Tb(2)-O(9)	2.290(6)
Tb(2)-O(11)	2.291(5)
Tb(2)-O(8)	2.338(6)
Tb(2)-O(10)	2.350(6)
Tb(2)-O(12)	2.353(5)
Tb(2)-O(7)	2.363(5)
Tb(2)-N(8)	2.611(6)
Tb(2)-N(7)#2	2.673(6)
Cu(1)-N(3)	1.995(6)
Cu(1)-N(5)	1.998(6)
Cu(1)-N(2)	2.019(6)
Cu(1)-N(4)	2.020(5)
O(1)-C(1)	1.253(10)
O(2)-C(3)	1.263(10)
O(3)-C(12)	1.249(9)
O(4)-C(14)	1.253(9)
O(5)-C(23)	1.228(11)
O(6)-C(25)	1.246(10)
O(7)-C(74)	1.261(10)
O(8)-C(76)	1.247(10)
O(9)-C(85)	1.286(11)
O(10)-C(87)	1.288(11)
O(11)-C(96)	1.246(10)
O(12)-C(98)	1.270(11)
N(1)-C(34)	1.313(12)
N(1)-C(38)	1.326(12)
N(2)-C(43)	1.368(9)
N(2)-C(40)	1.391(8)
N(3)-C(50)	1.371(9)
N(3)-C(53)	1.395(8)
N(4)-C(63)	1.375(9)
N(4)-C(60)	1.394(8)
N(5)-C(70)	1.380(10)
N(5)-C(73)	1.381(9)
N(6)-C(57)	1.331(10)
N(6)-C(59)	1.332(10)
N(7)-C(67)	1.325(10)
N(7)-C(69)	1.340(10)
N(8)-C(49)	1.338(10)
N(8)-C(47)	1.339(10)
C(1)-C(2)	1.396(14)
C(1)-C(4)	1.554(13)
C(1A)-C(99)	1.53(2)
C(1A)-H(1AA)	0.9800
C(1A)-H(1AB)	0.9800
C(1A)-H(1AC)	0.9800
C(1B)-C(103)	1.51(4)
C(1B)-H(1BA)	0.9800
C(1B)-H(1BB)	0.9800
C(1B)-H(1BC)	0.9800
C(1C)-C(103)	1.57(3)

C(1C)-H(1CA)	0.9800
C(1C)-H(1CB)	0.9800
C(1C)-H(1CC)	0.9800
C(1D)-C(103)	1.51(3)
C(1D)-H(1DA)	0.9800
C(1D)-H(1DB)	0.9800
C(1D)-H(1DC)	0.9800
C(2)-C(3)	1.409(14)
C(2)-H(2)	0.9500
C(3)-C(8)	1.545(14)
C(4)-C(6')	1.503(14)
C(4)-C(7)	1.511(16)
C(4)-C(5)	1.514(15)
C(4)-C(6)	1.521(15)
C(4)-C(5')	1.523(15)
C(4)-C(7')	1.530(15)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(5')-H(5'A)	0.9800
C(5')-H(5'B)	0.9800
C(5')-H(5'C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(6')-H(6'A)	0.9800
C(6')-H(6'B)	0.9800
C(6')-H(6'C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(7')-H(7'A)	0.9800
C(7')-H(7'B)	0.9800
C(7')-H(7'C)	0.9800
C(8)-C(11)	1.499(15)
C(8)-C(9)	1.525(15)
C(8)-C(10)	1.554(16)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.408(11)
C(12)-C(15)	1.559(10)
C(13)-C(14)	1.410(11)
C(13)-H(13)	0.9500
C(14)-C(19)	1.552(10)
C(15)-C(18)	1.504(12)
C(15)-C(16)	1.507(14)
C(15)-C(17)	1.531(12)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800

C(18)-H(18C)	0.9800
C(19)-C(22)	1.503(13)
C(19)-C(20)	1.508(13)
C(19)-C(21)	1.523(13)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.433(12)
C(23)-C(26)	1.556(12)
C(24)-C(25)	1.402(11)
C(24)-H(24)	0.9500
C(25)-C(30)	1.540(11)
C(26)-C(29)	1.507(15)
C(26)-C(28)	1.513(15)
C(26)-C(27)	1.526(15)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(32)	1.519(12)
C(30)-C(33)	1.519(13)
C(30)-C(31)	1.525(13)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.393(11)
C(34)-H(34)	0.9500
C(35)-C(36)	1.369(13)
C(35)-H(35)	0.9500
C(36)-C(37)	1.371(13)
C(36)-C(39)	1.503(9)
C(37)-C(38)	1.397(10)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(39)-C(73)	1.387(11)
C(39)-C(40)	1.388(10)
C(40)-C(41)	1.418(10)
C(41)-C(42)	1.354(11)
C(41)-H(41)	0.9500
C(42)-C(43)	1.443(9)
C(42)-H(42)	0.9500
C(43)-C(44)	1.408(10)
C(44)-C(50)	1.411(9)
C(44)-C(45)	1.485(10)
C(45)-C(46)	1.388(11)

C(45)-C(48)	1.389(11)
C(46)-C(47)	1.376(10)
C(46)-H(46)	0.9500
C(47)-H(47)	0.9500
C(48)-C(49)	1.397(11)
C(48)-H(48)	0.9500
C(49)-H(49)	0.9500
C(50)-C(51)	1.445(9)
C(51)-C(52)	1.339(10)
C(51)-H(51)	0.9500
C(52)-C(53)	1.432(10)
C(52)-H(52)	0.9500
C(53)-C(54)	1.379(10)
C(54)-C(60)	1.391(10)
C(54)-C(55)	1.494(8)
C(55)-C(58)	1.390(11)
C(55)-C(56)	1.402(11)
C(56)-C(57)	1.388(9)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(59)	1.374(10)
C(58)-H(58)	0.9500
C(59)-H(59)	0.9500
C(60)-C(61)	1.415(10)
C(61)-C(62)	1.348(10)
C(61)-H(61)	0.9500
C(62)-C(63)	1.437(9)
C(62)-H(62)	0.9500
C(63)-C(64)	1.403(10)
C(64)-C(70)	1.416(10)
C(64)-C(65)	1.480(10)
C(65)-C(66)	1.384(11)
C(65)-C(68)	1.395(11)
C(66)-C(67)	1.405(10)
C(66)-H(66)	0.9500
C(67)-H(67)	0.9500
C(68)-C(69)	1.367(11)
C(68)-H(68)	0.9500
C(69)-H(69)	0.9500
C(70)-C(71)	1.418(10)
C(71)-C(72)	1.355(11)
C(71)-H(71)	0.9500
C(72)-C(73)	1.440(11)
C(72)-H(72)	0.9500
C(74)-C(75)	1.394(13)
C(74)-C(77)	1.539(11)
C(75)-C(76)	1.399(13)
C(75)-H(75)	0.9500
C(76)-C(81)	1.529(14)
C(77)-C(78)	1.494(16)
C(77)-C(80)	1.528(16)
C(77)-C(79)	1.546(14)
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(80)-H(80A)	0.9800
C(80)-H(80B)	0.9800
C(80)-H(80C)	0.9800
C(81)-C(82)	1.516(13)

C(81)-C(83')	1.531(19)
C(81)-C(82')	1.532(19)
C(81)-C(84')	1.533(19)
C(81)-C(84)	1.535(14)
C(81)-C(83)	1.542(13)
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(82')-H(82D)	0.9800
C(82')-H(82E)	0.9800
C(82')-H(82F)	0.9800
C(83)-H(83A)	0.9800
C(83)-H(83B)	0.9800
C(83)-H(83C)	0.9800
C(83')-H(83D)	0.9800
C(83')-H(83E)	0.9800
C(83')-H(83F)	0.9800
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800
C(84')-H(84D)	0.9800
C(84')-H(84E)	0.9800
C(84')-H(84F)	0.9800
C(85)-C(86)	1.380(16)
C(85)-C(88')	1.52(10)
C(85)-C(88)	1.55(2)
C(86)-C(87)	1.367(16)
C(86)-H(86)	0.9500
C(87)-C(92)	1.531(18)
C(87)-C(92')	1.57(2)
C(88)-C(91)	1.505(14)
C(88)-C(90)	1.508(13)
C(88)-C(89)	1.531(13)
C(88')-C(91')	1.512(18)
C(88')-C(90')	1.519(18)
C(88')-C(89')	1.519(18)
C(89)-H(89A)	0.9800
C(89)-H(89B)	0.9800
C(89)-H(89C)	0.9800
C(89')-H(89D)	0.9800
C(89')-H(89E)	0.9800
C(89')-H(89F)	0.9800
C(90)-H(90A)	0.9800
C(90)-H(90B)	0.9800
C(90)-H(90C)	0.9800
C(90')-H(90D)	0.9800
C(90')-H(90E)	0.9800
C(90')-H(90F)	0.9800
C(91)-H(91A)	0.9800
C(91)-H(91B)	0.9800
C(91)-H(91C)	0.9800
C(91')-H(91D)	0.9800
C(91')-H(91E)	0.9800
C(91')-H(91F)	0.9800
C(92)-C(94)	1.491(15)
C(92)-C(93)	1.502(14)
C(92)-C(95)	1.517(14)
C(92')-C(93')	1.515(18)
C(92')-C(94')	1.516(18)
C(92')-C(95')	1.517(17)
C(93)-H(93A)	0.9800
C(93)-H(93B)	0.9800

C(93)-H(93C)	0.9800
C(93')-H(93D)	0.9800
C(93')-H(93E)	0.9800
C(93')-H(93F)	0.9800
C(94)-H(94A)	0.9800
C(94)-H(94B)	0.9800
C(94)-H(94C)	0.9800
C(94')-H(94D)	0.9800
C(94')-H(94E)	0.9800
C(94')-H(94F)	0.9800
C(95)-H(95A)	0.9800
C(95)-H(95B)	0.9800
C(95)-H(95C)	0.9800
C(95')-H(95D)	0.9800
C(95')-H(95E)	0.9800
C(95')-H(95F)	0.9800
C(96)-C(97)	1.388(14)
C(96)-C(99)	1.560(12)
C(97)-C(98)	1.385(14)
C(97)-H(97)	0.9500
C(98)-C(103)	1.542(14)
C(99)-C(100)	1.495(16)
C(99)-C(102)	1.501(16)
C(99)-C(101)	1.518(17)
C(100)-H(10D)	0.9800
C(100)-H(10E)	0.9800
C(100)-H(10F)	0.9800
C(101)-H(10G)	0.9800
C(101)-H(10H)	0.9800
C(101)-H(10I)	0.9800
C(102)-H(10J)	0.9800
C(102)-H(10K)	0.9800
C(102)-H(10L)	0.9800
C(103)-C(106)	1.46(2)
C(103)-C(105)	1.46(2)
C(103)-C(104)	1.56(2)
C(104)-H(10M)	0.9800
C(104)-H(10N)	0.9800
C(104)-H(10O)	0.9800
C(105)-H(10P)	0.9800
C(105)-H(10Q)	0.9800
C(105)-H(10R)	0.9800
C(106)-H(10S)	0.9800
C(106)-H(10T)	0.9800
C(106)-H(10U)	0.9800
Cs(1)-O(15)	2.914(7)
Cs(1)-O(13)	2.929(7)
Cs(1)-O(18)	2.950(7)
Cs(1)-O(16)	2.965(6)
Cs(1)-O(14)	2.970(6)
Cs(1)-O(17)	2.975(8)
Cs(1)-N(9)	3.078(9)
Cs(1)-N(10)	3.113(7)
O(13)-C(109)	1.411(13)
O(13)-C(108)	1.464(14)
O(14)-C(111)	1.422(12)
O(14)-C(110)	1.435(12)
O(15)-C(114)	1.395(15)
O(15)-C(115)	1.417(13)
O(16)-C(117)	1.376(12)
O(16)-C(116)	1.440(12)
O(17)-C(121)	1.444(15)

O(17)-C(120)	1.457(14)
O(18)-C(123)	1.415(13)
O(18)-C(122)	1.441(14)
N(9)-C(113)	1.426(17)
N(9)-C(119)	1.460(19)
N(9)-C(107)	1.477(14)
N(10)-C(124)	1.426(14)
N(10)-C(118)	1.454(13)
N(10)-C(112)	1.482(13)
C(107)-C(108)	1.519(17)
C(107)-H(10V)	0.9900
C(107)-H(10W)	0.9900
C(108)-H(10X)	0.9900
C(108)-H(10Y)	0.9900
C(109)-C(110)	1.482(18)
C(109)-H	0.9900
C(109)-H(10Z)	0.9900
C(110)-H(11D)	0.9900
C(110)-H(11E)	0.9900
C(111)-C(112)	1.510(15)
C(111)-H(11F)	0.9900
C(111)-H(11G)	0.9900
C(112)-H(11H)	0.9900
C(112)-H(11I)	0.9900
C(113)-C(114)	1.509(17)
C(113)-H(11J)	0.9900
C(113)-H(11K)	0.9900
C(114)-H(11L)	0.9900
C(114)-H(11M)	0.9900
C(115)-C(116)	1.495(16)
C(115)-H(11N)	0.9900
C(115)-H(11O)	0.9900
C(116)-H(11P)	0.9900
C(116)-H(11Q)	0.9900
C(117)-C(118)	1.469(16)
C(117)-H(11R)	0.9900
C(117)-H(11S)	0.9900
C(118)-H(11T)	0.9900
C(118)-H(11U)	0.9900
C(119)-C(120)	1.52(2)
C(119)-H(11V)	0.9900
C(119)-H(11W)	0.9900
C(120)-H(12A)	0.9900
C(120)-H(12B)	0.9900
C(121)-C(122)	1.464(18)
C(121)-H(12C)	0.9900
C(121)-H(12D)	0.9900
C(122)-H(12E)	0.9900
C(122)-H(12F)	0.9900
C(123)-C(124)	1.540(16)
C(123)-H(12G)	0.9900
C(123)-H(12H)	0.9900
C(124)-H(12I)	0.9900
C(124)-H(12J)	0.9900

O(4)-Tb(1)-O(1)	145.47(17)
O(4)-Tb(1)-O(2)	107.8(2)
O(1)-Tb(1)-O(2)	73.1(2)
O(4)-Tb(1)-O(3)	71.87(17)
O(1)-Tb(1)-O(3)	137.11(18)
O(2)-Tb(1)-O(3)	74.47(19)
O(4)-Tb(1)-O(5)	82.6(2)

O(1)-Tb(1)-O(5)	117.3(2)
O(2)-Tb(1)-O(5)	144.72(18)
O(3)-Tb(1)-O(5)	77.3(2)
O(4)-Tb(1)-O(6)	82.57(19)
O(1)-Tb(1)-O(6)	78.48(19)
O(2)-Tb(1)-O(6)	142.32(18)
O(3)-Tb(1)-O(6)	141.5(2)
O(5)-Tb(1)-O(6)	71.15(19)
O(4)-Tb(1)-N(1)	141.4(2)
O(1)-Tb(1)-N(1)	73.08(19)
O(2)-Tb(1)-N(1)	80.5(2)
O(3)-Tb(1)-N(1)	74.58(19)
O(5)-Tb(1)-N(1)	71.9(2)
O(6)-Tb(1)-N(1)	114.3(2)
O(4)-Tb(1)-N(6)#1	72.48(19)
O(1)-Tb(1)-N(6)#1	75.01(18)
O(2)-Tb(1)-N(6)#1	73.37(18)
O(3)-Tb(1)-N(6)#1	120.65(19)
O(5)-Tb(1)-N(6)#1	140.7(2)
O(6)-Tb(1)-N(6)#1	75.80(19)
N(1)-Tb(1)-N(6)#1	143.4(2)
O(9)-Tb(2)-O(11)	82.1(2)
O(9)-Tb(2)-O(8)	81.3(2)
O(11)-Tb(2)-O(8)	76.3(2)
O(9)-Tb(2)-O(10)	71.2(2)
O(11)-Tb(2)-O(10)	80.4(2)
O(8)-Tb(2)-O(10)	146.0(2)
O(9)-Tb(2)-O(12)	141.7(2)
O(11)-Tb(2)-O(12)	72.4(2)
O(8)-Tb(2)-O(12)	118.2(2)
O(10)-Tb(2)-O(12)	76.7(2)
O(9)-Tb(2)-O(7)	74.2(2)
O(11)-Tb(2)-O(7)	142.94(19)
O(8)-Tb(2)-O(7)	72.30(19)
O(10)-Tb(2)-O(7)	116.9(2)
O(12)-Tb(2)-O(7)	140.93(18)
O(9)-Tb(2)-N(8)	110.8(2)
O(11)-Tb(2)-N(8)	143.9(2)
O(8)-Tb(2)-N(8)	137.4(2)
O(10)-Tb(2)-N(8)	73.0(2)
O(12)-Tb(2)-N(8)	78.0(2)
O(7)-Tb(2)-N(8)	72.41(19)
O(9)-Tb(2)-N(7)#2	146.2(2)
O(11)-Tb(2)-N(7)#2	116.3(2)
O(8)-Tb(2)-N(7)#2	76.5(2)
O(10)-Tb(2)-N(7)#2	136.8(2)
O(12)-Tb(2)-N(7)#2	72.0(2)
O(7)-Tb(2)-N(7)#2	74.81(18)
N(8)-Tb(2)-N(7)#2	71.9(2)
N(3)-Cu(1)-N(5)	178.6(3)
N(3)-Cu(1)-N(2)	89.3(2)
N(5)-Cu(1)-N(2)	90.2(2)
N(3)-Cu(1)-N(4)	90.6(2)
N(5)-Cu(1)-N(4)	90.0(2)
N(2)-Cu(1)-N(4)	179.8(3)
C(1)-O(1)-Tb(1)	137.1(6)
C(3)-O(2)-Tb(1)	137.2(6)
C(12)-O(3)-Tb(1)	136.2(5)
C(14)-O(4)-Tb(1)	135.5(5)
C(23)-O(5)-Tb(1)	138.7(5)
C(25)-O(6)-Tb(1)	138.8(5)
C(74)-O(7)-Tb(2)	133.1(5)

C(76)-O(8)-Tb(2)	132.4(6)
C(85)-O(9)-Tb(2)	137.9(7)
C(87)-O(10)-Tb(2)	135.5(7)
C(96)-O(11)-Tb(2)	136.7(6)
C(98)-O(12)-Tb(2)	133.3(6)
C(34)-N(1)-C(38)	115.9(7)
C(34)-N(1)-Tb(1)	125.7(6)
C(38)-N(1)-Tb(1)	117.6(5)
C(43)-N(2)-C(40)	105.2(6)
C(43)-N(2)-Cu(1)	128.2(4)
C(40)-N(2)-Cu(1)	126.6(5)
C(50)-N(3)-C(53)	105.3(6)
C(50)-N(3)-Cu(1)	128.1(4)
C(53)-N(3)-Cu(1)	126.7(5)
C(63)-N(4)-C(60)	105.7(5)
C(63)-N(4)-Cu(1)	127.9(4)
C(60)-N(4)-Cu(1)	126.4(5)
C(70)-N(5)-C(73)	105.3(6)
C(70)-N(5)-Cu(1)	127.3(4)
C(73)-N(5)-Cu(1)	127.4(5)
C(57)-N(6)-C(59)	116.6(6)
C(57)-N(6)-Tb(1)#3	120.8(5)
C(59)-N(6)-Tb(1)#3	121.0(5)
C(67)-N(7)-C(69)	117.0(7)
C(67)-N(7)-Tb(2)#4	120.0(5)
C(69)-N(7)-Tb(2)#4	119.6(5)
C(49)-N(8)-C(47)	116.8(7)
C(49)-N(8)-Tb(2)	116.3(5)
C(47)-N(8)-Tb(2)	125.0(5)
O(1)-C(1)-C(2)	124.2(8)
O(1)-C(1)-C(4)	117.2(9)
C(2)-C(1)-C(4)	118.5(8)
C(99)-C(1A)-H(1AA)	109.5
C(99)-C(1A)-H(1AB)	109.5
H(1AA)-C(1A)-H(1AB)	109.5
C(99)-C(1A)-H(1AC)	109.5
H(1AA)-C(1A)-H(1AC)	109.5
H(1AB)-C(1A)-H(1AC)	109.5
C(103)-C(1B)-H(1BA)	109.5
C(103)-C(1B)-H(1BB)	109.5
H(1BA)-C(1B)-H(1BB)	109.5
C(103)-C(1B)-H(1BC)	109.5
H(1BA)-C(1B)-H(1BC)	109.5
H(1BB)-C(1B)-H(1BC)	109.5
C(103)-C(1C)-H(1CA)	109.5
C(103)-C(1C)-H(1CB)	109.5
H(1CA)-C(1C)-H(1CB)	109.5
C(103)-C(1C)-H(1CC)	109.5
H(1CA)-C(1C)-H(1CC)	109.5
H(1CB)-C(1C)-H(1CC)	109.5
C(103)-C(1D)-H(1DA)	109.5
C(103)-C(1D)-H(1DB)	109.5
H(1DA)-C(1D)-H(1DB)	109.5
C(103)-C(1D)-H(1DC)	109.5
H(1DA)-C(1D)-H(1DC)	109.5
H(1DB)-C(1D)-H(1DC)	109.5
C(1)-C(2)-C(3)	125.0(9)
C(1)-C(2)-H(2)	117.5
C(3)-C(2)-H(2)	117.5
O(2)-C(3)-C(2)	122.9(9)
O(2)-C(3)-C(8)	115.6(9)
C(2)-C(3)-C(8)	121.5(9)

C(7)-C(4)-C(5)	123(3)
C(7)-C(4)-C(6)	106(2)
C(5)-C(4)-C(6)	106.3(19)
C(6')-C(4)-C(5')	111.4(15)
C(6')-C(4)-C(7')	107.0(15)
C(5')-C(4)-C(7')	103(2)
C(6')-C(4)-C(1)	113.3(13)
C(7)-C(4)-C(1)	105.1(14)
C(5)-C(4)-C(1)	104.6(17)
C(6)-C(4)-C(1)	111.8(16)
C(5')-C(4)-C(1)	112.3(15)
C(7')-C(4)-C(1)	108.7(11)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(4)-C(5')-H(5'A)	109.5
C(4)-C(5')-H(5'B)	109.5
H(5'A)-C(5')-H(5'B)	109.5
C(4)-C(5')-H(5'C)	109.5
H(5'A)-C(5')-H(5'C)	109.5
H(5'B)-C(5')-H(5'C)	109.5
C(4)-C(6)-H(6A)	109.5
C(4)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(4)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(4)-C(6')-H(6'A)	109.5
C(4)-C(6')-H(6'B)	109.5
H(6'A)-C(6')-H(6'B)	109.5
C(4)-C(6')-H(6'C)	109.5
H(6'A)-C(6')-H(6'C)	109.5
H(6'B)-C(6')-H(6'C)	109.5
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(4)-C(7')-H(7'A)	109.5
C(4)-C(7')-H(7'B)	109.5
H(7'A)-C(7')-H(7'B)	109.5
C(4)-C(7')-H(7'C)	109.5
H(7'A)-C(7')-H(7'C)	109.5
H(7'B)-C(7')-H(7'C)	109.5
C(11)-C(8)-C(9)	110.7(11)
C(11)-C(8)-C(3)	108.9(8)
C(9)-C(8)-C(3)	105.9(8)
C(11)-C(8)-C(10)	109.8(10)
C(9)-C(8)-C(10)	108.9(11)
C(3)-C(8)-C(10)	112.5(10)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5

H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(3)-C(12)-C(13)	123.9(7)
O(3)-C(12)-C(15)	114.7(7)
C(13)-C(12)-C(15)	121.4(7)
C(12)-C(13)-C(14)	122.4(8)
C(12)-C(13)-H(13)	118.8
C(14)-C(13)-H(13)	118.8
O(4)-C(14)-C(13)	124.9(7)
O(4)-C(14)-C(19)	114.2(7)
C(13)-C(14)-C(19)	120.9(7)
C(18)-C(15)-C(16)	110.2(8)
C(18)-C(15)-C(17)	108.5(8)
C(16)-C(15)-C(17)	110.3(8)
C(18)-C(15)-C(12)	113.7(7)
C(16)-C(15)-C(12)	107.6(7)
C(17)-C(15)-C(12)	106.4(7)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(22)-C(19)-C(20)	108.9(9)
C(22)-C(19)-C(21)	108.4(9)
C(20)-C(19)-C(21)	110.3(9)
C(22)-C(19)-C(14)	107.1(7)
C(20)-C(19)-C(14)	113.9(7)
C(21)-C(19)-C(14)	108.0(7)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5

C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(5)-C(23)-C(24)	123.4(8)
O(5)-C(23)-C(26)	116.7(8)
C(24)-C(23)-C(26)	119.9(9)
C(25)-C(24)-C(23)	123.7(9)
C(25)-C(24)-H(24)	118.1
C(23)-C(24)-H(24)	118.1
O(6)-C(25)-C(24)	122.9(8)
O(6)-C(25)-C(30)	116.3(7)
C(24)-C(25)-C(30)	120.8(8)
C(29)-C(26)-C(28)	112.2(10)
C(29)-C(26)-C(27)	108.5(10)
C(28)-C(26)-C(27)	108.0(9)
C(29)-C(26)-C(23)	114.7(8)
C(28)-C(26)-C(23)	105.1(8)
C(27)-C(26)-C(23)	108.1(9)
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(32)-C(30)-C(33)	108.9(8)
C(32)-C(30)-C(31)	109.0(8)
C(33)-C(30)-C(31)	111.3(8)
C(32)-C(30)-C(25)	107.2(7)
C(33)-C(30)-C(25)	106.8(7)
C(31)-C(30)-C(25)	113.5(7)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5

N(1)-C(34)-C(35)	123.9(9)
N(1)-C(34)-H(34)	118.1
C(35)-C(34)-H(34)	118.1
C(36)-C(35)-C(34)	119.9(9)
C(36)-C(35)-H(35)	120.0
C(34)-C(35)-H(35)	120.0
C(35)-C(36)-C(37)	116.8(7)
C(35)-C(36)-C(39)	123.8(8)
C(37)-C(36)-C(39)	119.4(8)
C(36)-C(37)-C(38)	119.2(9)
C(36)-C(37)-H(37)	120.4
C(38)-C(37)-H(37)	120.4
N(1)-C(38)-C(37)	124.0(9)
N(1)-C(38)-H(38)	118.0
C(37)-C(38)-H(38)	118.0
C(73)-C(39)-C(40)	125.2(7)
C(73)-C(39)-C(36)	117.9(7)
C(40)-C(39)-C(36)	116.8(7)
C(39)-C(40)-N(2)	125.2(7)
C(39)-C(40)-C(41)	124.5(6)
N(2)-C(40)-C(41)	110.3(6)
C(42)-C(41)-C(40)	107.6(6)
C(42)-C(41)-H(41)	126.2
C(40)-C(41)-H(41)	126.2
C(41)-C(42)-C(43)	106.4(7)
C(41)-C(42)-H(42)	126.8
C(43)-C(42)-H(42)	126.8
N(2)-C(43)-C(44)	125.3(6)
N(2)-C(43)-C(42)	110.5(6)
C(44)-C(43)-C(42)	124.2(7)
C(43)-C(44)-C(50)	123.1(6)
C(43)-C(44)-C(45)	119.0(6)
C(50)-C(44)-C(45)	117.9(6)
C(46)-C(45)-C(48)	116.6(7)
C(46)-C(45)-C(44)	123.8(7)
C(48)-C(45)-C(44)	119.6(7)
C(47)-C(46)-C(45)	120.1(7)
C(47)-C(46)-H(46)	120.0
C(45)-C(46)-H(46)	120.0
N(8)-C(47)-C(46)	123.7(8)
N(8)-C(47)-H(47)	118.1
C(46)-C(47)-H(47)	118.1
C(45)-C(48)-C(49)	120.0(8)
C(45)-C(48)-H(48)	120.0
C(49)-C(48)-H(48)	120.0
N(8)-C(49)-C(48)	122.8(7)
N(8)-C(49)-H(49)	118.6
C(48)-C(49)-H(49)	118.6
N(3)-C(50)-C(44)	126.0(6)
N(3)-C(50)-C(51)	110.6(6)
C(44)-C(50)-C(51)	123.2(7)
C(52)-C(51)-C(50)	106.5(7)
C(52)-C(51)-H(51)	126.8
C(50)-C(51)-H(51)	126.8
C(51)-C(52)-C(53)	108.3(6)
C(51)-C(52)-H(52)	125.9
C(53)-C(52)-H(52)	125.9
C(54)-C(53)-N(3)	125.8(6)
C(54)-C(53)-C(52)	124.9(6)
N(3)-C(53)-C(52)	109.3(6)
C(53)-C(54)-C(60)	125.3(6)
C(53)-C(54)-C(55)	115.5(6)

C(60)-C(54)-C(55)	119.2(6)
C(58)-C(55)-C(56)	117.0(6)
C(58)-C(55)-C(54)	122.8(7)
C(56)-C(55)-C(54)	120.1(7)
C(57)-C(56)-C(55)	118.6(7)
C(57)-C(56)-H(56)	120.7
C(55)-C(56)-H(56)	120.7
N(6)-C(57)-C(56)	124.0(7)
N(6)-C(57)-H(57)	118.0
C(56)-C(57)-H(57)	118.0
C(59)-C(58)-C(55)	119.5(7)
C(59)-C(58)-H(58)	120.3
C(55)-C(58)-H(58)	120.3
N(6)-C(59)-C(58)	124.1(8)
N(6)-C(59)-H(59)	117.9
C(58)-C(59)-H(59)	117.9
C(54)-C(60)-N(4)	125.1(6)
C(54)-C(60)-C(61)	125.5(6)
N(4)-C(60)-C(61)	109.5(6)
C(62)-C(61)-C(60)	108.2(6)
C(62)-C(61)-H(61)	125.9
C(60)-C(61)-H(61)	125.9
C(61)-C(62)-C(63)	106.8(6)
C(61)-C(62)-H(62)	126.6
C(63)-C(62)-H(62)	126.6
N(4)-C(63)-C(64)	125.1(6)
N(4)-C(63)-C(62)	109.8(6)
C(64)-C(63)-C(62)	125.0(7)
C(63)-C(64)-C(70)	123.7(7)
C(63)-C(64)-C(65)	118.8(6)
C(70)-C(64)-C(65)	117.4(6)
C(66)-C(65)-C(68)	115.7(7)
C(66)-C(65)-C(64)	122.6(7)
C(68)-C(65)-C(64)	121.7(7)
C(65)-C(66)-C(67)	119.6(7)
C(65)-C(66)-H(66)	120.2
C(67)-C(66)-H(66)	120.2
N(7)-C(67)-C(66)	123.4(8)
N(7)-C(67)-H(67)	118.3
C(66)-C(67)-H(67)	118.3
C(69)-C(68)-C(65)	121.1(8)
C(69)-C(68)-H(68)	119.4
C(65)-C(68)-H(68)	119.4
N(7)-C(69)-C(68)	123.0(8)
N(7)-C(69)-H(69)	118.5
C(68)-C(69)-H(69)	118.5
N(5)-C(70)-C(64)	125.9(7)
N(5)-C(70)-C(71)	110.1(6)
C(64)-C(70)-C(71)	124.0(7)
C(72)-C(71)-C(70)	108.3(7)
C(72)-C(71)-H(71)	125.9
C(70)-C(71)-H(71)	125.9
C(71)-C(72)-C(73)	105.8(7)
C(71)-C(72)-H(72)	127.1
C(73)-C(72)-H(72)	127.1
N(5)-C(73)-C(39)	125.4(7)
N(5)-C(73)-C(72)	110.5(7)
C(39)-C(73)-C(72)	124.2(7)
O(7)-C(74)-C(75)	123.4(8)
O(7)-C(74)-C(77)	115.3(8)
C(75)-C(74)-C(77)	121.2(8)
C(74)-C(75)-C(76)	125.2(8)

C(74)-C(75)-H(75)	117.4
C(76)-C(75)-H(75)	117.4
O(8)-C(76)-C(75)	124.8(8)
O(8)-C(76)-C(81)	114.2(8)
C(75)-C(76)-C(81)	121.0(8)
C(78)-C(77)-C(80)	110.5(10)
C(78)-C(77)-C(74)	110.2(8)
C(80)-C(77)-C(74)	104.4(9)
C(78)-C(77)-C(79)	108.3(11)
C(80)-C(77)-C(79)	110.3(11)
C(74)-C(77)-C(79)	113.1(8)
C(77)-C(78)-H(78A)	109.5
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(77)-C(79)-H(79A)	109.5
C(77)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(77)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(77)-C(80)-H(80A)	109.5
C(77)-C(80)-H(80B)	109.5
H(80A)-C(80)-H(80B)	109.5
C(77)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5
H(80B)-C(80)-H(80C)	109.5
C(82)-C(81)-C(76)	115.9(9)
C(76)-C(81)-C(83')	105(8)
C(76)-C(81)-C(82')	102(8)
C(83')-C(81)-C(82')	114(4)
C(76)-C(81)-C(84')	105(8)
C(83')-C(81)-C(84')	114(4)
C(82')-C(81)-C(84')	114(4)
C(82)-C(81)-C(84)	110.2(13)
C(76)-C(81)-C(84)	105.7(10)
C(82)-C(81)-C(83)	107.9(12)
C(76)-C(81)-C(83)	108.7(9)
C(84)-C(81)-C(83)	108.1(14)
C(81)-C(82)-H(82A)	109.5
C(81)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(81)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(81)-C(82')-H(82D)	109.5
C(81)-C(82')-H(82E)	109.5
H(82D)-C(82')-H(82E)	109.5
C(81)-C(82')-H(82F)	109.5
H(82D)-C(82')-H(82F)	109.5
H(82E)-C(82')-H(82F)	109.5
C(81)-C(83)-H(83A)	109.5
C(81)-C(83)-H(83B)	109.5
H(83A)-C(83)-H(83B)	109.5
C(81)-C(83)-H(83C)	109.5
H(83A)-C(83)-H(83C)	109.5
H(83B)-C(83)-H(83C)	109.5
C(81)-C(83')-H(83D)	109.5
C(81)-C(83')-H(83E)	109.5
H(83D)-C(83')-H(83E)	109.5

C(81)-C(83')-H(83F)	109.5
H(83D)-C(83')-H(83F)	109.5
H(83E)-C(83')-H(83F)	109.5
C(81)-C(84)-H(84A)	109.5
C(81)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
C(81)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
C(81)-C(84')-H(84D)	109.5
C(81)-C(84')-H(84E)	109.5
H(84D)-C(84')-H(84E)	109.5
C(81)-C(84')-H(84F)	109.5
H(84D)-C(84')-H(84F)	109.5
H(84E)-C(84')-H(84F)	109.5
O(9)-C(85)-C(86)	123.3(9)
O(9)-C(85)-C(88')	122(2)
C(86)-C(85)-C(88')	113(2)
O(9)-C(85)-C(88)	112.3(11)
C(86)-C(85)-C(88)	124.3(10)
C(87)-C(86)-C(85)	124.8(10)
C(87)-C(86)-H(86)	117.6
C(85)-C(86)-H(86)	117.6
O(10)-C(87)-C(86)	123.8(10)
O(10)-C(87)-C(92)	119.6(11)
C(86)-C(87)-C(92)	115.6(10)
O(10)-C(87)-C(92')	107.7(17)
C(86)-C(87)-C(92')	127.5(16)
C(91)-C(88)-C(90)	104.3(14)
C(91)-C(88)-C(89)	110.8(16)
C(90)-C(88)-C(89)	111.5(13)
C(91)-C(88)-C(85)	109.6(11)
C(90)-C(88)-C(85)	114.5(13)
C(89)-C(88)-C(85)	106.2(11)
C(91')-C(88')-C(90')	109(6)
C(91')-C(88')-C(89')	98(5)
C(90')-C(88')-C(89')	125(8)
C(91')-C(88')-C(85)	102(5)
C(90')-C(88')-C(85)	114(6)
C(89')-C(88')-C(85)	105(6)
C(88)-C(89)-H(89A)	109.5
C(88)-C(89)-H(89B)	109.5
H(89A)-C(89)-H(89B)	109.5
C(88)-C(89)-H(89C)	109.5
H(89A)-C(89)-H(89C)	109.5
H(89B)-C(89)-H(89C)	109.5
C(88')-C(89')-H(89D)	109.5
C(88')-C(89')-H(89E)	109.5
H(89D)-C(89')-H(89E)	109.5
C(88')-C(89')-H(89F)	109.5
H(89D)-C(89')-H(89F)	109.5
H(89E)-C(89')-H(89F)	109.5
C(88)-C(90)-H(90A)	109.5
C(88)-C(90)-H(90B)	109.5
H(90A)-C(90)-H(90B)	109.5
C(88)-C(90)-H(90C)	109.5
H(90A)-C(90)-H(90C)	109.5
H(90B)-C(90)-H(90C)	109.5
C(88')-C(90')-H(90D)	109.5
C(88')-C(90')-H(90E)	109.5
H(90D)-C(90')-H(90E)	109.5
C(88')-C(90')-H(90F)	109.5

H(90D)-C(90')-H(90F)	109.5
H(90E)-C(90')-H(90F)	109.5
C(88)-C(91)-H(91A)	109.5
C(88)-C(91)-H(91B)	109.5
H(91A)-C(91)-H(91B)	109.5
C(88)-C(91)-H(91C)	109.5
H(91A)-C(91)-H(91C)	109.5
H(91B)-C(91)-H(91C)	109.5
C(88')-C(91')-H(91D)	109.5
C(88')-C(91')-H(91E)	109.5
H(91D)-C(91')-H(91E)	109.5
C(88')-C(91')-H(91F)	109.5
H(91D)-C(91')-H(91F)	109.5
H(91E)-C(91')-H(91F)	109.5
C(94)-C(92)-C(93)	110.1(18)
C(94)-C(92)-C(95)	112.7(15)
C(93)-C(92)-C(95)	110.8(18)
C(94)-C(92)-C(87)	102.4(12)
C(93)-C(92)-C(87)	112.6(15)
C(95)-C(92)-C(87)	108.0(13)
C(93')-C(92')-C(94')	99(3)
C(93')-C(92')-C(95')	99(3)
C(94')-C(92')-C(95')	103(3)
C(93')-C(92')-C(87)	119(3)
C(94')-C(92')-C(87)	121(3)
C(95')-C(92')-C(87)	113(2)
C(92)-C(93)-H(93A)	109.5
C(92)-C(93)-H(93B)	109.5
H(93A)-C(93)-H(93B)	109.5
C(92)-C(93)-H(93C)	109.5
H(93A)-C(93)-H(93C)	109.5
H(93B)-C(93)-H(93C)	109.5
C(92')-C(93')-H(93D)	109.5
C(92')-C(93')-H(93E)	109.5
H(93D)-C(93')-H(93E)	109.5
C(92')-C(93')-H(93F)	109.5
H(93D)-C(93')-H(93F)	109.5
H(93E)-C(93')-H(93F)	109.5
C(92)-C(94)-H(94A)	109.5
C(92)-C(94)-H(94B)	109.5
H(94A)-C(94)-H(94B)	109.5
C(92)-C(94)-H(94C)	109.5
H(94A)-C(94)-H(94C)	109.5
H(94B)-C(94)-H(94C)	109.5
C(92')-C(94')-H(94D)	109.5
C(92')-C(94')-H(94E)	109.5
H(94D)-C(94')-H(94E)	109.5
C(92')-C(94')-H(94F)	109.5
H(94D)-C(94')-H(94F)	109.5
H(94E)-C(94')-H(94F)	109.5
C(92)-C(95)-H(95A)	109.5
C(92)-C(95)-H(95B)	109.5
H(95A)-C(95)-H(95B)	109.5
C(92)-C(95)-H(95C)	109.5
H(95A)-C(95)-H(95C)	109.5
H(95B)-C(95)-H(95C)	109.5
C(92')-C(95')-H(95D)	109.5
C(92')-C(95')-H(95E)	109.5
H(95D)-C(95')-H(95E)	109.5
C(92')-C(95')-H(95F)	109.5
H(95D)-C(95')-H(95F)	109.5
H(95E)-C(95')-H(95F)	109.5

O(11)-C(96)-C(97)	123.2(9)
O(11)-C(96)-C(99)	116.0(9)
C(97)-C(96)-C(99)	120.8(8)
C(98)-C(97)-C(96)	125.5(9)
C(98)-C(97)-H(97)	117.3
C(96)-C(97)-H(97)	117.3
O(12)-C(98)-C(97)	123.9(9)
O(12)-C(98)-C(103)	115.7(9)
C(97)-C(98)-C(103)	120.4(9)
C(100)-C(99)-C(102)	107.7(11)
C(100)-C(99)-C(101)	102.1(16)
C(102)-C(99)-C(101)	120.0(16)
C(100)-C(99)-C(1A)	128(3)
C(102)-C(99)-C(1A)	94(3)
C(100)-C(99)-C(96)	108.3(9)
C(102)-C(99)-C(96)	105.3(9)
C(101)-C(99)-C(96)	112.9(11)
C(1A)-C(99)-C(96)	110.1(18)
C(99)-C(100)-H(10D)	109.5
C(99)-C(100)-H(10E)	109.5
H(10D)-C(100)-H(10E)	109.5
C(99)-C(100)-H(10F)	109.5
H(10D)-C(100)-H(10F)	109.5
H(10E)-C(100)-H(10F)	109.5
C(99)-C(101)-H(10G)	109.5
C(99)-C(101)-H(10H)	109.5
H(10G)-C(101)-H(10H)	109.5
C(99)-C(101)-H(10I)	109.5
H(10G)-C(101)-H(10I)	109.5
H(10H)-C(101)-H(10I)	109.5
C(99)-C(102)-H(10J)	109.5
C(99)-C(102)-H(10K)	109.5
H(10J)-C(102)-H(10K)	109.5
C(99)-C(102)-H(10L)	109.5
H(10J)-C(102)-H(10L)	109.5
H(10K)-C(102)-H(10L)	109.5
C(106)-C(103)-C(105)	112.2(15)
C(1B)-C(103)-C(1D)	106(2)
C(106)-C(103)-C(98)	110.0(10)
C(105)-C(103)-C(98)	102.8(12)
C(1B)-C(103)-C(98)	112.2(16)
C(1D)-C(103)-C(98)	114.2(13)
C(106)-C(103)-C(104)	112.1(18)
C(105)-C(103)-C(104)	108.7(17)
C(98)-C(103)-C(104)	110.6(11)
C(1B)-C(103)-C(1C)	106(2)
C(1D)-C(103)-C(1C)	107(2)
C(98)-C(103)-C(1C)	111.5(14)
C(103)-C(104)-H(10M)	109.5
C(103)-C(104)-H(10N)	109.5
H(10M)-C(104)-H(10N)	109.5
C(103)-C(104)-H(10O)	109.5
H(10M)-C(104)-H(10O)	109.5
H(10N)-C(104)-H(10O)	109.5
C(103)-C(105)-H(10P)	109.5
C(103)-C(105)-H(10Q)	109.5
H(10P)-C(105)-H(10Q)	109.5
C(103)-C(105)-H(10R)	109.5
H(10P)-C(105)-H(10R)	109.5
H(10Q)-C(105)-H(10R)	109.5
C(103)-C(106)-H(10S)	109.5
C(103)-C(106)-H(10T)	109.5

H(10S)-C(106)-H(10T)	109.5
C(103)-C(106)-H(10U)	109.5
H(10S)-C(106)-H(10U)	109.5
H(10T)-C(106)-H(10U)	109.5
O(15)-Cs(1)-O(13)	106.0(2)
O(15)-Cs(1)-O(18)	133.5(2)
O(13)-Cs(1)-O(18)	112.6(2)
O(15)-Cs(1)-O(16)	60.9(2)
O(13)-Cs(1)-O(16)	150.0(2)
O(18)-Cs(1)-O(16)	93.27(19)
O(15)-Cs(1)-O(14)	131.7(2)
O(13)-Cs(1)-O(14)	60.6(2)
O(18)-Cs(1)-O(14)	90.67(19)
O(16)-Cs(1)-O(14)	106.18(19)
O(15)-Cs(1)-O(17)	95.0(3)
O(13)-Cs(1)-O(17)	91.1(2)
O(18)-Cs(1)-O(17)	60.2(2)
O(16)-Cs(1)-O(17)	115.8(2)
O(14)-Cs(1)-O(17)	128.9(2)
O(15)-Cs(1)-N(9)	60.8(3)
O(13)-Cs(1)-N(9)	60.6(2)
O(18)-Cs(1)-N(9)	118.9(3)
O(16)-Cs(1)-N(9)	120.5(2)
O(14)-Cs(1)-N(9)	120.5(2)
O(17)-Cs(1)-N(9)	59.5(3)
O(15)-Cs(1)-N(10)	119.9(2)
O(13)-Cs(1)-N(10)	120.3(2)
O(18)-Cs(1)-N(10)	59.2(2)
O(16)-Cs(1)-N(10)	59.8(2)
O(14)-Cs(1)-N(10)	60.6(2)
O(17)-Cs(1)-N(10)	118.5(2)
N(9)-Cs(1)-N(10)	178.0(3)
C(109)-O(13)-C(108)	111.7(9)
C(109)-O(13)-Cs(1)	110.3(6)
C(108)-O(13)-Cs(1)	105.6(6)
C(111)-O(14)-C(110)	113.6(9)
C(111)-O(14)-Cs(1)	111.1(5)
C(110)-O(14)-Cs(1)	105.2(5)
C(114)-O(15)-C(115)	112.3(9)
C(114)-O(15)-Cs(1)	112.7(8)
C(115)-O(15)-Cs(1)	108.1(6)
C(117)-O(16)-C(116)	113.3(8)
C(117)-O(16)-Cs(1)	104.6(5)
C(116)-O(16)-Cs(1)	108.6(6)
C(121)-O(17)-C(120)	113.0(12)
C(121)-O(17)-Cs(1)	108.2(6)
C(120)-O(17)-Cs(1)	112.8(7)
C(123)-O(18)-C(122)	110.8(8)
C(123)-O(18)-Cs(1)	109.3(6)
C(122)-O(18)-Cs(1)	108.7(6)
C(113)-N(9)-C(119)	112.3(12)
C(113)-N(9)-C(107)	110.9(11)
C(119)-N(9)-C(107)	109.1(11)
C(113)-N(9)-Cs(1)	105.2(7)
C(119)-N(9)-Cs(1)	111.1(7)
C(107)-N(9)-Cs(1)	108.1(7)
C(124)-N(10)-C(118)	112.1(9)
C(124)-N(10)-C(112)	110.2(8)
C(118)-N(10)-C(112)	111.6(9)
C(124)-N(10)-Cs(1)	109.9(6)
C(118)-N(10)-Cs(1)	107.2(6)
C(112)-N(10)-Cs(1)	105.6(5)

N(9)-C(107)-C(108)	113.1(10)
N(9)-C(107)-Cs(1)	50.3(5)
C(108)-C(107)-Cs(1)	71.0(6)
N(9)-C(107)-H(10V)	109.0
C(108)-C(107)-H(10V)	109.0
Cs(1)-C(107)-H(10V)	151.2
N(9)-C(107)-H(10W)	109.0
C(108)-C(107)-H(10W)	109.0
Cs(1)-C(107)-H(10W)	98.9
H(10V)-C(107)-H(10W)	107.8
O(13)-C(108)-C(107)	106.5(10)
O(13)-C(108)-Cs(1)	51.4(4)
C(107)-C(108)-Cs(1)	85.5(6)
O(13)-C(108)-H(10X)	110.4
C(107)-C(108)-H(10X)	110.4
Cs(1)-C(108)-H(10X)	159.9
O(13)-C(108)-H(10Y)	110.4
C(107)-C(108)-H(10Y)	110.4
Cs(1)-C(108)-H(10Y)	75.2
H(10X)-C(108)-H(10Y)	108.6
O(13)-C(109)-C(110)	108.2(10)
O(13)-C(109)-Cs(1)	48.6(4)
C(110)-C(109)-Cs(1)	76.6(6)
O(13)-C(109)-H	110.1
C(110)-C(109)-H	110.1
Cs(1)-C(109)-H	88.1
O(13)-C(109)-H(10Z)	110.1
C(110)-C(109)-H(10Z)	110.1
Cs(1)-C(109)-H(10Z)	157.6
H-C(109)-H(10Z)	108.4
O(14)-C(110)-C(109)	109.5(10)
O(14)-C(110)-Cs(1)	52.3(4)
C(109)-C(110)-Cs(1)	80.0(6)
O(14)-C(110)-H(11D)	109.8
C(109)-C(110)-H(11D)	109.8
Cs(1)-C(110)-H(11D)	81.2
O(14)-C(110)-H(11E)	109.8
C(109)-C(110)-H(11E)	109.8
Cs(1)-C(110)-H(11E)	162.1
H(11D)-C(110)-H(11E)	108.2
O(14)-C(111)-C(112)	108.9(9)
O(14)-C(111)-Cs(1)	48.0(4)
C(112)-C(111)-Cs(1)	80.8(5)
O(14)-C(111)-H(11F)	109.9
C(112)-C(111)-H(11F)	109.9
Cs(1)-C(111)-H(11F)	157.9
O(14)-C(111)-H(11G)	109.9
C(112)-C(111)-H(11G)	109.9
Cs(1)-C(111)-H(11G)	84.7
H(11F)-C(111)-H(11G)	108.3
N(10)-C(112)-C(111)	115.0(8)
N(10)-C(112)-Cs(1)	52.3(4)
C(111)-C(112)-Cs(1)	76.0(5)
N(10)-C(112)-H(11H)	108.5
C(111)-C(112)-H(11H)	108.5
Cs(1)-C(112)-H(11H)	157.9
N(10)-C(112)-H(11I)	108.5
C(111)-C(112)-H(11I)	108.5
Cs(1)-C(112)-H(11I)	90.7
H(11H)-C(112)-H(11I)	107.5
N(9)-C(113)-C(114)	115.7(12)
N(9)-C(113)-Cs(1)	53.1(6)

C(114)-C(113)-Cs(1)	77.1(6)
N(9)-C(113)-H(11J)	108.4
C(114)-C(113)-H(11J)	108.4
Cs(1)-C(113)-H(11J)	159.4
N(9)-C(113)-H(11K)	108.4
C(114)-C(113)-H(11K)	108.4
Cs(1)-C(113)-H(11K)	88.9
H(11J)-C(113)-H(11K)	107.4
O(15)-C(114)-C(113)	110.6(11)
O(15)-C(114)-Cs(1)	46.8(5)
C(113)-C(114)-Cs(1)	79.4(6)
O(15)-C(114)-H(11L)	109.5
C(113)-C(114)-H(11L)	109.5
Cs(1)-C(114)-H(11L)	155.5
O(15)-C(114)-H(11M)	109.5
C(113)-C(114)-H(11M)	109.5
Cs(1)-C(114)-H(11M)	89.2
H(11L)-C(114)-H(11M)	108.1
O(15)-C(115)-C(116)	109.0(9)
O(15)-C(115)-Cs(1)	50.0(4)
C(116)-C(115)-Cs(1)	80.9(6)
O(15)-C(115)-H(11N)	109.9
C(116)-C(115)-H(11N)	109.9
Cs(1)-C(115)-H(11N)	82.4
O(15)-C(115)-H(11O)	109.9
C(116)-C(115)-H(11O)	109.9
Cs(1)-C(115)-H(11O)	159.9
H(11N)-C(115)-H(11O)	108.3
O(16)-C(116)-C(115)	110.0(8)
O(16)-C(116)-Cs(1)	49.7(4)
C(115)-C(116)-Cs(1)	75.5(5)
O(16)-C(116)-H(11P)	109.7
C(115)-C(116)-H(11P)	109.7
Cs(1)-C(116)-H(11P)	89.7
O(16)-C(116)-H(11Q)	109.7
C(115)-C(116)-H(11Q)	109.7
Cs(1)-C(116)-H(11Q)	157.5
H(11P)-C(116)-H(11Q)	108.2
O(16)-C(117)-C(118)	112.6(10)
O(16)-C(117)-Cs(1)	53.5(4)
C(118)-C(117)-Cs(1)	87.7(5)
O(16)-C(117)-H(11R)	109.1
C(118)-C(117)-H(11R)	109.1
Cs(1)-C(117)-H(11R)	160.5
O(16)-C(117)-H(11S)	109.1
C(118)-C(117)-H(11S)	109.1
Cs(1)-C(117)-H(11S)	74.5
H(11R)-C(117)-H(11S)	107.8
N(10)-C(118)-C(117)	116.7(9)
N(10)-C(118)-Cs(1)	51.4(4)
C(117)-C(118)-Cs(1)	69.6(5)
N(10)-C(118)-H(11T)	108.1
C(117)-C(118)-H(11T)	108.1
Cs(1)-C(118)-H(11T)	145.5
N(10)-C(118)-H(11U)	108.1
C(117)-C(118)-H(11U)	108.1
Cs(1)-C(118)-H(11U)	105.8
H(11T)-C(118)-H(11U)	107.3
N(9)-C(119)-C(120)	114.0(11)
N(9)-C(119)-Cs(1)	48.2(5)
C(120)-C(119)-Cs(1)	76.1(6)
N(9)-C(119)-H(11V)	108.8

C(120)-C(119)-H(11V)	108.8
Cs(1)-C(119)-H(11V)	152.7
N(9)-C(119)-H(11W)	108.8
C(120)-C(119)-H(11W)	108.8
Cs(1)-C(119)-H(11W)	95.4
H(11V)-C(119)-H(11W)	107.7
O(17)-C(120)-C(119)	109.5(13)
O(17)-C(120)-Cs(1)	46.4(5)
C(119)-C(120)-Cs(1)	81.0(7)
O(17)-C(120)-H(12A)	109.8
C(119)-C(120)-H(12A)	109.8
Cs(1)-C(120)-H(12A)	155.9
O(17)-C(120)-H(12B)	109.8
C(119)-C(120)-H(12B)	109.8
Cs(1)-C(120)-H(12B)	86.9
H(12A)-C(120)-H(12B)	108.2
O(17)-C(121)-C(122)	107.7(10)
O(17)-C(121)-Cs(1)	50.0(5)
C(122)-C(121)-Cs(1)	78.0(7)
O(17)-C(121)-H(12C)	110.2
C(122)-C(121)-H(12C)	110.2
Cs(1)-C(121)-H(12C)	84.5
O(17)-C(121)-H(12D)	110.2
C(122)-C(121)-H(12D)	110.2
Cs(1)-C(121)-H(12D)	159.9
H(12C)-C(121)-H(12D)	108.5
O(18)-C(122)-C(121)	110.2(10)
O(18)-C(122)-Cs(1)	49.5(5)
C(121)-C(122)-Cs(1)	79.1(7)
O(18)-C(122)-H(12E)	109.6
C(121)-C(122)-H(12E)	109.6
Cs(1)-C(122)-H(12E)	85.9
O(18)-C(122)-H(12F)	109.6
C(121)-C(122)-H(12F)	109.6
Cs(1)-C(122)-H(12F)	158.7
H(12E)-C(122)-H(12F)	108.1
O(18)-C(123)-C(124)	108.8(9)
O(18)-C(123)-Cs(1)	49.4(5)
C(124)-C(123)-Cs(1)	84.5(6)
O(18)-C(123)-H(12G)	109.9
C(124)-C(123)-H(12G)	109.9
Cs(1)-C(123)-H(12G)	158.8
O(18)-C(123)-H(12H)	109.9
C(124)-C(123)-H(12H)	109.9
Cs(1)-C(123)-H(12H)	79.6
H(12G)-C(123)-H(12H)	108.3
N(10)-C(124)-C(123)	113.9(9)
N(10)-C(124)-Cs(1)	49.6(5)
C(123)-C(124)-Cs(1)	72.0(5)
N(10)-C(124)-H(12I)	108.8
C(123)-C(124)-H(12I)	108.8
Cs(1)-C(124)-H(12I)	150.3
N(10)-C(124)-H(12J)	108.8
C(123)-C(124)-H(12J)	108.8
Cs(1)-C(124)-H(12J)	99.6
H(12I)-C(124)-H(12J)	107.7

Symmetry transformations used to generate equivalent atoms:
#1 x-1,-y+1/2,z-1/2 #2 x,-y+1/2,z+1/2 #3 x+1,-y+1/2,z+1/2
#4 x,-y+1/2,z-1/2

Table S6. Bond lengths [E] and angles [°] for **3**.

Tb(1)-O(1)	2.311(3)
Tb(1)-O(4)	2.313(4)
Tb(1)-O(5)	2.327(3)
Tb(1)-O(3)	2.339(4)
Tb(1)-O(6)	2.349(4)
Tb(1)-O(2)	2.349(3)
Tb(1)-N(1)	2.604(4)
Tb(1)-N(6)#1	2.637(4)
Tb(2)-O(8)	2.299(4)
Tb(2)-O(10)	2.309(4)
Tb(2)-O(11)	2.323(3)
Tb(2)-O(9)	2.340(4)
Tb(2)-O(12)	2.341(3)
Tb(2)-O(7)	2.373(4)
Tb(2)-N(8)#2	2.580(4)
Tb(2)-N(7)	2.598(4)
Cs(1)-O(18')	2.832(10)
Cs(1)-O(13)	2.932(13)
Cs(1)-O(17)	3.020(8)
Cs(1)-O(18)	3.042(11)
Cs(1)-O(13')	3.06(2)
Cs(1)-O(14)	3.102(11)
Cs(1)-O(14')	3.200(14)
Cs(1)-N(5)	3.207(4)
Cs(1)-O(17')	3.227(12)
Cs(1)-N(10')	3.23(2)
Cs(1)-C(40)	3.287(5)
Cs(1)-N(9)	3.309(16)
Cs(2)-O(23)	2.991(7)
Cs(2)-O(21)	2.993(10)
Cs(2)-O(24)	3.020(6)
Cs(2)-O(22)	3.147(10)
Cs(2)-N(11)	3.218(6)
Cs(2)-N(12)	3.252(8)
Cs(2)-N(3)	3.293(5)
Cs(2)-N(4)	3.386(4)
Cs(2)-C(53)	3.527(5)
Cs(2)-C(142)	3.551(10)
Cs(2)-C(131)	3.60(2)
Cs(2)-C(136)	3.665(8)
Cs(2')-O(23')	2.99(2)
Cs(2')-O(24')	3.03(3)
Cs(2')-O(22')	3.032(19)
Cs(2')-O(21')	3.13(4)
Cs(2')-N(3)	3.184(5)
Cs(2')-N(11)	3.256(6)
Cs(2')-N(12')	3.285(19)
Cs(2')-N(4)	3.360(5)
Cs(2')-C(23A)	3.60(2)
Cs(2')-C(141)	3.604(7)
Cs(2')-C(24A)	3.68(6)
Cs(2')-C(53)	3.706(6)
O(1)-C(1)	1.262(6)
O(2)-C(3)	1.276(6)
O(3)-C(12)	1.270(8)
O(4)-C(14)	1.261(7)
O(5)-C(23)	1.254(7)
O(6)-C(25)	1.279(6)
O(7)-C(74)	1.267(7)
O(8)-C(76)	1.264(7)

O(9)-C(85)	1.259(7)
O(10)-C(87)	1.266(7)
O(11)-C(96)	1.267(7)
O(12)-C(98)	1.275(7)
O(13)-C(108)	1.39(2)
O(13)-C(109)	1.50(3)
O(13')-C(2A)	1.29(4)
O(13')-C(3A)	1.50(4)
O(14)-C(110)	1.37(2)
O(14)-C(111)	1.56(2)
O(14')-C(4A)	1.32(3)
O(14')-C(5A)	1.63(3)
O(15)-C(114)	1.398(10)
O(15)-C(115)	1.435(9)
O(16)-C(116)	1.404(8)
O(16)-C(117)	1.416(8)
O(17)-C(121)	1.361(19)
O(17)-C(120)	1.47(3)
O(17')-C(11A)	1.37(3)
O(17')-C(10A)	1.46(2)
O(18)-C(123)	1.38(2)
O(18)-C(122)	1.46(3)
O(18')-C(13A)	1.36(4)
O(18')-C(12A)	1.48(2)
O(19)-C(127)	1.343(12)
O(19)-C(126)	1.400(14)
O(19')-C(16A)	1.394(13)
O(19')-C(127)	1.521(12)
O(20)-C(129)	1.397(9)
O(20)-C(128)	1.436(10)
O(20')-C(129)	1.36(2)
O(20')-C(17A)	1.45(4)
O(21)-C(133)	1.369(18)
O(21)-C(132)	1.451(18)
O(21')-C(20A)	1.41(6)
O(21')-C(21A)	1.44(6)
O(22)-C(135)	1.385(14)
O(22)-C(134)	1.435(14)
O(22')-C(22A)	1.55(2)
O(22')-C(136)	1.563(17)
O(23)-C(138)	1.398(17)
O(23)-C(139)	1.441(16)
O(23')-C(25A)	1.41(4)
O(23')-C(26A)	1.44(4)
O(24)-C(140)	1.446(16)
O(24)-C(141)	1.446(10)
O(24')-C(28A)	1.37(5)
O(24')-C(27A)	1.52(6)
N(1)-C(34)	1.329(7)
N(1)-C(38)	1.347(7)
N(2)-C(70)	1.383(7)
N(2)-C(73)	1.394(6)
N(2)-H(2)	0.8800
N(3)-C(60)	1.378(7)
N(3)-C(63)	1.385(7)
N(3)-H(3)	0.8800
N(4)-C(50)	1.393(6)
N(4)-C(53)	1.399(6)
N(4)-H(4)	0.8800
N(5)-C(40)	1.372(7)
N(5)-C(43)	1.387(6)
N(5)-H(5)	0.8800

N(6)-C(49)	1.336(6)
N(6)-C(47)	1.354(6)
N(7)-C(57)	1.335(7)
N(7)-C(59)	1.354(7)
N(8)-C(67)	1.312(7)
N(8)-C(69)	1.348(7)
N(9)-C(113)	1.44(3)
N(9)-C(119)	1.45(2)
N(9)-C(107)	1.54(3)
N(9')-C(9A)	1.40(4)
N(9')-C(1A)	1.48(3)
N(9')-C(7A)	1.56(4)
N(10)-C(112)	1.43(2)
N(10)-C(118)	1.48(3)
N(10)-C(124)	1.55(4)
N(10')-C(6A)	1.42(3)
N(10')-C(8A)	1.48(3)
N(10')-C(14A)	1.49(3)
N(11)-C(24A)	1.25(6)
N(11)-C(125)	1.444(18)
N(11)-C(131)	1.453(12)
N(11)-C(19A)	1.460(19)
N(11)-C(15A)	1.51(6)
N(11)-C(137)	1.572(17)
N(12)-C(142)	1.435(12)
N(12)-C(130)	1.478(11)
N(12)-C(136)	1.483(11)
N(12')-C(18A)	1.459(19)
N(12')-C(23A)	1.463(19)
N(12')-C(141)	1.473(17)
C(1)-C(2)	1.402(8)
C(1)-C(4)	1.542(7)
C(1A)-C(2A)	1.46(5)
C(1A)-H(1AA)	0.9900
C(1A)-H(1AB)	0.9900
C(2)-C(3)	1.380(8)
C(2)-H(2A)	0.9500
C(2A)-H(2AA)	0.9900
C(2A)-H(2AB)	0.9900
C(3)-C(8)	1.552(7)
C(3A)-C(4A)	1.548(19)
C(3A)-H(3AA)	0.9900
C(3A)-H(3AB)	0.9900
C(4)-C(7)	1.527(8)
C(4)-C(5)	1.528(9)
C(4)-C(6)	1.549(9)
C(4A)-H(4AA)	0.9900
C(4A)-H(4AB)	0.9900
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(5A)-C(6A)	1.27(3)
C(5A)-H(5AA)	0.9900
C(5A)-H(5AB)	0.9900
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(6A)-H(6AA)	0.9900
C(6A)-H(6AB)	0.9900
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800

C(7A)-C(114)	1.573(19)
C(7A)-H(7AA)	0.9900
C(7A)-H(7AB)	0.9900
C(8)-C(11)	1.526(8)
C(8)-C(10)	1.529(9)
C(8)-C(9)	1.536(8)
C(8A)-C(117)	1.515(15)
C(8A)-H(8AA)	0.9900
C(8A)-H(8AB)	0.9900
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(9A)-C(10A)	1.55(4)
C(9A)-H(9AA)	0.9900
C(9A)-H(9AB)	0.9900
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(10A)-H(10D)	0.9900
C(10A)-H(10E)	0.9900
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(11A)-C(12A)	1.52(3)
C(11A)-H(11D)	0.9900
C(11A)-H(11E)	0.9900
C(12)-C(13)	1.384(10)
C(12)-C(15')	1.548(13)
C(12)-C(15)	1.587(13)
C(12A)-H(12A)	0.9900
C(12A)-H(12B)	0.9900
C(13)-C(14)	1.405(9)
C(13)-H(13)	0.9500
C(13A)-C(14A)	1.52(3)
C(13A)-H(13A)	0.9900
C(13A)-H(13B)	0.9900
C(14)-C(19)	1.540(8)
C(14A)-H(14A)	0.9900
C(14A)-H(14B)	0.9900
C(15)-C(18)	1.514(14)
C(15)-C(16)	1.520(13)
C(15)-C(17)	1.522(13)
C(15')-C(18')	1.508(13)
C(15')-C(16')	1.528(13)
C(15')-C(17')	1.529(12)
C(15A)-C(16A)	1.576(15)
C(15A)-H(15A)	0.9900
C(15A)-H(15B)	0.9900
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(16')-H(16D)	0.9800
C(16')-H(16E)	0.9800
C(16')-H(16F)	0.9800
C(16A)-H(16G)	0.9900
C(16A)-H(16H)	0.9900
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(17')-H(17D)	0.9800
C(17')-H(17E)	0.9800
C(17')-H(17F)	0.9800

C(17A)-C(127)	1.36(2)
C(17A)-H(17G)	0.9900
C(17A)-H(17H)	0.9900
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(18')-H(18D)	0.9800
C(18')-H(18E)	0.9800
C(18')-H(18F)	0.9800
C(18A)-C(129)	1.42(3)
C(18A)-H(18G)	0.9900
C(18A)-H(18H)	0.9900
C(19)-C(21)	1.521(10)
C(19)-C(22)	1.546(10)
C(19)-C(20)	1.551(9)
C(19A)-C(20A)	1.61(6)
C(19A)-H(19A)	0.9900
C(19A)-H(19B)	0.9900
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(20A)-H(20D)	0.9900
C(20A)-H(20E)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(21A)-C(22A)	1.37(6)
C(21A)-H(21D)	0.9900
C(21A)-H(21E)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(22A)-H(22D)	0.9900
C(22A)-H(22E)	0.9900
C(23)-C(24)	1.386(8)
C(23)-C(26)	1.547(8)
C(23A)-C(136)	1.40(3)
C(23A)-H(23A)	0.9900
C(23A)-H(23B)	0.9900
C(24)-C(25)	1.402(8)
C(24)-H(24)	0.9500
C(24A)-C(25A)	1.43(6)
C(24A)-H(24A)	0.9900
C(24A)-H(24B)	0.9900
C(25)-C(30)	1.538(8)
C(25A)-H(25A)	0.9900
C(25A)-H(25B)	0.9900
C(26)-C(27)	1.497(13)
C(26)-C(29)	1.510(10)
C(26)-C(28)	1.518(11)
C(26A)-C(27A)	1.45(6)
C(26A)-H(26A)	0.9900
C(26A)-H(26B)	0.9900
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(27A)-H(27D)	0.9900
C(27A)-H(27E)	0.9900
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(28A)-C(141)	1.51(3)

C(28A)-H(28D)	0.9900
C(28A)-H(28E)	0.9900
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(33)	1.520(8)
C(30)-C(31)	1.530(9)
C(30)-C(32)	1.538(9)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.373(8)
C(34)-H(34)	0.9500
C(35)-C(36)	1.372(8)
C(35)-H(35)	0.9500
C(36)-C(37)	1.386(8)
C(36)-C(39)	1.499(7)
C(37)-C(38)	1.386(8)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(39)-C(73)	1.357(7)
C(39)-C(40)	1.458(7)
C(40)-C(41)	1.414(7)
C(41)-C(42)	1.389(8)
C(41)-H(41)	0.9500
C(42)-C(43)	1.410(7)
C(42)-H(42)	0.9500
C(43)-C(44)	1.453(7)
C(44)-C(50)	1.382(7)
C(44)-C(45)	1.483(7)
C(45)-C(48)	1.398(7)
C(45)-C(46)	1.400(7)
C(46)-C(47)	1.384(7)
C(46)-H(46)	0.9500
C(47)-H(47)	0.9500
C(48)-C(49)	1.397(7)
C(48)-H(48)	0.9500
C(49)-H(49)	0.9500
C(50)-C(51)	1.440(7)
C(51)-C(52)	1.351(7)
C(51)-H(51)	0.9500
C(52)-C(53)	1.431(7)
C(52)-H(52)	0.9500
C(53)-C(54)	1.376(7)
C(54)-C(60)	1.451(8)
C(54)-C(55)	1.487(7)
C(55)-C(56)	1.385(7)
C(55)-C(58)	1.403(7)
C(56)-C(57)	1.383(7)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-C(59)	1.383(8)
C(58)-H(58)	0.9500
C(59)-H(59)	0.9500
C(60)-C(61)	1.406(7)
C(61)-C(62)	1.382(8)

C(61)-H(61)	0.9500
C(62)-C(63)	1.409(7)
C(62)-H(62)	0.9500
C(63)-C(64)	1.449(8)
C(64)-C(70)	1.389(7)
C(64)-C(65)	1.492(7)
C(65)-C(68)	1.383(8)
C(65)-C(66)	1.399(7)
C(66)-C(67)	1.384(8)
C(66)-H(66)	0.9500
C(67)-H(67)	0.9500
C(68)-C(69)	1.391(8)
C(68)-H(68)	0.9500
C(69)-H(69)	0.9500
C(70)-C(71)	1.446(8)
C(71)-C(72)	1.356(8)
C(71)-H(71)	0.9500
C(72)-C(73)	1.452(7)
C(72)-H(72)	0.9500
C(74)-C(75)	1.411(9)
C(74)-C(77)	1.534(10)
C(75)-C(76)	1.404(10)
C(75)-H(75)	0.9500
C(76)-C(81)	1.550(9)
C(77)-C(78)	1.519(9)
C(77)-C(80)	1.527(10)
C(77)-C(79)	1.541(11)
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(80)-H(80A)	0.9800
C(80)-H(80B)	0.9800
C(80)-H(80C)	0.9800
C(81)-C(82)	1.513(10)
C(81)-C(83)	1.522(9)
C(81)-C(84)	1.531(12)
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(83)-H(83A)	0.9800
C(83)-H(83B)	0.9800
C(83)-H(83C)	0.9800
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800
C(85)-C(86)	1.413(9)
C(85)-C(88)	1.542(10)
C(86)-C(87)	1.392(9)
C(86)-H(86)	0.9500
C(87)-C(92)	1.549(9)
C(88)-C(90)	1.504(11)
C(88)-C(91)	1.506(10)
C(88)-C(89)	1.521(12)
C(89)-H(89A)	0.9800
C(89)-H(89B)	0.9800
C(89)-H(89C)	0.9800
C(90)-H(90A)	0.9800
C(90)-H(90B)	0.9800
C(90)-H(90C)	0.9800

C(91)-H(91A)	0.9800
C(91)-H(91B)	0.9800
C(91)-H(91C)	0.9800
C(92)-C(93)	1.525(9)
C(92)-C(95)	1.529(11)
C(92)-C(94)	1.543(10)
C(93)-H(93A)	0.9800
C(93)-H(93B)	0.9800
C(93)-H(93C)	0.9800
C(94)-H(94A)	0.9800
C(94)-H(94B)	0.9800
C(94)-H(94C)	0.9800
C(95)-H(95A)	0.9800
C(95)-H(95B)	0.9800
C(95)-H(95C)	0.9800
C(96)-C(97)	1.413(8)
C(96)-C(99)	1.539(8)
C(97)-C(98)	1.385(8)
C(97)-H(97)	0.9500
C(98)-C(103)	1.529(7)
C(99)-C(100)	1.502(10)
C(99)-C(102)	1.524(8)
C(99)-C(101)	1.536(10)
C(100)-H(10F)	0.9800
C(100)-H(10G)	0.9800
C(100)-H(10H)	0.9800
C(101)-H(10I)	0.9800
C(101)-H(10J)	0.9800
C(101)-H(10K)	0.9800
C(102)-H(10L)	0.9800
C(102)-H(10M)	0.9800
C(102)-H(10N)	0.9800
C(103)-C(106)	1.512(10)
C(103)-C(104)	1.533(10)
C(103)-C(105)	1.538(10)
C(104)-H(10O)	0.9800
C(104)-H(10P)	0.9800
C(104)-H(10Q)	0.9800
C(105)-H(10R)	0.9800
C(105)-H(10S)	0.9800
C(105)-H(10T)	0.9800
C(106)-H(10U)	0.9800
C(106)-H(10V)	0.9800
C(106)-H(10W)	0.9800
C(107)-C(108)	1.58(3)
C(107)-H(10X)	0.9900
C(107)-H(10Y)	0.9900
C(108)-H	0.9900
C(108)-H(10Z)	0.9900
C(109)-C(110)	1.566(17)
C(109)-H(10)	0.9900
C(109)-HA	0.9900
C(110)-H(11F)	0.9900
C(110)-H(11G)	0.9900
C(111)-C(112)	1.40(3)
C(111)-H(11H)	0.9900
C(111)-H(11I)	0.9900
C(112)-H(11J)	0.9900
C(112)-H(11K)	0.9900
C(113)-C(114)	1.546(15)
C(113)-H(11L)	0.9900
C(113)-H(11M)	0.9900

C(114)-H(11N)	0.9900
C(114)-H(11O)	0.9900
C(114)-H(11P)	0.9900
C(114)-H(11Q)	0.9900
C(115)-C(116)	1.471(11)
C(115)-H(11R)	0.9900
C(115)-H(11S)	0.9900
C(116)-H(11T)	0.9900
C(116)-H(11U)	0.9900
C(117)-C(118)	1.523(15)
C(117)-H(11V)	0.9900
C(117)-H(11W)	0.9900
C(117)-H(11X)	0.9900
C(117)-H(11Y)	0.9900
C(118)-H(11Z)	0.9900
C(118)-HB	0.9900
C(119)-C(120)	1.51(3)
C(119)-H(11)	0.9900
C(119)-HC	0.9900
C(120)-H(12C)	0.9900
C(120)-H(12D)	0.9900
C(121)-C(122)	1.49(3)
C(121)-H(12E)	0.9900
C(121)-H(12F)	0.9900
C(122)-H(12G)	0.9900
C(122)-H(12H)	0.9900
C(123)-C(124)	1.49(3)
C(123)-H(12I)	0.9900
C(123)-H(12J)	0.9900
C(124)-H(12K)	0.9900
C(124)-H(12L)	0.9900
C(125)-C(126)	1.588(12)
C(125)-H(12M)	0.9900
C(125)-H(12N)	0.9900
C(126)-H(12O)	0.9900
C(126)-H(12P)	0.9900
C(127)-C(128)	1.432(14)
C(127)-H(12S)	0.9900
C(127)-H(12T)	0.9900
C(127)-H(12Q)	0.9900
C(127)-H(12R)	0.9900
C(128)-H(12U)	0.9900
C(128)-H(12V)	0.9900
C(129)-C(130)	1.485(12)
C(129)-H(12W)	0.9900
C(129)-H(12X)	0.9900
C(129)-H(12Y)	0.9900
C(129)-HD	0.9900
C(130)-H(13C)	0.9900
C(130)-H(13D)	0.9900
C(131)-C(132)	1.45(2)
C(131)-H(13E)	0.9900
C(131)-H(13F)	0.9900
C(132)-H(13G)	0.9900
C(132)-H(13H)	0.9900
C(133)-C(134)	1.475(16)
C(133)-H(13I)	0.9900
C(133)-H(13J)	0.9900
C(134)-H(13K)	0.9900
C(134)-H(13L)	0.9900
C(135)-C(136)	1.474(12)
C(135)-H(13M)	0.9900

C(135)-H(13N)	0.9900
C(136)-H(13O)	0.9900
C(136)-H(13P)	0.9900
C(136)-H(13Q)	0.9900
C(136)-H(13R)	0.9900
C(137)-C(138)	1.52(2)
C(137)-H(13S)	0.9900
C(137)-H(13T)	0.9900
C(138)-H(13U)	0.9900
C(138)-H(13V)	0.9900
C(139)-C(140)	1.46(3)
C(139)-H(13W)	0.9900
C(139)-H(13X)	0.9900
C(140)-H(14C)	0.9900
C(140)-H(14D)	0.9900
C(141)-C(142)	1.514(14)
C(141)-H(14E)	0.9900
C(141)-H(14F)	0.9900
C(141)-H(14G)	0.9900
C(141)-H(14H)	0.9900
C(142)-H(14I)	0.9900
C(142)-H(14J)	0.9900
C(1S)-C(2S)	1.354(12)
C(1S)-C(6S)	1.380(12)
C(1S)-C(7S)	1.521(14)
C(2S)-C(3S)	1.386(12)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.393(12)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.361(15)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.381(15)
C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500
C(7S)-H(7SA)	0.9800
C(7S)-H(7SB)	0.9800
C(7S)-H(7SC)	0.9800
C(8S)-C(13S)	1.358(13)
C(8S)-C(13')	1.362(11)
C(8S)-C(9')	1.367(11)
C(8S)-C(9S)	1.391(13)
C(8S)-C(14S)	1.439(18)
C(8S)-H(8S)	0.9500
C(9')-C(10')	1.365(11)
C(9')-H(9')	0.9500
C(9S)-C(10S)	1.377(14)
C(9S)-H(9S)	0.9500
C(10')-C(11')	1.368(11)
C(10')-H(10')	0.9500
C(10S)-C(11S)	1.345(14)
C(10S)-H(1)	0.9500
C(11')-C(12')	1.367(12)
C(11')-H(11')	0.9500
C(11S)-C(12S)	1.379(14)
C(11S)-H(6)	0.9500
C(12')-C(13')	1.370(11)
C(12')-H(12')	0.9500
C(12S)-C(13S)	1.378(14)
C(12S)-H(12Z)	0.9500
C(13')-C(14')	1.47(2)
C(13S)-H(13Y)	0.9500
C(14')-H(14K)	0.9800

C(14')-H(14L)	0.9800
C(14')-H(14M)	0.9800
C(14S)-H(14N)	0.9800
C(14S)-H(14O)	0.9800
C(14S)-H(14P)	0.9800
C(15S)-C(16S)	1.388(10)
C(15S)-C(20S)	1.389(11)
C(15S)-C(21S)	1.507(10)
C(16S)-C(17S)	1.378(11)
C(16S)-H(16S)	0.9500
C(17S)-C(18S)	1.343(13)
C(17S)-H(17S)	0.9500
C(18S)-C(19S)	1.414(14)
C(18S)-H(18S)	0.9500
C(19S)-C(20S)	1.375(13)
C(19S)-H(19S)	0.9500
C(20S)-H(20S)	0.9500
C(21S)-H(21F)	0.9800
C(21S)-H(21G)	0.9800
C(21S)-H(21H)	0.9800

O(1)-Tb(1)-O(4)	77.31(13)
O(1)-Tb(1)-O(5)	147.26(12)
O(4)-Tb(1)-O(5)	82.55(14)
O(1)-Tb(1)-O(3)	117.93(14)
O(4)-Tb(1)-O(3)	72.36(14)
O(5)-Tb(1)-O(3)	79.05(14)
O(1)-Tb(1)-O(6)	79.14(12)
O(4)-Tb(1)-O(6)	77.24(13)
O(5)-Tb(1)-O(6)	71.36(13)
O(3)-Tb(1)-O(6)	139.78(12)
O(1)-Tb(1)-O(2)	72.13(12)
O(4)-Tb(1)-O(2)	116.24(14)
O(5)-Tb(1)-O(2)	140.53(12)
O(3)-Tb(1)-O(2)	75.00(12)
O(6)-Tb(1)-O(2)	143.68(12)
O(1)-Tb(1)-N(1)	138.15(12)
O(4)-Tb(1)-N(1)	141.59(13)
O(5)-Tb(1)-N(1)	70.53(13)
O(3)-Tb(1)-N(1)	75.93(15)
O(6)-Tb(1)-N(1)	116.98(14)
O(2)-Tb(1)-N(1)	74.62(13)
O(1)-Tb(1)-N(6)#1	74.53(13)
O(4)-Tb(1)-N(6)#1	143.24(13)
O(5)-Tb(1)-N(6)#1	109.83(14)
O(3)-Tb(1)-N(6)#1	142.73(13)
O(6)-Tb(1)-N(6)#1	74.66(12)
O(2)-Tb(1)-N(6)#1	76.60(13)
N(1)-Tb(1)-N(6)#1	73.63(13)
O(8)-Tb(2)-O(10)	86.40(15)
O(8)-Tb(2)-O(11)	74.62(14)
O(10)-Tb(2)-O(11)	147.07(14)
O(8)-Tb(2)-O(9)	81.37(17)
O(10)-Tb(2)-O(9)	72.16(15)
O(11)-Tb(2)-O(9)	78.46(14)
O(8)-Tb(2)-O(12)	143.15(15)
O(10)-Tb(2)-O(12)	112.57(14)
O(11)-Tb(2)-O(12)	72.91(12)
O(9)-Tb(2)-O(12)	75.52(14)
O(8)-Tb(2)-O(7)	71.37(15)
O(10)-Tb(2)-O(7)	76.37(14)
O(11)-Tb(2)-O(7)	120.46(13)

O(9)-Tb(2)-O(7)	139.26(14)
O(12)-Tb(2)-O(7)	141.93(13)
O(8)-Tb(2)-N(8)#2	144.02(15)
O(10)-Tb(2)-N(8)#2	72.05(14)
O(11)-Tb(2)-N(8)#2	136.70(13)
O(9)-Tb(2)-N(8)#2	116.90(14)
O(12)-Tb(2)-N(8)#2	72.79(14)
O(7)-Tb(2)-N(8)#2	75.66(14)
O(8)-Tb(2)-N(7)	104.32(16)
O(10)-Tb(2)-N(7)	141.13(15)
O(11)-Tb(2)-N(7)	70.86(14)
O(9)-Tb(2)-N(7)	145.67(14)
O(12)-Tb(2)-N(7)	80.97(13)
O(7)-Tb(2)-N(7)	72.24(13)
N(8)#2-Tb(2)-N(7)	78.37(14)
O(13)-Cs(1)-O(17)	113.6(3)
O(13)-Cs(1)-O(18)	142.7(3)
O(17)-Cs(1)-O(18)	54.4(3)
O(18')-Cs(1)-O(13')	146.1(4)
O(13)-Cs(1)-O(14)	56.4(4)
O(17)-Cs(1)-O(14)	135.1(2)
O(18)-Cs(1)-O(14)	104.7(3)
O(18')-Cs(1)-O(14')	109.4(4)
O(13')-Cs(1)-O(14')	53.3(5)
O(18')-Cs(1)-N(5)	92.4(2)
O(13)-Cs(1)-N(5)	118.8(2)
O(17)-Cs(1)-N(5)	100.18(19)
O(18)-Cs(1)-N(5)	98.5(2)
O(13')-Cs(1)-N(5)	121.4(4)
O(14)-Cs(1)-N(5)	123.50(19)
O(14')-Cs(1)-N(5)	126.9(2)
O(18')-Cs(1)-O(17')	52.8(3)
O(13')-Cs(1)-O(17')	107.4(5)
O(14')-Cs(1)-O(17')	121.1(3)
N(5)-Cs(1)-O(17')	110.7(2)
O(18')-Cs(1)-N(10')	54.8(4)
O(13')-Cs(1)-N(10')	103.5(5)
O(14')-Cs(1)-N(10')	54.8(4)
N(5)-Cs(1)-N(10')	120.0(3)
O(17')-Cs(1)-N(10')	88.7(4)
O(18')-Cs(1)-C(40)	116.7(3)
O(13)-Cs(1)-C(40)	95.7(3)
O(17)-Cs(1)-C(40)	105.10(19)
O(18)-Cs(1)-C(40)	121.1(2)
O(13')-Cs(1)-C(40)	97.1(4)
O(14)-Cs(1)-C(40)	118.9(2)
O(14')-Cs(1)-C(40)	115.5(3)
N(5)-Cs(1)-C(40)	24.35(12)
O(17')-Cs(1)-C(40)	122.2(2)
N(10')-Cs(1)-C(40)	135.3(3)
O(13)-Cs(1)-N(9)	56.4(4)
O(17)-Cs(1)-N(9)	57.2(4)
O(18)-Cs(1)-N(9)	102.9(4)
O(14)-Cs(1)-N(9)	99.4(4)
N(5)-Cs(1)-N(9)	124.6(3)
C(40)-Cs(1)-N(9)	106.6(3)
O(23)-Cs(2)-O(21)	111.6(3)
O(23)-Cs(2)-O(24)	55.9(2)
O(21)-Cs(2)-O(24)	134.1(3)
O(23)-Cs(2)-O(22)	145.3(2)
O(21)-Cs(2)-O(22)	53.5(3)
O(24)-Cs(2)-O(22)	108.8(2)

O(23)-Cs(2)-N(11)	58.1(2)
O(21)-Cs(2)-N(11)	54.8(3)
O(24)-Cs(2)-N(11)	104.91(19)
O(22)-Cs(2)-N(11)	105.1(2)
O(23)-Cs(2)-N(12)	107.2(2)
O(21)-Cs(2)-N(12)	103.4(3)
O(24)-Cs(2)-N(12)	53.8(2)
O(22)-Cs(2)-N(12)	56.8(2)
N(11)-Cs(2)-N(12)	128.39(17)
O(23)-Cs(2)-N(3)	88.76(17)
O(21)-Cs(2)-N(3)	98.4(3)
O(24)-Cs(2)-N(3)	122.78(16)
O(22)-Cs(2)-N(3)	122.25(17)
N(11)-Cs(2)-N(3)	86.08(13)
N(12)-Cs(2)-N(3)	145.49(15)
O(23)-Cs(2)-N(4)	116.19(18)
O(21)-Cs(2)-N(4)	122.3(3)
O(24)-Cs(2)-N(4)	99.66(15)
O(22)-Cs(2)-N(4)	96.11(19)
N(11)-Cs(2)-N(4)	139.88(13)
N(12)-Cs(2)-N(4)	91.72(15)
N(3)-Cs(2)-N(4)	53.86(10)
O(23)-Cs(2)-C(53)	134.88(18)
O(21)-Cs(2)-C(53)	99.2(3)
O(24)-Cs(2)-C(53)	120.52(16)
O(22)-Cs(2)-C(53)	79.66(18)
N(11)-Cs(2)-C(53)	130.28(14)
N(12)-Cs(2)-C(53)	96.24(17)
N(3)-Cs(2)-C(53)	53.66(12)
N(4)-Cs(2)-C(53)	23.24(10)
O(23)-Cs(2)-C(142)	98.4(3)
O(21)-Cs(2)-C(142)	126.8(3)
O(24)-Cs(2)-C(142)	42.9(3)
O(22)-Cs(2)-C(142)	76.7(3)
N(11)-Cs(2)-C(142)	141.9(2)
N(12)-Cs(2)-C(142)	23.8(2)
N(3)-Cs(2)-C(142)	125.92(17)
N(4)-Cs(2)-C(142)	75.63(17)
C(53)-Cs(2)-C(142)	87.75(19)
O(23)-Cs(2)-C(131)	78.3(3)
O(21)-Cs(2)-C(131)	42.0(4)
O(24)-Cs(2)-C(131)	128.7(3)
O(22)-Cs(2)-C(131)	95.4(3)
N(11)-Cs(2)-C(131)	23.8(3)
N(12)-Cs(2)-C(131)	139.6(3)
N(3)-Cs(2)-C(131)	72.6(2)
N(4)-Cs(2)-C(131)	122.5(3)
C(53)-Cs(2)-C(131)	107.7(3)
C(142)-Cs(2)-C(131)	161.3(3)
O(23)-Cs(2)-C(136)	131.0(2)
O(21)-Cs(2)-C(136)	91.5(3)
O(24)-Cs(2)-C(136)	76.7(2)
O(22)-Cs(2)-C(136)	38.7(2)
N(11)-Cs(2)-C(136)	135.45(17)
N(12)-Cs(2)-C(136)	23.80(19)
N(3)-Cs(2)-C(136)	131.37(13)
N(4)-Cs(2)-C(136)	80.72(13)
C(53)-Cs(2)-C(136)	77.80(14)
C(142)-Cs(2)-C(136)	38.4(2)
C(131)-Cs(2)-C(136)	133.3(3)
O(23')-Cs(2')-O(24')	55.5(10)
O(23')-Cs(2')-O(22')	133.1(7)

O(24')-Cs(2')-O(22')	108.1(8)
O(23')-Cs(2')-O(21')	105.2(10)
O(24')-Cs(2')-O(21')	139.6(9)
O(22')-Cs(2')-O(21')	56.3(9)
O(23')-Cs(2')-N(3)	99.2(6)
O(24')-Cs(2')-N(3)	127.7(7)
O(22')-Cs(2')-N(3)	119.9(4)
O(21')-Cs(2')-N(3)	87.3(8)
O(23')-Cs(2')-N(11)	49.5(6)
O(24')-Cs(2')-N(11)	100.6(8)
O(22')-Cs(2')-N(11)	104.3(4)
O(21')-Cs(2')-N(11)	56.7(8)
N(3)-Cs(2')-N(11)	87.26(14)
O(23')-Cs(2')-N(12')	103.6(6)
O(24')-Cs(2')-N(12')	55.7(8)
O(22')-Cs(2')-N(12')	54.2(4)
O(21')-Cs(2')-N(12')	106.0(9)
N(3)-Cs(2')-N(12')	149.4(3)
N(11)-Cs(2')-N(12')	123.2(3)
O(23')-Cs(2')-N(4)	141.1(6)
O(24')-Cs(2')-N(4)	114.1(7)
O(22')-Cs(2')-N(4)	85.3(3)
O(21')-Cs(2')-N(4)	102.2(8)
N(3)-Cs(2')-N(4)	55.01(11)
N(11)-Cs(2')-N(4)	139.30(15)
N(12')-Cs(2')-N(4)	94.8(3)
O(23')-Cs(2')-C(23A)	127.6(7)
O(24')-Cs(2')-C(23A)	77.0(9)
O(22')-Cs(2')-C(23A)	40.6(6)
O(21')-Cs(2')-C(23A)	96.9(10)
N(3)-Cs(2')-C(23A)	129.2(4)
N(11)-Cs(2')-C(23A)	136.3(5)
N(12')-Cs(2')-C(23A)	24.0(3)
N(4)-Cs(2')-C(23A)	74.8(4)
O(23')-Cs(2')-C(141)	93.5(6)
O(24')-Cs(2')-C(141)	38.7(8)
O(22')-Cs(2')-C(141)	77.0(4)
O(21')-Cs(2')-C(141)	130.1(8)
N(3)-Cs(2')-C(141)	135.40(18)
N(11)-Cs(2')-C(141)	131.15(17)
N(12')-Cs(2')-C(141)	24.1(3)
N(4)-Cs(2')-C(141)	89.47(14)
C(23A)-Cs(2')-C(141)	39.4(4)
O(23')-Cs(2')-C(24A)	39.5(10)
O(24')-Cs(2')-C(24A)	94.9(12)
O(22')-Cs(2')-C(24A)	123.7(8)
O(21')-Cs(2')-C(24A)	72.7(11)
N(3)-Cs(2')-C(24A)	75.8(9)
N(11)-Cs(2')-C(24A)	19.6(7)
N(12')-Cs(2')-C(24A)	134.2(10)
N(4)-Cs(2')-C(24A)	130.8(10)
C(23A)-Cs(2')-C(24A)	153.3(10)
C(141)-Cs(2')-C(24A)	132.1(10)
O(23')-Cs(2')-C(53)	151.4(6)
O(24')-Cs(2')-C(53)	135.1(7)
O(22')-Cs(2')-C(53)	73.5(3)
O(21')-Cs(2')-C(53)	80.1(8)
N(3)-Cs(2')-C(53)	52.55(12)
N(11)-Cs(2')-C(53)	122.99(17)
N(12')-Cs(2')-C(53)	101.7(3)
N(4)-Cs(2')-C(53)	22.15(10)
C(23A)-Cs(2')-C(53)	78.3(4)

C(141)-Cs(2')-C(53)	104.47(15)
C(24A)-Cs(2')-C(53)	122.2(10)
C(1)-O(1)-Tb(1)	138.3(3)
C(3)-O(2)-Tb(1)	136.7(3)
C(12)-O(3)-Tb(1)	135.7(4)
C(14)-O(4)-Tb(1)	138.7(4)
C(23)-O(5)-Tb(1)	136.0(4)
C(25)-O(6)-Tb(1)	134.0(3)
C(74)-O(7)-Tb(2)	132.6(4)
C(76)-O(8)-Tb(2)	133.6(4)
C(85)-O(9)-Tb(2)	137.5(4)
C(87)-O(10)-Tb(2)	138.8(4)
C(96)-O(11)-Tb(2)	136.3(3)
C(98)-O(12)-Tb(2)	134.9(3)
C(108)-O(13)-C(109)	108.7(15)
C(108)-O(13)-Cs(1)	126.6(12)
C(109)-O(13)-Cs(1)	119.3(10)
C(2A)-O(13')-C(3A)	123(3)
C(2A)-O(13')-Cs(1)	119(2)
C(3A)-O(13')-Cs(1)	117.2(14)
C(110)-O(14)-C(111)	113.7(12)
C(110)-O(14)-Cs(1)	98.5(10)
C(111)-O(14)-Cs(1)	93.5(8)
C(4A)-O(14')-C(5A)	114.0(17)
C(4A)-O(14')-Cs(1)	99.0(15)
C(5A)-O(14')-Cs(1)	89.2(10)
C(114)-O(15)-C(115)	113.4(6)
C(116)-O(16)-C(117)	114.2(5)
C(121)-O(17)-C(120)	110.8(12)
C(121)-O(17)-Cs(1)	120.6(10)
C(120)-O(17)-Cs(1)	119.3(10)
C(11A)-O(17')-C(10A)	112.4(18)
C(11A)-O(17')-Cs(1)	88.6(13)
C(10A)-O(17')-Cs(1)	114.0(11)
C(123)-O(18)-C(122)	116.6(16)
C(123)-O(18)-Cs(1)	117.9(11)
C(122)-O(18)-Cs(1)	111.9(10)
C(13A)-O(18')-C(12A)	113.1(17)
C(13A)-O(18')-Cs(1)	126.5(15)
C(12A)-O(18')-Cs(1)	120.3(9)
C(127)-O(19)-C(126)	102.4(11)
C(16A)-O(19')-C(127)	111.2(10)
C(129)-O(20)-C(128)	113.7(7)
C(129)-O(20')-C(17A)	123(3)
C(133)-O(21)-C(132)	116.5(11)
C(133)-O(21)-Cs(2)	124.7(9)
C(132)-O(21)-Cs(2)	115.6(8)
C(20A)-O(21')-C(21A)	110(3)
C(20A)-O(21')-Cs(2')	126(3)
C(21A)-O(21')-Cs(2')	114(3)
C(135)-O(22)-C(134)	112.0(9)
C(135)-O(22)-Cs(2)	117.5(6)
C(134)-O(22)-Cs(2)	114.6(7)
C(22A)-O(22')-C(136)	121(2)
C(22A)-O(22')-Cs(2')	113(2)
C(136)-O(22')-Cs(2')	116.7(10)
C(138)-O(23)-C(139)	111.8(10)
C(138)-O(23)-Cs(2)	121.8(8)
C(139)-O(23)-Cs(2)	119.5(8)
C(25A)-O(23')-C(26A)	114(3)
C(25A)-O(23')-Cs(2')	120(2)
C(26A)-O(23')-Cs(2')	117.8(19)

C(140)-O(24)-C(141)	115.2(9)
C(140)-O(24)-Cs(2)	111.8(8)
C(141)-O(24)-Cs(2)	113.5(5)
C(28A)-O(24')-C(27A)	113(3)
C(28A)-O(24')-Cs(2')	123(2)
C(27A)-O(24')-Cs(2')	117(2)
C(34)-N(1)-C(38)	117.0(5)
C(34)-N(1)-Tb(1)	120.3(4)
C(38)-N(1)-Tb(1)	122.1(4)
C(70)-N(2)-C(73)	110.5(4)
C(70)-N(2)-Cs(1)	127.6(3)
C(73)-N(2)-Cs(1)	86.1(3)
C(70)-N(2)-H(2)	124.7
C(73)-N(2)-H(2)	124.7
Cs(1)-N(2)-H(2)	61.5
C(60)-N(3)-C(63)	104.5(4)
C(60)-N(3)-Cs(2')	105.9(3)
C(63)-N(3)-Cs(2')	125.8(3)
C(60)-N(3)-Cs(2)	96.3(3)
C(63)-N(3)-Cs(2)	128.5(3)
C(60)-N(3)-H(3)	127.8
C(63)-N(3)-H(3)	127.8
Cs(2)-N(3)-H(3)	53.3
C(50)-N(4)-C(53)	110.5(4)
C(50)-N(4)-Cs(2')	110.9(3)
C(53)-N(4)-Cs(2')	92.9(3)
C(50)-N(4)-Cs(2)	110.5(3)
C(53)-N(4)-Cs(2)	84.1(3)
C(50)-N(4)-H(4)	124.7
C(53)-N(4)-H(4)	124.7
Cs(2)-N(4)-H(4)	77.5
C(40)-N(5)-C(43)	105.6(4)
C(40)-N(5)-Cs(1)	81.1(3)
C(43)-N(5)-Cs(1)	93.1(3)
C(40)-N(5)-Cs(2')	124.0(3)
C(43)-N(5)-Cs(2')	115.6(3)
Cs(1)-N(5)-Cs(2')	129.78(13)
C(40)-N(5)-H(5)	127.2
C(43)-N(5)-H(5)	127.2
Cs(1)-N(5)-H(5)	94.8
Cs(2')-N(5)-H(5)	35.0
C(49)-N(6)-C(47)	115.6(4)
C(49)-N(6)-Tb(1)#1	121.3(3)
C(47)-N(6)-Tb(1)#1	122.0(3)
C(57)-N(7)-C(59)	116.4(4)
C(57)-N(7)-Tb(2)	118.7(3)
C(59)-N(7)-Tb(2)	122.4(3)
C(67)-N(8)-C(69)	117.4(5)
C(67)-N(8)-Tb(2)#2	124.3(3)
C(69)-N(8)-Tb(2)#2	117.8(4)
C(113)-N(9)-C(119)	111.4(14)
C(113)-N(9)-C(107)	109.5(16)
C(119)-N(9)-C(107)	105.8(16)
C(113)-N(9)-Cs(1)	140.2(11)
C(119)-N(9)-Cs(1)	91.8(10)
C(107)-N(9)-Cs(1)	93.5(11)
C(9A)-N(9')-C(1A)	115(3)
C(9A)-N(9')-C(7A)	116.9(19)
C(1A)-N(9')-C(7A)	109(2)
C(9A)-N(9')-Cs(1)	87.4(17)
C(1A)-N(9')-Cs(1)	87.2(12)
C(7A)-N(9')-Cs(1)	138.7(14)

C(112)-N(10)-C(118)	113.4(14)
C(112)-N(10)-C(124)	112.0(14)
C(118)-N(10)-C(124)	115.3(15)
C(112)-N(10)-Cs(1)	105.2(10)
C(118)-N(10)-Cs(1)	117.4(10)
C(124)-N(10)-Cs(1)	91.3(12)
C(6A)-N(10')-C(8A)	110(2)
C(6A)-N(10')-C(14A)	111.9(18)
C(8A)-N(10')-C(14A)	108.6(16)
C(6A)-N(10')-Cs(1)	109.0(15)
C(8A)-N(10')-Cs(1)	121.7(13)
C(14A)-N(10')-Cs(1)	95.2(11)
C(125)-N(11)-C(131)	118.7(12)
C(24A)-N(11)-C(19A)	110(4)
C(24A)-N(11)-C(15A)	104(3)
C(19A)-N(11)-C(15A)	102(4)
C(125)-N(11)-C(137)	113.9(13)
C(131)-N(11)-C(137)	108.4(10)
C(125)-N(11)-Cs(2)	123.7(6)
C(131)-N(11)-Cs(2)	92.9(11)
C(137)-N(11)-Cs(2)	95.4(7)
C(24A)-N(11)-Cs(2')	100(2)
C(19A)-N(11)-Cs(2')	98(3)
C(15A)-N(11)-Cs(2')	141.7(11)
C(142)-N(12)-C(130)	114.7(8)
C(142)-N(12)-C(136)	109.0(8)
C(130)-N(12)-C(136)	113.3(8)
C(142)-N(12)-Cs(2)	89.8(6)
C(130)-N(12)-Cs(2)	132.3(6)
C(136)-N(12)-Cs(2)	93.9(5)
C(18A)-N(12')-C(23A)	110(2)
C(18A)-N(12')-C(141)	115.3(19)
C(23A)-N(12')-C(141)	111.6(17)
C(18A)-N(12')-Cs(2')	136.2(16)
C(23A)-N(12')-Cs(2')	90.0(12)
C(141)-N(12')-Cs(2')	90.2(8)
O(1)-C(1)-C(2)	124.2(5)
O(1)-C(1)-C(4)	114.6(5)
C(2)-C(1)-C(4)	121.2(4)
C(2A)-C(1A)-N(9')	117(2)
C(2A)-C(1A)-Cs(1)	87.8(17)
N(9')-C(1A)-Cs(1)	68.8(11)
C(2A)-C(1A)-H(1AA)	108.0
N(9')-C(1A)-H(1AA)	108.0
Cs(1)-C(1A)-H(1AA)	162.8
C(2A)-C(1A)-H(1AB)	108.0
N(9')-C(1A)-H(1AB)	108.0
Cs(1)-C(1A)-H(1AB)	60.0
H(1AA)-C(1A)-H(1AB)	107.3
C(3)-C(2)-C(1)	124.3(5)
C(3)-C(2)-H(2A)	117.9
C(1)-C(2)-H(2A)	117.9
O(13')-C(2A)-C(1A)	114(3)
O(13')-C(2A)-Cs(1)	43.8(18)
C(1A)-C(2A)-Cs(1)	70.1(16)
O(13')-C(2A)-H(2AA)	108.8
C(1A)-C(2A)-H(2AA)	108.8
Cs(1)-C(2A)-H(2AA)	122.7
O(13')-C(2A)-H(2AB)	108.8
C(1A)-C(2A)-H(2AB)	108.8
Cs(1)-C(2A)-H(2AB)	127.4
H(2AA)-C(2A)-H(2AB)	107.7

O(2)-C(3)-C(2)	124.3(5)
O(2)-C(3)-C(8)	113.8(5)
C(2)-C(3)-C(8)	121.9(5)
O(13')-C(3A)-C(4A)	108(2)
O(13')-C(3A)-H(3AA)	110.1
C(4A)-C(3A)-H(3AA)	110.1
O(13')-C(3A)-H(3AB)	110.1
C(4A)-C(3A)-H(3AB)	110.1
H(3AA)-C(3A)-H(3AB)	108.4
C(7)-C(4)-C(5)	109.5(5)
C(7)-C(4)-C(1)	115.0(5)
C(5)-C(4)-C(1)	107.7(5)
C(7)-C(4)-C(6)	109.0(5)
C(5)-C(4)-C(6)	108.4(6)
C(1)-C(4)-C(6)	107.0(5)
O(14')-C(4A)-C(3A)	103(2)
O(14')-C(4A)-Cs(1)	60.1(12)
C(3A)-C(4A)-Cs(1)	90.5(14)
O(14')-C(4A)-H(4AA)	111.1
C(3A)-C(4A)-H(4AA)	111.1
Cs(1)-C(4A)-H(4AA)	158.3
O(14')-C(4A)-H(4AB)	111.1
C(3A)-C(4A)-H(4AB)	111.1
Cs(1)-C(4A)-H(4AB)	61.8
H(4AA)-C(4A)-H(4AB)	109.1
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(6A)-C(5A)-O(14')	112(2)
C(6A)-C(5A)-Cs(1)	96.8(15)
O(14')-C(5A)-Cs(1)	63.6(9)
C(6A)-C(5A)-H(5AA)	109.3
O(14')-C(5A)-H(5AA)	109.3
Cs(1)-C(5A)-H(5AA)	153.4
C(6A)-C(5A)-H(5AB)	109.3
O(14')-C(5A)-H(5AB)	109.3
Cs(1)-C(5A)-H(5AB)	56.4
H(5AA)-C(5A)-H(5AB)	108.0
C(4)-C(6)-H(6A)	109.5
C(4)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(4)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5A)-C(6A)-N(10')	115(2)
C(5A)-C(6A)-H(6AA)	108.5
N(10')-C(6A)-H(6AA)	108.5
C(5A)-C(6A)-H(6AB)	108.5
N(10')-C(6A)-H(6AB)	108.5
H(6AA)-C(6A)-H(6AB)	107.5
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(9')-C(7A)-C(114)	111.1(18)
N(9')-C(7A)-H(7AA)	109.4
C(114)-C(7A)-H(7AA)	109.4

N(9')-C(7A)-H(7AB)	109.4
C(114)-C(7A)-H(7AB)	109.4
H(7AA)-C(7A)-H(7AB)	108.0
C(11)-C(8)-C(10)	110.4(5)
C(11)-C(8)-C(9)	109.4(5)
C(10)-C(8)-C(9)	109.6(5)
C(11)-C(8)-C(3)	107.4(5)
C(10)-C(8)-C(3)	107.3(5)
C(9)-C(8)-C(3)	112.8(5)
N(10')-C(8A)-C(117)	110.3(19)
N(10')-C(8A)-H(8AA)	109.6
C(117)-C(8A)-H(8AA)	109.6
N(10')-C(8A)-H(8AB)	109.6
C(117)-C(8A)-H(8AB)	109.6
H(8AA)-C(8A)-H(8AB)	108.1
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(9')-C(9A)-C(10A)	116(3)
N(9')-C(9A)-Cs(1)	69.8(14)
C(10A)-C(9A)-Cs(1)	94.8(16)
N(9')-C(9A)-H(9AA)	108.4
C(10A)-C(9A)-H(9AA)	108.4
Cs(1)-C(9A)-H(9AA)	154.1
N(9')-C(9A)-H(9AB)	108.4
C(10A)-C(9A)-H(9AB)	108.4
Cs(1)-C(9A)-H(9AB)	52.5
H(9AA)-C(9A)-H(9AB)	107.4
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
O(17')-C(10A)-C(9A)	109.4(17)
O(17')-C(10A)-H(10D)	109.8
C(9A)-C(10A)-H(10D)	109.8
O(17')-C(10A)-H(10E)	109.8
C(9A)-C(10A)-H(10E)	109.8
H(10D)-C(10A)-H(10E)	108.2
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(17')-C(11A)-C(12A)	110(2)
O(17')-C(11A)-Cs(1)	68.2(11)
C(12A)-C(11A)-Cs(1)	90.4(13)
O(17')-C(11A)-H(11D)	109.8
C(12A)-C(11A)-H(11D)	109.8
Cs(1)-C(11A)-H(11D)	158.5
O(17')-C(11A)-H(11E)	109.8
C(12A)-C(11A)-H(11E)	109.8
Cs(1)-C(11A)-H(11E)	55.9
H(11D)-C(11A)-H(11E)	108.2
O(3)-C(12)-C(13)	124.8(6)
O(3)-C(12)-C(15')	121.4(8)
C(13)-C(12)-C(15')	113.1(8)

O(3)-C(12)-C(15)	110.4(8)
C(13)-C(12)-C(15)	123.7(8)
O(18')-C(12A)-C(11A)	105.2(14)
O(18')-C(12A)-Cs(1)	40.0(6)
C(11A)-C(12A)-Cs(1)	66.0(11)
O(18')-C(12A)-H(12A)	110.7
C(11A)-C(12A)-H(12A)	110.7
Cs(1)-C(12A)-H(12A)	117.1
O(18')-C(12A)-H(12B)	110.7
C(11A)-C(12A)-H(12B)	110.7
Cs(1)-C(12A)-H(12B)	131.9
H(12A)-C(12A)-H(12B)	108.8
C(12)-C(13)-C(14)	124.9(6)
C(12)-C(13)-H(13)	117.5
C(14)-C(13)-H(13)	117.5
O(18')-C(13A)-C(14A)	111(3)
O(18')-C(13A)-Cs(1)	36.8(12)
C(14A)-C(13A)-Cs(1)	73.8(17)
O(18')-C(13A)-H(13A)	109.5
C(14A)-C(13A)-H(13A)	109.5
Cs(1)-C(13A)-H(13A)	124.2
O(18')-C(13A)-H(13B)	109.5
C(14A)-C(13A)-H(13B)	109.5
Cs(1)-C(13A)-H(13B)	123.5
H(13A)-C(13A)-H(13B)	108.1
O(4)-C(14)-C(13)	122.6(6)
O(4)-C(14)-C(19)	115.8(5)
C(13)-C(14)-C(19)	121.6(5)
N(10')-C(14A)-C(13A)	111(2)
N(10')-C(14A)-Cs(1)	61.0(9)
C(13A)-C(14A)-Cs(1)	82.8(17)
N(10')-C(14A)-H(14A)	109.5
C(13A)-C(14A)-H(14A)	109.5
Cs(1)-C(14A)-H(14A)	69.9
N(10')-C(14A)-H(14B)	109.5
C(13A)-C(14A)-H(14B)	109.5
Cs(1)-C(14A)-H(14B)	167.1
H(14A)-C(14A)-H(14B)	108.0
C(18)-C(15)-C(16)	106.5(15)
C(18)-C(15)-C(17)	111.8(17)
C(16)-C(15)-C(17)	106.7(13)
C(18)-C(15)-C(12)	113.0(13)
C(16)-C(15)-C(12)	108.0(12)
C(17)-C(15)-C(12)	110.4(13)
C(18')-C(15')-C(16')	109.7(13)
C(18')-C(15')-C(17')	110.6(14)
C(16')-C(15')-C(17')	110.3(12)
C(18')-C(15')-C(12)	100.1(12)
C(16')-C(15')-C(12)	118.1(12)
C(17')-C(15')-C(12)	107.6(11)
N(11)-C(15A)-C(16A)	108(3)
N(11)-C(15A)-H(15A)	110.1
C(16A)-C(15A)-H(15A)	110.1
N(11)-C(15A)-H(15B)	110.1
C(16A)-C(15A)-H(15B)	110.1
H(15A)-C(15A)-H(15B)	108.4
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

C(15')-C(16')-H(16D)	109.5
C(15')-C(16')-H(16E)	109.5
H(16D)-C(16')-H(16E)	109.5
C(15')-C(16')-H(16F)	109.5
H(16D)-C(16')-H(16F)	109.5
H(16E)-C(16')-H(16F)	109.5
O(19')-C(16A)-C(15A)	123(3)
O(19')-C(16A)-H(16G)	106.7
C(15A)-C(16A)-H(16G)	106.7
O(19')-C(16A)-H(16H)	106.7
C(15A)-C(16A)-H(16H)	106.7
H(16G)-C(16A)-H(16H)	106.6
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15')-C(17')-H(17D)	109.5
C(15')-C(17')-H(17E)	109.5
H(17D)-C(17')-H(17E)	109.5
C(15')-C(17')-H(17F)	109.5
H(17D)-C(17')-H(17F)	109.5
H(17E)-C(17')-H(17F)	109.5
C(127)-C(17A)-O(20')	99(2)
C(127)-C(17A)-H(17G)	111.9
O(20')-C(17A)-H(17G)	111.9
C(127)-C(17A)-H(17H)	111.9
O(20')-C(17A)-H(17H)	111.9
H(17G)-C(17A)-H(17H)	109.6
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(15')-C(18')-H(18D)	109.5
C(15')-C(18')-H(18E)	109.5
H(18D)-C(18')-H(18E)	109.5
C(15')-C(18')-H(18F)	109.5
H(18D)-C(18')-H(18F)	109.5
H(18E)-C(18')-H(18F)	109.5
C(129)-C(18A)-N(12')	114(2)
C(129)-C(18A)-H(18G)	108.7
N(12')-C(18A)-H(18G)	108.7
C(129)-C(18A)-H(18H)	108.7
N(12')-C(18A)-H(18H)	108.7
H(18G)-C(18A)-H(18H)	107.6
C(21)-C(19)-C(14)	109.9(5)
C(21)-C(19)-C(22)	110.1(6)
C(14)-C(19)-C(22)	113.2(6)
C(21)-C(19)-C(20)	109.0(6)
C(14)-C(19)-C(20)	106.1(5)
C(22)-C(19)-C(20)	108.2(6)
N(11)-C(19A)-C(20A)	123(4)
N(11)-C(19A)-Cs(2')	60(3)
C(20A)-C(19A)-Cs(2')	92(3)
N(11)-C(19A)-H(19A)	106.6
C(20A)-C(19A)-H(19A)	106.6
Cs(2')-C(19A)-H(19A)	161.3
N(11)-C(19A)-H(19B)	106.6
C(20A)-C(19A)-H(19B)	106.6

Cs(2')-C(19A)-H(19B)	68.9
H(19A)-C(19A)-H(19B)	106.6
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(21')-C(20A)-C(19A)	100(4)
O(21')-C(20A)-H(20D)	111.7
C(19A)-C(20A)-H(20D)	111.7
O(21')-C(20A)-H(20E)	111.7
C(19A)-C(20A)-H(20E)	111.7
H(20D)-C(20A)-H(20E)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(22A)-C(21A)-O(21')	117(3)
C(22A)-C(21A)-H(21D)	108.2
O(21')-C(21A)-H(21D)	108.2
C(22A)-C(21A)-H(21E)	108.2
O(21')-C(21A)-H(21E)	108.2
H(21D)-C(21A)-H(21E)	107.3
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21A)-C(22A)-O(22')	109(3)
C(21A)-C(22A)-Cs(2')	81(2)
O(22')-C(22A)-Cs(2')	45.4(16)
C(21A)-C(22A)-H(22D)	109.9
O(22')-C(22A)-H(22D)	109.9
Cs(2')-C(22A)-H(22D)	155.2
C(21A)-C(22A)-H(22E)	109.9
O(22')-C(22A)-H(22E)	109.9
Cs(2')-C(22A)-H(22E)	87.1
H(22D)-C(22A)-H(22E)	108.3
O(5)-C(23)-C(24)	123.9(5)
O(5)-C(23)-C(26)	114.7(5)
C(24)-C(23)-C(26)	121.4(5)
C(136)-C(23A)-N(12')	122(2)
C(136)-C(23A)-Cs(2')	95.6(11)
N(12')-C(23A)-Cs(2')	66.0(11)
C(136)-C(23A)-H(23A)	106.7
N(12')-C(23A)-H(23A)	106.7
Cs(2')-C(23A)-H(23A)	156.3
C(136)-C(23A)-H(23B)	106.7
N(12')-C(23A)-H(23B)	106.7
Cs(2')-C(23A)-H(23B)	57.9
H(23A)-C(23A)-H(23B)	106.6
C(23)-C(24)-C(25)	124.7(5)
C(23)-C(24)-H(24)	117.7
C(25)-C(24)-H(24)	117.7
N(11)-C(24A)-C(25A)	114(5)
N(11)-C(24A)-Cs(2')	61(2)
C(25A)-C(24A)-Cs(2')	87(3)
N(11)-C(24A)-H(24A)	108.7

C(25A)-C(24A)-H(24A)	108.7
Cs(2')-C(24A)-H(24A)	67.9
N(11)-C(24A)-H(24B)	108.7
C(25A)-C(24A)-H(24B)	108.7
Cs(2')-C(24A)-H(24B)	163.8
H(24A)-C(24A)-H(24B)	107.6
O(6)-C(25)-C(24)	122.9(5)
O(6)-C(25)-C(30)	117.6(5)
C(24)-C(25)-C(30)	119.5(5)
O(23')-C(25A)-C(24A)	111(3)
O(23')-C(25A)-Cs(2')	42.1(17)
C(24A)-C(25A)-Cs(2')	71(3)
O(23')-C(25A)-H(25A)	109.4
C(24A)-C(25A)-H(25A)	109.4
Cs(2')-C(25A)-H(25A)	136.1
O(23')-C(25A)-H(25B)	109.4
C(24A)-C(25A)-H(25B)	109.4
Cs(2')-C(25A)-H(25B)	113.0
H(25A)-C(25A)-H(25B)	108.0
C(27)-C(26)-C(29)	109.1(8)
C(27)-C(26)-C(28)	109.7(9)
C(29)-C(26)-C(28)	109.4(7)
C(27)-C(26)-C(23)	106.8(6)
C(29)-C(26)-C(23)	112.4(6)
C(28)-C(26)-C(23)	109.4(6)
O(23')-C(26A)-C(27A)	106(3)
O(23')-C(26A)-Cs(2')	43.0(14)
C(27A)-C(26A)-Cs(2')	82.3(18)
O(23')-C(26A)-H(26A)	110.5
C(27A)-C(26A)-H(26A)	110.5
Cs(2')-C(26A)-H(26A)	86.8
O(23')-C(26A)-H(26B)	110.5
C(27A)-C(26A)-H(26B)	110.5
Cs(2')-C(26A)-H(26B)	153.5
H(26A)-C(26A)-H(26B)	108.7
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26A)-C(27A)-O(24')	112(3)
C(26A)-C(27A)-H(27D)	109.3
O(24')-C(27A)-H(27D)	109.3
C(26A)-C(27A)-H(27E)	109.3
O(24')-C(27A)-H(27E)	109.3
H(27D)-C(27A)-H(27E)	107.9
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(24')-C(28A)-C(141)	103(2)
O(24')-C(28A)-H(28D)	111.1
C(141)-C(28A)-H(28D)	111.1
O(24')-C(28A)-H(28E)	111.1
C(141)-C(28A)-H(28E)	111.1
H(28D)-C(28A)-H(28E)	109.1
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5

C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(33)-C(30)-C(31)	109.4(5)
C(33)-C(30)-C(25)	110.7(4)
C(31)-C(30)-C(25)	109.3(5)
C(33)-C(30)-C(32)	109.7(6)
C(31)-C(30)-C(32)	108.9(5)
C(25)-C(30)-C(32)	108.9(5)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
N(1)-C(34)-C(35)	123.6(5)
N(1)-C(34)-H(34)	118.2
C(35)-C(34)-H(34)	118.2
C(36)-C(35)-C(34)	120.4(5)
C(36)-C(35)-H(35)	119.8
C(34)-C(35)-H(35)	119.8
C(35)-C(36)-C(37)	116.5(5)
C(35)-C(36)-C(39)	121.9(5)
C(37)-C(36)-C(39)	121.6(5)
C(36)-C(37)-C(38)	120.5(5)
C(36)-C(37)-H(37)	119.8
C(38)-C(37)-H(37)	119.8
N(1)-C(38)-C(37)	122.0(5)
N(1)-C(38)-H(38)	119.0
C(37)-C(38)-H(38)	119.0
C(73)-C(39)-C(40)	127.9(5)
C(73)-C(39)-C(36)	116.6(4)
C(40)-C(39)-C(36)	115.5(4)
C(73)-C(39)-Cs(1)	89.9(3)
C(40)-C(39)-Cs(1)	60.4(3)
C(36)-C(39)-Cs(1)	121.5(3)
N(5)-C(40)-C(41)	111.0(4)
N(5)-C(40)-C(39)	125.2(4)
C(41)-C(40)-C(39)	123.8(5)
N(5)-C(40)-Cs(1)	74.5(3)
C(41)-C(40)-Cs(1)	95.2(3)
C(39)-C(40)-Cs(1)	96.9(3)
C(42)-C(41)-C(40)	106.2(5)
C(42)-C(41)-Cs(1)	85.0(4)
C(40)-C(41)-Cs(1)	62.4(3)
C(42)-C(41)-H(41)	126.9
C(40)-C(41)-H(41)	126.9
Cs(1)-C(41)-H(41)	117.3
C(41)-C(42)-C(43)	107.0(5)
C(41)-C(42)-Cs(1)	73.8(4)

C(43)-C(42)-Cs(1)	68.4(3)
C(41)-C(42)-H(42)	126.5
C(43)-C(42)-H(42)	126.5
Cs(1)-C(42)-H(42)	122.9
N(5)-C(43)-C(42)	110.2(4)
N(5)-C(43)-C(44)	125.1(4)
C(42)-C(43)-C(44)	124.7(5)
N(5)-C(43)-Cs(1)	64.0(3)
C(42)-C(43)-Cs(1)	90.0(4)
C(44)-C(43)-Cs(1)	113.2(3)
C(50)-C(44)-C(43)	124.6(5)
C(50)-C(44)-C(45)	117.0(5)
C(43)-C(44)-C(45)	118.3(4)
C(48)-C(45)-C(46)	115.4(5)
C(48)-C(45)-C(44)	122.8(4)
C(46)-C(45)-C(44)	121.8(4)
C(47)-C(46)-C(45)	120.7(5)
C(47)-C(46)-H(46)	119.7
C(45)-C(46)-H(46)	119.7
N(6)-C(47)-C(46)	123.8(5)
N(6)-C(47)-H(47)	118.1
C(46)-C(47)-H(47)	118.1
C(49)-C(48)-C(45)	120.2(5)
C(49)-C(48)-H(48)	119.9
C(45)-C(48)-H(48)	119.9
N(6)-C(49)-C(48)	124.2(5)
N(6)-C(49)-H(49)	117.9
C(48)-C(49)-H(49)	117.9
C(44)-C(50)-N(4)	125.3(5)
C(44)-C(50)-C(51)	129.1(5)
N(4)-C(50)-C(51)	105.5(4)
C(52)-C(51)-C(50)	108.9(5)
C(52)-C(51)-H(51)	125.5
C(50)-C(51)-H(51)	125.5
C(51)-C(52)-C(53)	109.4(5)
C(51)-C(52)-H(52)	125.3
C(53)-C(52)-H(52)	125.3
C(54)-C(53)-N(4)	126.8(5)
C(54)-C(53)-C(52)	127.7(5)
N(4)-C(53)-C(52)	105.5(4)
C(54)-C(53)-Cs(2)	85.5(3)
N(4)-C(53)-Cs(2)	72.7(3)
C(52)-C(53)-Cs(2)	111.1(3)
C(54)-C(53)-Cs(2')	88.0(3)
N(4)-C(53)-Cs(2')	64.9(3)
C(52)-C(53)-Cs(2')	115.8(3)
C(53)-C(54)-C(60)	126.9(5)
C(53)-C(54)-C(55)	117.4(5)
C(60)-C(54)-C(55)	115.6(4)
C(53)-C(54)-Cs(2)	72.7(3)
C(60)-C(54)-Cs(2)	79.6(3)
C(55)-C(54)-Cs(2)	126.3(3)
C(53)-C(54)-Cs(2')	71.4(3)
C(60)-C(54)-Cs(2')	75.1(3)
C(55)-C(54)-Cs(2')	134.0(3)
C(56)-C(55)-C(58)	116.0(5)
C(56)-C(55)-C(54)	123.8(5)
C(58)-C(55)-C(54)	120.2(5)
C(57)-C(56)-C(55)	120.8(5)
C(57)-C(56)-H(56)	119.6
C(55)-C(56)-H(56)	119.6
N(7)-C(57)-C(56)	123.4(5)

N(7)-C(57)-H(57)	118.3
C(56)-C(57)-H(57)	118.3
C(59)-C(58)-C(55)	119.8(5)
C(59)-C(58)-H(58)	120.1
C(55)-C(58)-H(58)	120.1
N(7)-C(59)-C(58)	123.5(5)
N(7)-C(59)-H(59)	118.3
C(58)-C(59)-H(59)	118.3
N(3)-C(60)-C(61)	111.3(5)
N(3)-C(60)-C(54)	125.1(4)
C(61)-C(60)-C(54)	123.6(5)
N(3)-C(60)-Cs(2)	62.0(3)
C(61)-C(60)-Cs(2)	137.4(3)
C(54)-C(60)-Cs(2)	77.8(3)
N(3)-C(60)-Cs(2')	53.7(3)
C(61)-C(60)-Cs(2')	138.7(3)
C(54)-C(60)-Cs(2')	83.3(3)
C(62)-C(61)-C(60)	106.7(5)
C(62)-C(61)-H(61)	126.6
C(60)-C(61)-H(61)	126.6
C(61)-C(62)-C(63)	106.4(5)
C(61)-C(62)-H(62)	126.8
C(63)-C(62)-H(62)	126.8
N(3)-C(63)-C(62)	111.1(5)
N(3)-C(63)-C(64)	125.3(4)
C(62)-C(63)-C(64)	123.6(5)
C(70)-C(64)-C(63)	124.7(5)
C(70)-C(64)-C(65)	119.3(5)
C(63)-C(64)-C(65)	116.0(4)
C(68)-C(65)-C(66)	116.6(5)
C(68)-C(65)-C(64)	122.9(5)
C(66)-C(65)-C(64)	120.3(5)
C(67)-C(66)-C(65)	119.4(5)
C(67)-C(66)-H(66)	120.3
C(65)-C(66)-H(66)	120.3
N(8)-C(67)-C(66)	124.1(5)
N(8)-C(67)-H(67)	118.0
C(66)-C(67)-H(67)	118.0
C(65)-C(68)-C(69)	120.1(5)
C(65)-C(68)-H(68)	120.0
C(69)-C(68)-H(68)	120.0
N(8)-C(69)-C(68)	122.4(5)
N(8)-C(69)-H(69)	118.8
C(68)-C(69)-H(69)	118.8
N(2)-C(70)-C(64)	124.6(5)
N(2)-C(70)-C(71)	106.9(4)
C(64)-C(70)-C(71)	128.5(5)
C(72)-C(71)-C(70)	107.8(5)
C(72)-C(71)-H(71)	126.1
C(70)-C(71)-H(71)	126.1
C(71)-C(72)-C(73)	109.5(5)
C(71)-C(72)-H(72)	125.3
C(73)-C(72)-H(72)	125.3
C(39)-C(73)-N(2)	127.0(5)
C(39)-C(73)-C(72)	127.6(5)
N(2)-C(73)-C(72)	105.3(4)
O(7)-C(74)-C(75)	123.2(6)
O(7)-C(74)-C(77)	116.3(6)
C(75)-C(74)-C(77)	120.5(6)
C(76)-C(75)-C(74)	124.1(5)
C(76)-C(75)-H(75)	118.0
C(74)-C(75)-H(75)	118.0

O(8)-C(76)-C(75)	123.5(6)
O(8)-C(76)-C(81)	113.7(6)
C(75)-C(76)-C(81)	122.8(5)
C(78)-C(77)-C(80)	110.4(6)
C(78)-C(77)-C(74)	114.2(7)
C(80)-C(77)-C(74)	107.3(6)
C(78)-C(77)-C(79)	108.6(7)
C(80)-C(77)-C(79)	108.7(7)
C(74)-C(77)-C(79)	107.5(6)
C(77)-C(78)-H(78A)	109.5
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(77)-C(79)-H(79A)	109.5
C(77)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(77)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(77)-C(80)-H(80A)	109.5
C(77)-C(80)-H(80B)	109.5
H(80A)-C(80)-H(80B)	109.5
C(77)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5
H(80B)-C(80)-H(80C)	109.5
C(82)-C(81)-C(83)	110.7(6)
C(82)-C(81)-C(84)	110.2(7)
C(83)-C(81)-C(84)	108.4(7)
C(82)-C(81)-C(76)	112.6(7)
C(83)-C(81)-C(76)	107.4(5)
C(84)-C(81)-C(76)	107.4(5)
C(81)-C(82)-H(82A)	109.5
C(81)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(81)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(81)-C(83)-H(83A)	109.5
C(81)-C(83)-H(83B)	109.5
H(83A)-C(83)-H(83B)	109.5
C(81)-C(83)-H(83C)	109.5
H(83A)-C(83)-H(83C)	109.5
H(83B)-C(83)-H(83C)	109.5
C(81)-C(84)-H(84A)	109.5
C(81)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
C(81)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
O(9)-C(85)-C(86)	123.3(6)
O(9)-C(85)-C(88)	115.5(6)
C(86)-C(85)-C(88)	121.2(5)
C(87)-C(86)-C(85)	124.8(6)
C(87)-C(86)-H(86)	117.6
C(85)-C(86)-H(86)	117.6
O(10)-C(87)-C(86)	123.3(6)
O(10)-C(87)-C(92)	113.4(6)
C(86)-C(87)-C(92)	123.3(6)
C(90)-C(88)-C(91)	112.6(8)
C(90)-C(88)-C(89)	108.8(8)

C(91)-C(88)-C(89)	106.6(8)
C(90)-C(88)-C(85)	108.0(6)
C(91)-C(88)-C(85)	110.6(6)
C(89)-C(88)-C(85)	110.2(6)
C(88)-C(89)-H(89A)	109.5
C(88)-C(89)-H(89B)	109.5
H(89A)-C(89)-H(89B)	109.5
C(88)-C(89)-H(89C)	109.5
H(89A)-C(89)-H(89C)	109.5
H(89B)-C(89)-H(89C)	109.5
C(88)-C(90)-H(90A)	109.5
C(88)-C(90)-H(90B)	109.5
H(90A)-C(90)-H(90B)	109.5
C(88)-C(90)-H(90C)	109.5
H(90A)-C(90)-H(90C)	109.5
H(90B)-C(90)-H(90C)	109.5
C(88)-C(91)-H(91A)	109.5
C(88)-C(91)-H(91B)	109.5
H(91A)-C(91)-H(91B)	109.5
C(88)-C(91)-H(91C)	109.5
H(91A)-C(91)-H(91C)	109.5
H(91B)-C(91)-H(91C)	109.5
C(93)-C(92)-C(95)	109.0(6)
C(93)-C(92)-C(94)	110.0(6)
C(95)-C(92)-C(94)	109.5(6)
C(93)-C(92)-C(87)	112.9(6)
C(95)-C(92)-C(87)	106.5(5)
C(94)-C(92)-C(87)	108.8(5)
C(92)-C(93)-H(93A)	109.5
C(92)-C(93)-H(93B)	109.5
H(93A)-C(93)-H(93B)	109.5
C(92)-C(93)-H(93C)	109.5
H(93A)-C(93)-H(93C)	109.5
H(93B)-C(93)-H(93C)	109.5
C(92)-C(94)-H(94A)	109.5
C(92)-C(94)-H(94B)	109.5
H(94A)-C(94)-H(94B)	109.5
C(92)-C(94)-H(94C)	109.5
H(94A)-C(94)-H(94C)	109.5
H(94B)-C(94)-H(94C)	109.5
C(92)-C(95)-H(95A)	109.5
C(92)-C(95)-H(95B)	109.5
H(95A)-C(95)-H(95B)	109.5
C(92)-C(95)-H(95C)	109.5
H(95A)-C(95)-H(95C)	109.5
H(95B)-C(95)-H(95C)	109.5
O(11)-C(96)-C(97)	124.2(5)
O(11)-C(96)-C(99)	114.6(5)
C(97)-C(96)-C(99)	121.1(5)
C(98)-C(97)-C(96)	124.0(5)
C(98)-C(97)-H(97)	118.0
C(96)-C(97)-H(97)	118.0
O(12)-C(98)-C(97)	125.4(5)
O(12)-C(98)-C(103)	113.3(5)
C(97)-C(98)-C(103)	121.4(5)
C(100)-C(99)-C(102)	109.3(6)
C(100)-C(99)-C(101)	111.3(7)
C(102)-C(99)-C(101)	108.8(6)
C(100)-C(99)-C(96)	108.0(5)
C(102)-C(99)-C(96)	114.0(5)
C(101)-C(99)-C(96)	105.4(5)
C(99)-C(100)-H(10F)	109.5

C(99)-C(100)-H(10G)	109.5
H(10F)-C(100)-H(10G)	109.5
C(99)-C(100)-H(10H)	109.5
H(10F)-C(100)-H(10H)	109.5
H(10G)-C(100)-H(10H)	109.5
C(99)-C(101)-H(10I)	109.5
C(99)-C(101)-H(10J)	109.5
H(10I)-C(101)-H(10J)	109.5
C(99)-C(101)-H(10K)	109.5
H(10I)-C(101)-H(10K)	109.5
H(10J)-C(101)-H(10K)	109.5
C(99)-C(102)-H(10L)	109.5
C(99)-C(102)-H(10M)	109.5
H(10L)-C(102)-H(10M)	109.5
C(99)-C(102)-H(10N)	109.5
H(10L)-C(102)-H(10N)	109.5
H(10M)-C(102)-H(10N)	109.5
C(106)-C(103)-C(98)	108.3(5)
C(106)-C(103)-C(104)	107.5(6)
C(98)-C(103)-C(104)	114.0(5)
C(106)-C(103)-C(105)	110.3(7)
C(98)-C(103)-C(105)	107.8(5)
C(104)-C(103)-C(105)	108.9(6)
C(103)-C(104)-H(10O)	109.5
C(103)-C(104)-H(10P)	109.5
H(10O)-C(104)-H(10P)	109.5
C(103)-C(104)-H(10Q)	109.5
H(10O)-C(104)-H(10Q)	109.5
H(10P)-C(104)-H(10Q)	109.5
C(103)-C(105)-H(10R)	109.5
C(103)-C(105)-H(10S)	109.5
H(10R)-C(105)-H(10S)	109.5
C(103)-C(105)-H(10T)	109.5
H(10R)-C(105)-H(10T)	109.5
H(10S)-C(105)-H(10T)	109.5
C(103)-C(106)-H(10U)	109.5
C(103)-C(106)-H(10V)	109.5
H(10U)-C(106)-H(10V)	109.5
C(103)-C(106)-H(10W)	109.5
H(10U)-C(106)-H(10W)	109.5
H(10V)-C(106)-H(10W)	109.5
N(9)-C(107)-C(108)	109.9(15)
N(9)-C(107)-Cs(1)	62.2(10)
C(108)-C(107)-Cs(1)	84.8(10)
N(9)-C(107)-H(10X)	109.7
C(108)-C(107)-H(10X)	109.7
Cs(1)-C(107)-H(10X)	66.5
N(9)-C(107)-H(10Y)	109.7
C(108)-C(107)-H(10Y)	109.7
Cs(1)-C(107)-H(10Y)	165.4
H(10X)-C(107)-H(10Y)	108.2
O(13)-C(108)-C(107)	106.2(15)
O(13)-C(108)-H	110.5
C(107)-C(108)-H	110.5
O(13)-C(108)-H(10Z)	110.5
C(107)-C(108)-H(10Z)	110.5
H-C(108)-H(10Z)	108.7
O(13)-C(109)-C(110)	103.6(15)
O(13)-C(109)-Cs(1)	41.1(7)
C(110)-C(109)-Cs(1)	66.6(9)
O(13)-C(109)-H(10)	111.0
C(110)-C(109)-H(10)	111.0

Cs(1)-C(109)-H(10)	140.8
O(13)-C(109)-HA	111.0
C(110)-C(109)-HA	111.0
Cs(1)-C(109)-HA	107.8
H(10)-C(109)-HA	109.0
O(14)-C(110)-C(109)	105.4(14)
O(14)-C(110)-Cs(1)	59.2(8)
C(109)-C(110)-Cs(1)	89.7(10)
O(14)-C(110)-H(11F)	110.7
C(109)-C(110)-H(11F)	110.7
Cs(1)-C(110)-H(11F)	159.5
O(14)-C(110)-H(11G)	110.7
C(109)-C(110)-H(11G)	110.7
Cs(1)-C(110)-H(11G)	63.9
H(11F)-C(110)-H(11G)	108.8
C(112)-C(111)-O(14)	109.8(13)
C(112)-C(111)-Cs(1)	98.2(10)
O(14)-C(111)-Cs(1)	60.5(7)
C(112)-C(111)-H(11H)	109.7
O(14)-C(111)-H(11H)	109.7
Cs(1)-C(111)-H(11H)	152.0
C(112)-C(111)-H(11I)	109.7
O(14)-C(111)-H(11I)	109.7
Cs(1)-C(111)-H(11I)	58.2
H(11H)-C(111)-H(11I)	108.2
C(111)-C(112)-N(10)	116.0(13)
C(111)-C(112)-H(11J)	108.3
N(10)-C(112)-H(11J)	108.3
C(111)-C(112)-H(11K)	108.3
N(10)-C(112)-H(11K)	108.3
H(11J)-C(112)-H(11K)	107.4
N(9)-C(113)-C(114)	117.0(14)
N(9)-C(113)-H(11L)	108.0
C(114)-C(113)-H(11L)	108.0
N(9)-C(113)-H(11M)	108.0
C(114)-C(113)-H(11M)	108.0
H(11L)-C(113)-H(11M)	107.3
O(15)-C(114)-C(113)	118.5(12)
O(15)-C(114)-C(7A)	94.6(11)
O(15)-C(114)-H(11N)	107.7
C(113)-C(114)-H(11N)	107.7
O(15)-C(114)-H(11O)	107.7
C(113)-C(114)-H(11O)	107.7
H(11N)-C(114)-H(11O)	107.1
O(15)-C(114)-H(11P)	112.8
C(7A)-C(114)-H(11P)	112.8
O(15)-C(114)-H(11Q)	112.8
C(7A)-C(114)-H(11Q)	112.8
H(11P)-C(114)-H(11Q)	110.3
O(15)-C(115)-C(116)	117.4(6)
O(15)-C(115)-H(11R)	107.9
C(116)-C(115)-H(11R)	107.9
O(15)-C(115)-H(11S)	107.9
C(116)-C(115)-H(11S)	107.9
H(11R)-C(115)-H(11S)	107.2
O(16)-C(116)-C(115)	116.5(7)
O(16)-C(116)-H(11T)	108.2
C(115)-C(116)-H(11T)	108.2
O(16)-C(116)-H(11U)	108.2
C(115)-C(116)-H(11U)	108.2
H(11T)-C(116)-H(11U)	107.3
O(16)-C(117)-C(8A)	115.1(13)

O(16)-C(117)-C(118)	103.3(10)
O(16)-C(117)-H(11V)	111.1
C(118)-C(117)-H(11V)	111.1
O(16)-C(117)-H(11W)	111.1
C(118)-C(117)-H(11W)	111.1
H(11V)-C(117)-H(11W)	109.1
O(16)-C(117)-H(11X)	108.5
C(8A)-C(117)-H(11X)	108.5
O(16)-C(117)-H(11Y)	108.5
C(8A)-C(117)-H(11Y)	108.5
H(11X)-C(117)-H(11Y)	107.5
N(10)-C(118)-C(117)	107.6(15)
N(10)-C(118)-H(11Z)	110.2
C(117)-C(118)-H(11Z)	110.2
N(10)-C(118)-HB	110.2
C(117)-C(118)-HB	110.2
H(11Z)-C(118)-HB	108.5
N(9)-C(119)-C(120)	113.7(17)
N(9)-C(119)-Cs(1)	64.8(8)
C(120)-C(119)-Cs(1)	89.9(11)
N(9)-C(119)-H(11)	108.8
C(120)-C(119)-H(11)	108.8
Cs(1)-C(119)-H(11)	160.9
N(9)-C(119)-HC	108.8
C(120)-C(119)-HC	108.8
Cs(1)-C(119)-HC	61.1
H(11)-C(119)-HC	107.7
O(17)-C(120)-C(119)	106.9(13)
O(17)-C(120)-H(12C)	110.3
C(119)-C(120)-H(12C)	110.3
O(17)-C(120)-H(12D)	110.3
C(119)-C(120)-H(12D)	110.3
H(12C)-C(120)-H(12D)	108.6
O(17)-C(121)-C(122)	108.3(14)
O(17)-C(121)-Cs(1)	41.9(7)
C(122)-C(121)-Cs(1)	76.6(10)
O(17)-C(121)-H(12E)	110.0
C(122)-C(121)-H(12E)	110.0
Cs(1)-C(121)-H(12E)	96.9
O(17)-C(121)-H(12F)	110.0
C(122)-C(121)-H(12F)	110.0
Cs(1)-C(121)-H(12F)	148.8
H(12E)-C(121)-H(12F)	108.4
O(18)-C(122)-C(121)	105.3(16)
O(18)-C(122)-Cs(1)	47.4(8)
C(121)-C(122)-Cs(1)	81.1(10)
O(18)-C(122)-H(12G)	110.7
C(121)-C(122)-H(12G)	110.7
Cs(1)-C(122)-H(12G)	82.6
O(18)-C(122)-H(12H)	110.7
C(121)-C(122)-H(12H)	110.7
Cs(1)-C(122)-H(12H)	158.0
H(12G)-C(122)-H(12H)	108.8
O(18)-C(123)-C(124)	112.9(19)
O(18)-C(123)-Cs(1)	43.8(8)
C(124)-C(123)-Cs(1)	73.9(14)
O(18)-C(123)-H(12I)	109.0
C(124)-C(123)-H(12I)	109.0
Cs(1)-C(123)-H(12I)	143.3
O(18)-C(123)-H(12J)	109.0
C(124)-C(123)-H(12J)	109.0
Cs(1)-C(123)-H(12J)	105.4

H(12I)-C(123)-H(12J)	107.8
C(123)-C(124)-N(10)	113.6(18)
C(123)-C(124)-Cs(1)	83.7(14)
N(10)-C(124)-Cs(1)	64.4(11)
C(123)-C(124)-H(12K)	108.8
N(10)-C(124)-H(12K)	108.8
Cs(1)-C(124)-H(12K)	167.4
C(123)-C(124)-H(12L)	108.8
N(10)-C(124)-H(12L)	108.8
Cs(1)-C(124)-H(12L)	66.9
H(12K)-C(124)-H(12L)	107.7
N(11)-C(125)-C(126)	103.4(11)
N(11)-C(125)-H(12M)	111.1
C(126)-C(125)-H(12M)	111.1
N(11)-C(125)-H(12N)	111.1
C(126)-C(125)-H(12N)	111.1
H(12M)-C(125)-H(12N)	109.0
O(19)-C(126)-C(125)	109.3(14)
O(19)-C(126)-Cs(2)	156.5(10)
C(125)-C(126)-Cs(2)	94.0(9)
O(19)-C(126)-H(12O)	109.8
C(125)-C(126)-H(12O)	109.8
Cs(2)-C(126)-H(12O)	62.2
O(19)-C(126)-H(12P)	109.8
C(125)-C(126)-H(12P)	109.8
Cs(2)-C(126)-H(12P)	57.7
H(12O)-C(126)-H(12P)	108.3
O(19)-C(127)-C(128)	113.3(12)
C(17A)-C(127)-O(19')	108(3)
C(17A)-C(127)-H(12S)	110.1
O(19')-C(127)-H(12S)	110.1
C(17A)-C(127)-H(12T)	110.1
O(19')-C(127)-H(12T)	110.1
H(12S)-C(127)-H(12T)	108.4
O(19)-C(127)-H(12Q)	108.9
C(128)-C(127)-H(12Q)	108.9
O(19)-C(127)-H(12R)	108.9
C(128)-C(127)-H(12R)	108.9
H(12Q)-C(127)-H(12R)	107.7
C(127)-C(128)-O(20)	117.4(10)
C(127)-C(128)-H(12U)	108.0
O(20)-C(128)-H(12U)	108.0
C(127)-C(128)-H(12V)	108.0
O(20)-C(128)-H(12V)	108.0
H(12U)-C(128)-H(12V)	107.2
O(20')-C(129)-C(18A)	118(2)
O(20)-C(129)-C(130)	110.5(7)
O(20)-C(129)-H(12W)	109.5
C(130)-C(129)-H(12W)	109.5
O(20)-C(129)-H(12X)	109.5
C(130)-C(129)-H(12X)	109.5
H(12W)-C(129)-H(12X)	108.1
O(20')-C(129)-H(12Y)	107.9
C(18A)-C(129)-H(12Y)	107.9
O(20')-C(129)-HD	107.9
C(18A)-C(129)-HD	107.9
H(12Y)-C(129)-HD	107.2
N(12)-C(130)-C(129)	114.3(8)
N(12)-C(130)-H(13C)	108.7
C(129)-C(130)-H(13C)	108.7
N(12)-C(130)-H(13D)	108.7
C(129)-C(130)-H(13D)	108.7

H(13C)-C(130)-H(13D)	107.6
C(132)-C(131)-N(11)	111.2(10)
C(132)-C(131)-Cs(2)	88.7(11)
N(11)-C(131)-Cs(2)	63.3(9)
C(132)-C(131)-H(13E)	109.4
N(11)-C(131)-H(13E)	109.4
Cs(2)-C(131)-H(13E)	62.6
C(132)-C(131)-H(13F)	109.4
N(11)-C(131)-H(13F)	109.4
Cs(2)-C(131)-H(13F)	161.8
H(13E)-C(131)-H(13F)	108.0
C(131)-C(132)-O(21)	113.5(13)
C(131)-C(132)-Cs(2)	69.1(10)
O(21)-C(132)-Cs(2)	44.5(6)
C(131)-C(132)-H(13G)	108.9
O(21)-C(132)-H(13G)	108.9
Cs(2)-C(132)-H(13G)	127.9
C(131)-C(132)-H(13H)	108.9
O(21)-C(132)-H(13H)	108.9
Cs(2)-C(132)-H(13H)	122.5
H(13G)-C(132)-H(13H)	107.7
O(21)-C(133)-C(134)	109.1(10)
O(21)-C(133)-H(13I)	109.9
C(134)-C(133)-H(13I)	109.9
O(21)-C(133)-H(13J)	109.9
C(134)-C(133)-H(13J)	109.9
H(13I)-C(133)-H(13J)	108.3
O(22)-C(134)-C(133)	111.4(9)
O(22)-C(134)-H(13K)	109.3
C(133)-C(134)-H(13K)	109.3
O(22)-C(134)-H(13L)	109.3
C(133)-C(134)-H(13L)	109.3
H(13K)-C(134)-H(13L)	108.0
O(22)-C(135)-C(136)	107.7(8)
O(22)-C(135)-H(13M)	110.2
C(136)-C(135)-H(13M)	110.2
O(22)-C(135)-H(13N)	110.2
C(136)-C(135)-H(13N)	110.2
H(13M)-C(135)-H(13N)	108.5
C(135)-C(136)-N(12)	116.2(6)
C(23A)-C(136)-O(22')	105.2(13)
C(135)-C(136)-Cs(2)	91.3(5)
N(12)-C(136)-Cs(2)	62.3(4)
C(135)-C(136)-H(13O)	108.2
N(12)-C(136)-H(13O)	108.2
Cs(2)-C(136)-H(13O)	160.4
C(135)-C(136)-H(13P)	108.2
N(12)-C(136)-H(13P)	108.2
Cs(2)-C(136)-H(13P)	63.5
H(13O)-C(136)-H(13P)	107.4
C(23A)-C(136)-H(13Q)	110.7
O(22')-C(136)-H(13Q)	110.7
C(23A)-C(136)-H(13R)	110.7
O(22')-C(136)-H(13R)	110.7
H(13Q)-C(136)-H(13R)	108.8
C(138)-C(137)-N(11)	112.7(15)
C(138)-C(137)-Cs(2)	86.0(10)
N(11)-C(137)-Cs(2)	59.6(7)
C(138)-C(137)-H(13S)	109.1
N(11)-C(137)-H(13S)	109.1
Cs(2)-C(137)-H(13S)	164.4
C(138)-C(137)-H(13T)	109.1

N(11)-C(137)-H(13T)	109.1
Cs(2)-C(137)-H(13T)	69.4
H(13S)-C(137)-H(13T)	107.8
O(23)-C(138)-C(137)	109.6(13)
O(23)-C(138)-Cs(2)	40.5(6)
C(137)-C(138)-Cs(2)	71.2(9)
O(23)-C(138)-H(13U)	109.8
C(137)-C(138)-H(13U)	109.8
Cs(2)-C(138)-H(13U)	112.0
O(23)-C(138)-H(13V)	109.8
C(137)-C(138)-H(13V)	109.8
Cs(2)-C(138)-H(13V)	136.6
H(13U)-C(138)-H(13V)	108.2
O(23)-C(139)-C(140)	109.5(11)
O(23)-C(139)-Cs(2)	41.8(6)
C(140)-C(139)-Cs(2)	75.1(8)
O(23)-C(139)-H(13W)	109.8
C(140)-C(139)-H(13W)	109.8
Cs(2)-C(139)-H(13W)	146.0
O(23)-C(139)-H(13X)	109.8
C(140)-C(139)-H(13X)	109.8
Cs(2)-C(139)-H(13X)	100.9
H(13W)-C(139)-H(13X)	108.2
O(24)-C(140)-C(139)	108.9(11)
O(24)-C(140)-Cs(2)	47.5(6)
C(139)-C(140)-Cs(2)	83.1(8)
O(24)-C(140)-H(14C)	109.9
C(139)-C(140)-H(14C)	109.9
Cs(2)-C(140)-H(14C)	157.4
O(24)-C(140)-H(14D)	109.9
C(139)-C(140)-H(14D)	109.9
Cs(2)-C(140)-H(14D)	83.0
H(14C)-C(140)-H(14D)	108.3
N(12')-C(141)-C(28A)	112.4(15)
O(24)-C(141)-C(142)	111.8(6)
N(12')-C(141)-Cs(2')	65.7(8)
C(28A)-C(141)-Cs(2')	91.3(10)
O(24)-C(141)-Cs(2)	46.2(3)
C(142)-C(141)-Cs(2)	67.8(5)
O(24)-C(141)-H(14E)	109.3
C(142)-C(141)-H(14E)	109.3
Cs(2)-C(141)-H(14E)	111.8
O(24)-C(141)-H(14F)	109.3
C(142)-C(141)-H(14F)	109.3
Cs(2)-C(141)-H(14F)	138.6
H(14E)-C(141)-H(14F)	107.9
N(12')-C(141)-H(14G)	109.1
C(28A)-C(141)-H(14G)	109.1
Cs(2')-C(141)-H(14G)	158.9
N(12')-C(141)-H(14H)	109.1
C(28A)-C(141)-H(14H)	109.1
Cs(2')-C(141)-H(14H)	58.6
H(14G)-C(141)-H(14H)	107.9
N(12)-C(142)-C(141)	113.5(8)
N(12)-C(142)-Cs(2)	66.3(5)
C(141)-C(142)-Cs(2)	88.9(5)
N(12)-C(142)-H(14I)	108.9
C(141)-C(142)-H(14I)	108.9
Cs(2)-C(142)-H(14I)	161.5
N(12)-C(142)-H(14J)	108.9
C(141)-C(142)-H(14J)	108.9
Cs(2)-C(142)-H(14J)	60.2

H(14I)-C(142)-H(14J)	107.7
C(2S)-C(1S)-C(6S)	119.0(10)
C(2S)-C(1S)-C(7S)	120.5(8)
C(6S)-C(1S)-C(7S)	120.5(9)
C(1S)-C(2S)-C(3S)	120.7(9)
C(1S)-C(2S)-H(2S)	119.7
C(3S)-C(2S)-H(2S)	119.7
C(2S)-C(3S)-C(4S)	120.7(9)
C(2S)-C(3S)-H(3S)	119.6
C(4S)-C(3S)-H(3S)	119.6
C(5S)-C(4S)-C(3S)	117.6(10)
C(5S)-C(4S)-H(4S)	121.2
C(3S)-C(4S)-H(4S)	121.2
C(4S)-C(5S)-C(6S)	121.7(10)
C(4S)-C(5S)-H(5S)	119.2
C(6S)-C(5S)-H(5S)	119.2
C(1S)-C(6S)-C(5S)	120.2(10)
C(1S)-C(6S)-H(6S)	119.9
C(5S)-C(6S)-H(6S)	119.9
C(1S)-C(7S)-H(7SA)	109.5
C(1S)-C(7S)-H(7SB)	109.5
H(7SA)-C(7S)-H(7SB)	109.5
C(1S)-C(7S)-H(7SC)	109.5
H(7SA)-C(7S)-H(7SC)	109.5
H(7SB)-C(7S)-H(7SC)	109.5
C(13')-C(8S)-C(9')	130.1(13)
C(13S)-C(8S)-C(9S)	109.2(13)
C(13S)-C(8S)-C(14S)	127.0(18)
C(9S)-C(8S)-C(14S)	123.5(18)
C(13')-C(8S)-H(8S)	114.9
C(9')-C(8S)-H(8S)	114.9
C(10')-C(9')-C(8S)	112.2(15)
C(10')-C(9')-H(9')	123.9
C(8S)-C(9')-H(9')	123.9
C(10S)-C(9S)-C(8S)	129.2(19)
C(10S)-C(9S)-H(9S)	115.4
C(8S)-C(9S)-H(9S)	115.4
C(9')-C(10')-C(11')	122.4(18)
C(9')-C(10')-H(10')	118.8
C(11')-C(10')-H(10')	118.8
C(11S)-C(10S)-C(9S)	117(2)
C(11S)-C(10S)-H(1)	121.6
C(9S)-C(10S)-H(1)	121.6
C(12')-C(11')-C(10')	120.5(19)
C(12')-C(11')-H(11')	119.7
C(10')-C(11')-H(11')	119.7
C(10S)-C(11S)-C(12S)	119(2)
C(10S)-C(11S)-H(6)	120.6
C(12S)-C(11S)-H(6)	120.6
C(11')-C(12')-C(13')	121.1(18)
C(11')-C(12')-H(12')	119.4
C(13')-C(12')-H(12')	119.4
C(11S)-C(12S)-C(13S)	120(2)
C(11S)-C(12S)-H(12Z)	120.0
C(13S)-C(12S)-H(12Z)	120.0
C(8S)-C(13')-C(12')	112.9(14)
C(8S)-C(13')-C(14')	121.8(17)
C(12')-C(13')-C(14')	125.2(16)
C(8S)-C(13S)-C(12S)	125.9(18)
C(8S)-C(13S)-H(13Y)	117.1
C(12S)-C(13S)-H(13Y)	117.1
C(13')-C(14')-H(14K)	109.5

C(13')-C(14')-H(14L)	109.5
H(14K)-C(14')-H(14L)	109.5
C(13')-C(14')-H(14M)	109.5
H(14K)-C(14')-H(14M)	109.5
H(14L)-C(14')-H(14M)	109.5
C(8S)-C(14S)-H(14N)	109.5
C(8S)-C(14S)-H(14O)	109.5
H(14N)-C(14S)-H(14O)	109.5
C(8S)-C(14S)-H(14P)	109.5
H(14N)-C(14S)-H(14P)	109.5
H(14O)-C(14S)-H(14P)	109.5
C(16S)-C(15S)-C(20S)	117.3(7)
C(16S)-C(15S)-C(21S)	119.9(8)
C(20S)-C(15S)-C(21S)	122.8(7)
C(17S)-C(16S)-C(15S)	121.4(9)
C(17S)-C(16S)-H(16S)	119.3
C(15S)-C(16S)-H(16S)	119.3
C(18S)-C(17S)-C(16S)	121.0(9)
C(18S)-C(17S)-H(17S)	119.5
C(16S)-C(17S)-H(17S)	119.5
C(17S)-C(18S)-C(19S)	119.5(9)
C(17S)-C(18S)-H(18S)	120.3
C(19S)-C(18S)-H(18S)	120.3
C(20S)-C(19S)-C(18S)	119.1(9)
C(20S)-C(19S)-H(19S)	120.4
C(18S)-C(19S)-H(19S)	120.4
C(19S)-C(20S)-C(15S)	121.7(8)
C(19S)-C(20S)-H(20S)	119.2
C(15S)-C(20S)-H(20S)	119.2
C(15S)-C(21S)-H(21F)	109.5
C(15S)-C(21S)-H(21G)	109.5
H(21F)-C(21S)-H(21G)	109.5
C(15S)-C(21S)-H(21H)	109.5
H(21F)-C(21S)-H(21H)	109.5
H(21G)-C(21S)-H(21H)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x,-y,-z+1

Theoretical calculations.

Optimization of the molecular structures was performed using the PBE exchange-correlation functional[3] and with the extended basis set Cu: [9s9p8d/5s5p4d], O,N,C : [5s5p2d/3s3p2d], H :[5s1p/3s1p] for valence electrons and the SBK pseudopotential[4] implemented in the PRIRODA package[5]. The Hirschfeld method[6] was used to calculate atomic charges. All quantum chemical calculations were performed using the computing capabilities of the Joint supercomputer center of the National Research Center "Kurchatov Institute".

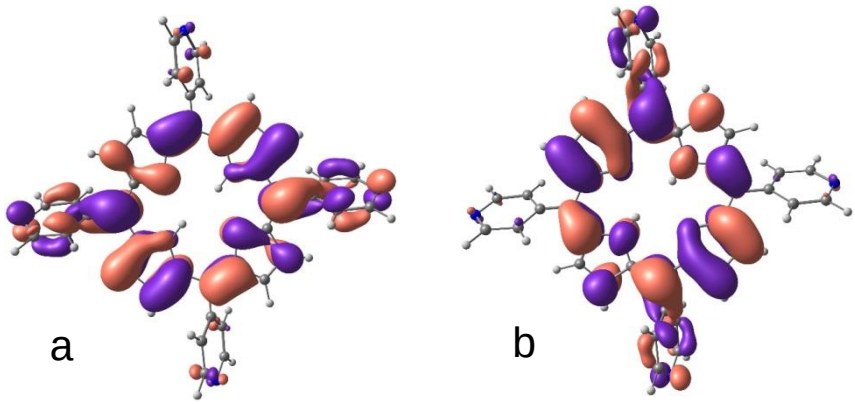

Fig. S22. Structure of α-orbitals for $H_2TPyP^{\bullet-}$ radical anions: (a) HOMO; (b) LUMO. To elucidate the regions with small degree of localization the small value 0.02 for contour plots was used.

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Cartesian coordinate of the structures optimized

The [{Cu^{II}TPyP}$^{-}$ anion (S = 1)

7	-1.44282242	-1.43504474	-0.04562011
6	-2.79685366	-1.23098003	-0.30607863
6	-3.47376937	-2.49219427	-0.40082073
1	-4.52735089	-2.62736249	-0.62471251
6	-2.53154963	-3.46889656	-0.19416449
1	-2.67871613	-4.54308133	-0.22597009
6	-1.27381992	-2.80206078	0.03813500
7	7.69879248	-0.00216048	1.23243762
6	7.17880631	0.32143451	0.03412364
1	7.90058155	0.58376006	-0.74637713
6	5.80891224	0.33429667	-0.24863636
1	5.45254521	0.60529954	-1.24360404
6	4.89113452	-0.00935652	0.75903395
6	5.42933115	-0.34677949	2.01304946
1	4.76788056	-0.61721175	2.83748789
6	6.81618729	-0.32791114	2.19465037
1	7.24342148	-0.58677309	3.16902212
7	-1.39609921	1.45062446	-0.30581777
6	-1.19469703	2.81335460	-0.38358831
6	-2.44595360	3.48084637	-0.65375950
1	-2.57384417	4.54897183	-0.79205688
6	-3.41509395	2.51183271	-0.71455657
1	-4.47752090	2.65087163	-0.88809091
6	-2.76028157	1.25080558	-0.51036750
7	1.44355855	1.43538394	0.04050311
6	2.79756648	1.23167765	0.30087872
6	3.47538823	2.49311478	0.38882052
1	4.52919331	2.62891119	0.61119669
6	2.53375658	3.46927603	0.17751444
1	2.68216015	4.54343131	0.20369184
6	1.27512173	2.80178901	-0.04967964
7	-7.70514293	-0.00003243	-1.19634751
6	-7.17449368	-0.32690217	-0.00355784
1	-7.88923854	-0.59326777	0.78201862
6	-5.80228597	-0.33875891	0.26753535
1	-5.43710378	-0.61359286	1.25823270
6	-4.89343642	0.01022935	-0.74642933
6	-5.44279103	0.35184900	-1.99448667
1	-4.78871379	0.62629409	-2.82347812
6	-6.83108699	0.33074170	-2.16466059
1	-7.26680891	0.59213506	-3.13459333
7	-0.11887066	-7.81863678	0.55174601

6	0.07329743	4.95827915	-0.37050172
6	-0.69691820	5.78733026	0.47394469
1	-1.32792384	5.34434156	1.24587878
6	-0.63710020	7.17540363	0.33412035
1	-1.23033665	7.81439296	0.99723058
7	0.12397094	7.81731449	-0.57430866
6	0.86098276	7.02657684	-1.37973904
1	1.47527632	7.54385294	-2.12470895
6	0.87207662	5.63166497	-1.32029315
1	1.48822697	5.06124584	-2.01700574
6	0.04945124	3.47972726	-0.26715817
6	3.41790630	-0.01058196	0.50987020
6	-0.86316321	-7.03131788	1.35382005
1	-1.48239751	-7.55163014	2.09257143
6	-3.41844903	0.01183377	-0.50815083
6	0.70721991	-5.78428422	-0.48391835
1	1.34360044	-5.33805173	-1.24953840
6	2.44477558	-3.47927174	0.65861826
1	2.57243121	-4.54709535	0.79951769
6	1.19493749	-2.81271515	0.38029959
7	1.39624422	-1.44998200	0.30172037
6	2.75936134	-1.24943815	0.51283652
6	3.41324432	-2.50976921	0.72364198
1	4.47461752	-2.64824490	0.90394620
6	-0.04833751	-3.47992345	0.25742668
6	-0.07094774	-4.95869720	0.35683183
6	0.64835233	-7.17279384	-0.34878020
1	1.24771270	-7.80892221	-1.00911942
6	-0.87593087	-5.63626543	1.29845540
1	-1.49833014	-5.06903879	1.99219162
29	0.00015662	0.00013221	-0.00232306

The $[\{H_2TPyP\}^-$ radical anion (S = 1/2)

7	-1.49887219	-1.52958679	0.02914193
1	-0.74396572	-0.84768250	0.13671621
6	-2.82143074	-1.24707456	-0.28021394
6	-3.48231061	-2.50151658	-0.41408179
1	-4.52755801	-2.62901605	-0.67422149
6	-2.55159659	-3.50881991	-0.19548799
1	-2.72386585	-4.57747372	-0.25610603
6	-1.29398026	-2.89337185	0.08296989
7	7.68922647	-0.02795557	1.16852944
6	7.15359535	0.34531597	-0.00937442
1	7.86533893	0.64528600	-0.78551532
6	5.78160730	0.36197611	-0.27689121

1	5.41503767	0.67336415	-1.25626253
6	4.87391182	-0.03565247	0.72157375
6	5.42937319	-0.41944892	1.95589717
1	4.77899406	-0.72768946	2.77569572
6	6.81784416	-0.40065756	2.12335844
1	7.25589827	-0.69867417	3.08172895
7	-1.38126872	1.49396726	-0.31301036
6	-1.20436717	2.84870293	-0.40110840
6	-2.47350861	3.51889196	-0.67979945
1	-2.62014207	4.58359194	-0.83234339
6	-3.42367385	2.54221839	-0.73585787
1	-4.48713792	2.67369350	-0.91158658
6	-2.73262697	1.27780308	-0.51552524
7	1.49743754	1.52962853	-0.02650343
1	0.74393311	0.84752440	-0.14193941
6	2.82308612	1.24627442	0.26788653
6	3.48561887	2.50043547	0.39723477
1	4.53202658	2.62698018	0.65318269
6	2.55415819	3.50827353	0.18469482
1	2.72607222	4.57690570	0.24726513
6	1.29442428	2.89337382	-0.08600906
7	-7.68222650	0.02594883	-1.21317405
6	-7.15529716	-0.35029193	-0.03223512
1	-7.87266284	-0.65346502	0.73746161
6	-5.78536728	-0.36690493	0.24560384
1	-5.42606022	-0.68184596	1.22652400
6	-4.87035873	0.03519879	-0.74439032
6	-5.41671939	0.42261468	-1.98160361
1	-4.76039252	0.73442814	-2.79529022
6	-6.80379560	0.40242274	-2.16007445
1	-7.23472482	0.70286843	-3.12091134
7	-0.10051188	-7.87495047	0.60169148
6	0.05236753	5.01502108	-0.38278413
6	-0.75516876	5.82917784	0.44219447
1	-1.40820668	5.37311790	1.18742107
6	-0.70019233	7.21910234	0.32013406
1	-1.32420963	7.84588836	0.96642200
7	0.09129541	7.87713550	-0.54937295
6	0.86644733	7.10112015	-1.33356728
1	1.50666936	7.63168526	-2.04661485
6	0.88635629	5.70612999	-1.28943070
1	1.53206206	5.14903671	-1.96988647
6	0.03817320	3.53652492	-0.29581763
6	3.39833501	-0.03645090	0.48350737
6	-0.88530275	-7.08933690	1.36657579

1	-1.53576907	-7.61109897	2.07687516
6	-3.39655924	0.03570026	-0.49588327
6	0.76125932	-5.83843595	-0.40077805
1	1.42629371	-5.39210116	-1.14121984
6	2.47201257	-3.51741177	0.69397160
1	2.61911206	-4.58071054	0.85525982
6	1.20355850	-2.84868204	0.40890099
7	1.38187490	-1.49476169	0.31034024
6	2.73351753	-1.27802521	0.51124184
6	3.42340353	-2.54147422	0.74034741
1	4.48679546	-2.67322380	0.91606342
6	-0.03923993	-3.53650410	0.30393689
6	-0.05621674	-5.01389329	0.40418540
6	0.70337012	-7.22683711	-0.26401656
1	1.33550362	-7.86095577	-0.89505780
6	-0.90279186	-5.69493391	1.30714974
1	-1.55791244	-5.13041353	1.97226291