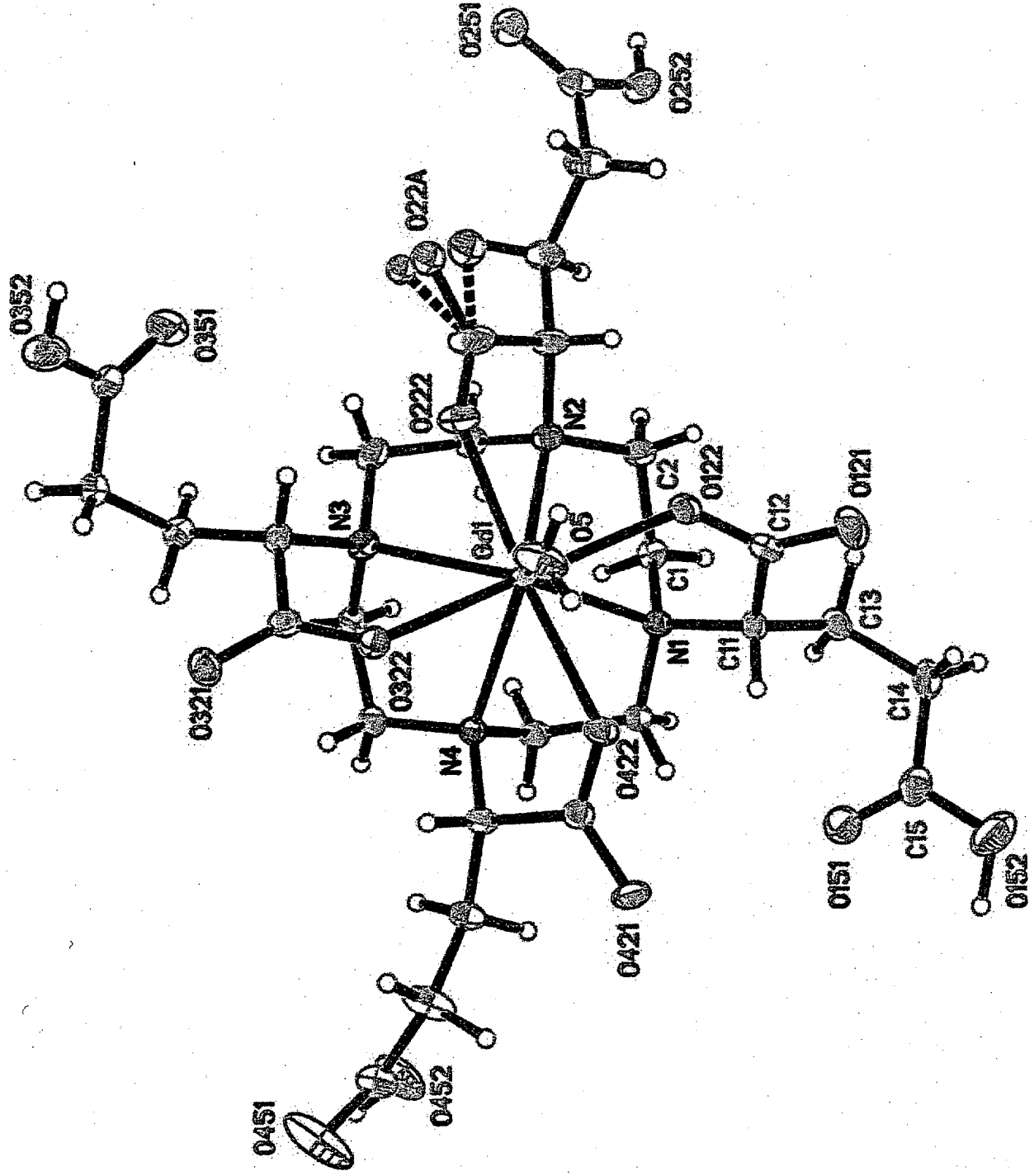
© 2000 American Chemical Society, J. Am. Chem. Soc., Woods ja994492v Supporting Info Page 1 of 2

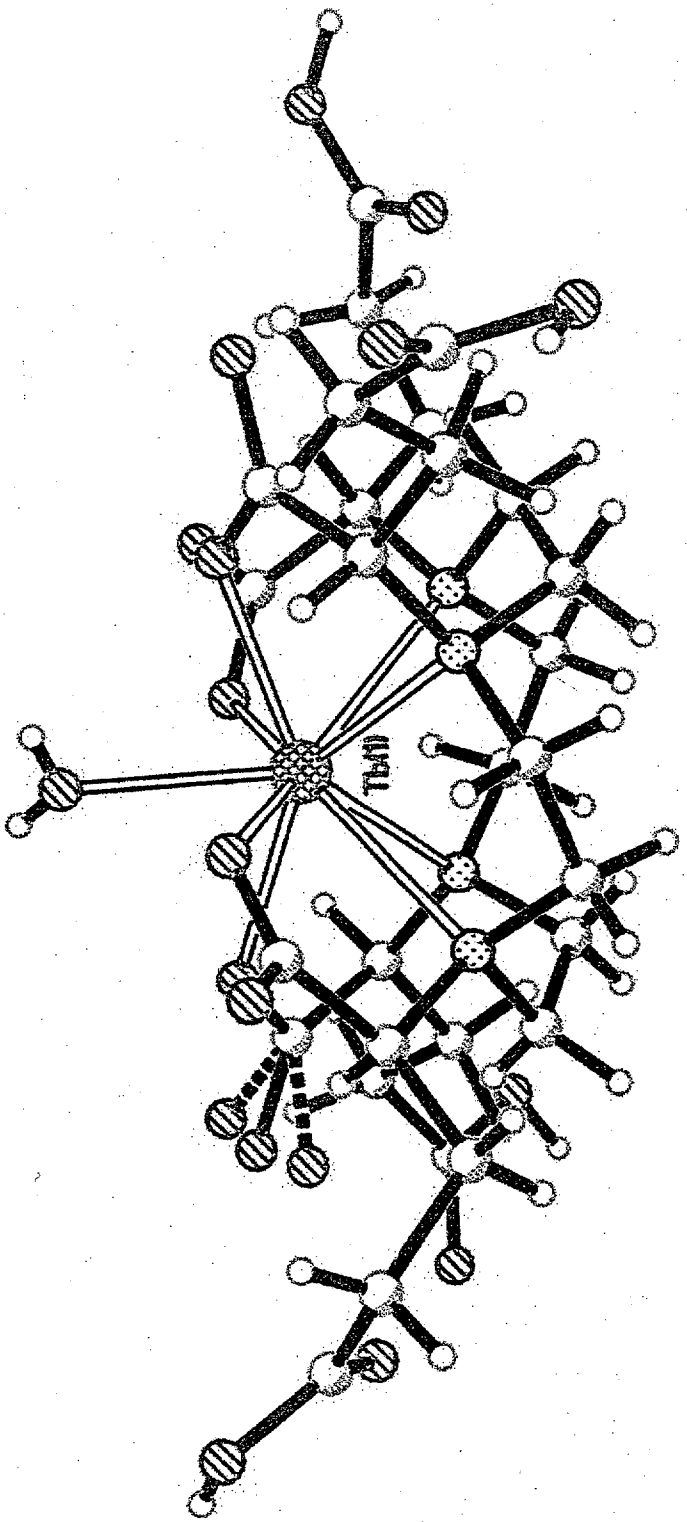
SUPPORTING INFORMATION

-25-355

Selected crystal data for the europium, terbium and gadolinium complexes of 1,4,7,10-tetrakis(carboxyethyl)-1,4,7,10-tetraazacyclododecane.

Empirical formula	C28 H49 Eu N4 O20.25	C28 H49 N4 O23 Tb	C28 H49 Gd N4 O20
Formula weight	917.67	920.63	918.96
Temperature	150(2) K	150(2) K	150(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1
Cell dimensions (Å/°)	a = 9.637(2) α = 102.47(2)	a =9.6289(1) α=102.7389(8)	a =9.6460(5) α=102.652(4)
	b = 12.690(4) β = 101.28(2)	b=12.6877(2) β=101.2348(9)	b=12.6915(7) β=101.192(4)
	c = 16.186(5) γ = 110.42(2)	c=16.2170(2) γ=110.5812(4)	c=16.2000(11) γ=110.446(3)
Volume	1729.84(3) $Å^3$	1726.76(4) $Å^3$	1731.9(2) $Å^3$
Z	2	2	2
Density (calculated)	1.762 g/cm^3	1.771 g/cm^3	1.762 g/cm^3
Absorption coefficient	1.906 mm^{-1}	2.141 mm^{-1}	2.007 mm^{-1}
Absorption correction	Integration	Semi-empirical - Sadabs	Multiscan – Sadabs
Max. & min. transmiss.	0.835 and 0.713	0.677 and 0.419	0.610 and 0.491
F(000)	940	940	938
Crystal size	0.16 x 0.16 x 0.10 mm^3	0.10 x 0.20 x 0.25 mm^3	0.34 x 0.32 x 0.18 mm^3
θ range for collection	1.35 to 27.45°.	1.35 to 27.53°.	1.35 to 27.50°.
Index ranges	-11<=h<=12,	-11<=h<=12,	-12<=h<=12,
	-15<=k<=16,	-16<=k<=16,	-16<=k<=16,
	-20<=l<=20	-21<=l<=20	-13<=l<=21
Reflections collected	13944	13969	14872
Independent reflects.	7826 [R(int) = 0.0310]	7856 [R(int) = 0.0381]	7843 [R(int) = 0.0251]
Refinement method	Full-matr least-squares on F^2	Full-matr least-squares on F^2	Full-matr least-squares on F^2
Data/restrs/parameters	7797 / 0 / 627	7856 / 0 / 610	7843 / 0 / 651
Goodness-of-fit on F^2	1.094	1.085	1.046
R indices [I>2σ(I)]	R1 = 0.0305, wR2 = 0.0670	R1 = 0.0442, wR2 = 0.1057	R1 = 0.0211, wR2 = 0.0511
R indices (all data)	R1 = 0.0364, wR2 = 0.0747	R1 = 0.0601, wR2 = 0.1177	R1 = 0.0242, wR2 = 0.0523
Extinction coefficient	not refined	not refined?	not refined?
Largest residuals	0.979 and -0.950 $e.Å^{-3}$	2.683 and -2.362 $e.Å^{-3}$	0.656 and -0.714 $e.Å^{-3}$


0251
0252
022A
0352
0351
0222
N2
C2
0122
0121
N3
Gd1
O5
C12
C1
C13
0321
0322
N1
C11
C14
N4
0422
0151
C15
0152
0421
0451
0452


Tb(III)

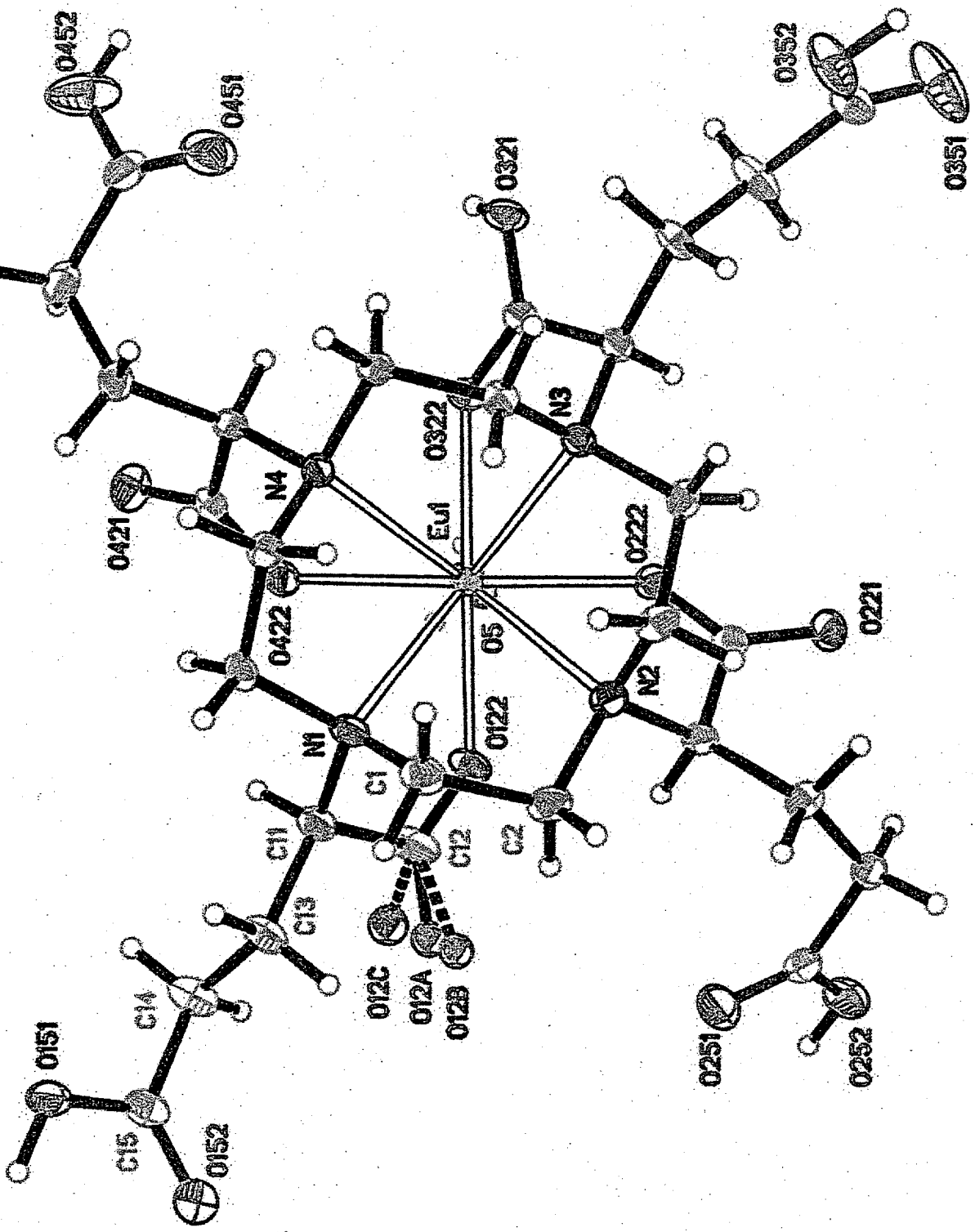

0452
0451
0321
0352
0351
0421
N4
0322
N3
Eu1
0222
0422
05
0221
N2
N1
0122
C1
C11
C12
C2
C13
012C
012A
012B
C14
0151
C15
0152
0251
0252

Table 1. Crystal data and structure refinement for 97srv139.

Empirical formula	C28 H49 Eu N4 O20.25	
Formula weight	917.67	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P(-1)	
Unit cell dimensions	a = 9.637(2) Å	α= 102.47(2)°.
	b = 12.690(4) Å	β= 101.28(2)°.
	c = 16.186(5) Å	γ = 110.42(2)°.
Volume	1729.84(3) $Å^3$	
Z	2	
Density (calculated)	1.762 Mg/m^3	
Absorption coefficient	1.906 mm^{-1}	
F(000)	940	
Crystal size	0.16 x 0.16 x 0.10 mm^3	
Theta range for data collection	1.35 to 27.45°.	
Index ranges	-11<=h<=12, -15<=k<=16, -20<=l<=20	
Reflections collected	13944	
Independent reflections	7826 [R(int) = 0.0310]	
Absorption correction	Integration	
Max. and min. transmission	0.835 and 0.713	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7797 / 0 / 627	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0305, wR2 = 0.0670	
R indices (all data)	R1 = 0.0364, wR2 = 0.0747	
Extinction coefficient	not refined	
Largest diff. peak and hole	0.979 and -0.950 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 97srv139. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Eu(1)	4179(1)	2765(1)	2664(1)	12(1)
O(5)	1958(4)	3118(3)	2960(3)	29(1)
O(12A)	6645(7)	6099(5)	4956(3)	18(1)
O(12B)	7164(10)	5885(7)	5062(5)	16(2)
O(12C)	6325(16)	6337(12)	4732(9)	24(3)
O(122)	5037(3)	4390(2)	3985(2)	22(1)
O(151)	10854(3)	9080(2)	3929(2)	25(1)
O(152)	10813(3)	9216(2)	5316(2)	28(1)
O(221)	3539(3)	795(2)	4634(2)	25(1)
O(222)	3240(3)	1607(2)	3553(2)	17(1)
O(251)	7682(3)	4467(2)	6461(2)	32(1)
O(252)	6139(3)	3806(2)	7275(2)	28(1)
O(321)	719(4)	-461(2)	445(2)	28(1)
O(322)	1951(3)	1311(2)	1470(2)	17(1)
O(351)	386(4)	-4377(3)	1393(3)	55(1)
O(352)	2209(4)	-3773(3)	745(2)	36(1)
O(421)	2991(3)	4414(2)	616(2)	29(1)
O(422)	3780(3)	4092(2)	1892(2)	18(1)
O(451)	2692(4)	813(3)	-1269(2)	41(1)
O(452)	1180(4)	1294(3)	-2199(2)	51(1)
O(1SA)	10045(5)	9130(4)	6817(3)	52(1)
O(1SB)	10457(19)	8960(14)	7000(11)	46(4)
O(2SA)	139(12)	3580(9)	1920(7)	37(2)
O(2SB)	-215(13)	3199(10)	802(7)	71(3)
O(3SB)	-1001(10)	1666(8)	1452(6)	72(2)
O(3SA)	-968(11)	1872(8)	1881(7)	48(2)
O(3SC)	-1631(15)	1284(11)	882(9)	50(3)
N(1)	7001(3)	4447(2)	2955(2)	18(1)
N(2)	6387(3)	2543(2)	3835(2)	17(1)
N(3)	4369(3)	705(2)	2075(2)	14(1)
N(4)	4998(3)	2594(2)	1175(2)	14(1)
C(1)	8215(4)	4111(3)	3397(2)	23(1)
C(2)	7875(4)	3626(3)	4149(2)	24(1)
C(3)	6682(4)	1505(3)	3422(2)	21(1)
C(4)	5236(4)	438(3)	2822(2)	17(1)
C(5)	5229(4)	766(3)	1408(2)	16(1)
C(6)	4770(4)	1350(3)	741(2)	16(1)
C(7)	6678(4)	3375(3)	1388(2)	17(1)
C(8)	7214(4)	4566(3)	2080(2)	19(1)
C(11)	7053(4)	5576(3)	3507(2)	21(1)
C(12)	6233(5)	5322(3)	4207(2)	31(1)
C(13)	8661(4)	6616(3)	3895(3)	25(1)
C(14)	8555(4)	7816(3)	4111(3)	30(1)
C(15)	10178(4)	8782(3)	4515(2)	23(1)
C(21)	5756(4)	2391(3)	4603(2)	16(1)
C(22)	4043(4)	1516(3)	4240(2)	17(1)
C(23)	6724(4)	2094(3)	5314(2)	19(1)
C(24)	6399(4)	2362(3)	6205(2)	20(1)
C(25)	6825(4)	3656(3)	6647(2)	22(1)
C(31)	2735(4)	-226(3)	1705(2)	16(1)
C(32)	1735(4)	256(3)	1168(2)	16(1)
C(33)	2577(4)	-1466(3)	1237(2)	20(1)
C(34)	1092(4)	-2449(3)	1241(3)	28(1)
C(35)	1173(4)	-3640(3)	1134(2)	24(1)
C(41)	3967(4)	2927(3)	558(2)	16(1)
C(42)	3562(4)	3906(3)	1054(2)	18(1)
C(43)	4537(4)	3190(3)	-231(2)	19(1)
C(44)	3243(5)	2868(3)	-1074(2)	25(1)
C(45)	2349(5)	1553(3)	-1514(2)	26(1)

© 2000 American Chemical Society, J. Am. Chem. Soc., Woods ja994492v Supporting Info Page 7

Table 3. Bond lengths [Å] and angles [°] for 97srv139.

Eu(1)-O(222)	2.354(2)	C(2)-H(2A)	0.96(4)	O(422)-Eu(1)-O(322)	83.23(8)
Eu(1)-O(422)	2.391(2)	C(2)-H(2B)	1.01(5)	O(122)-Eu(1)-O(322)	144.73(8)
Eu(1)-O(122)	2.393(2)	C(3)-C(4)	1.518(5)	O(222)-Eu(1)-O(5)	72.73(9)
Eu(1)-O(322)	2.412(2)	C(3)-H(3B)	0.99	O(422)-Eu(1)-O(5)	72.52(9)
Eu(1)-O(5)	2.447(3)	C(3)-H(3A)	0.99	O(122)-Eu(1)-O(5)	70.15(11)
Eu(1)-N(3)	2.664(3)	C(4)-H(4B)	1.00(4)	O(322)-Eu(1)-O(5)	74.58(10)
Eu(1)-N(4)	2.667(3)	C(4)-H(4A)	0.99(4)	O(222)-Eu(1)-N(3)	72.75(8)
Eu(1)-N(1)	2.681(3)	C(5)-C(6)	1.516(4)	O(422)-Eu(1)-N(3)	130.35(8)
Eu(1)-N(2)	2.696(3)	C(5)-H(5B)	0.97(4)	O(122)-Eu(1)-N(3)	140.88(9)
Eu(1)-H(5D)	2.81(6)	C(5)-H(5A)	0.93(4)	O(322)-Eu(1)-N(3)	65.85(8)
O(5)-H(5D)	0.64(6)	C(6)-H(6A)	1.03(4)	O(5)-Eu(1)-N(3)	128.46(9)
O(5)-H(5C)	0.76(9)	C(6)-H(6B)	0.93(3)	O(222)-Eu(1)-N(4)	140.90(8)
O(12A)-O(12B)	0.660(8)	C(7)-C(8)	1.518(5)	O(422)-Eu(1)-N(4)	65.16(8)
O(12A)-O(12C)	0.622(13)	C(7)-H(7B)	0.99(4)	O(122)-Eu(1)-N(4)	131.41(8)
O(12A)-C(12)	1.274(6)	C(7)-H(7A)	1.00(4)	O(322)-Eu(1)-N(4)	72.43(8)
O(12B)-O(12C)	1.25(2)	C(8)-H(8B)	0.96(4)	O(5)-Eu(1)-N(4)	128.38(11)
O(12B)-C(12)	1.367(9)	C(8)-H(8A)	1.00(4)	N(3)-Eu(1)-N(4)	68.80(8)
O(12C)-C(12)	1.343(14)	C(11)-C(12)	1.530(5)	O(222)-Eu(1)-N(1)	129.88(8)
O(122)-C(12)	1.249(4)	C(11)-C(13)	1.540(5)	O(422)-Eu(1)-N(1)	74.11(8)
O(151)-C(15)	1.300(4)	C(11)-H(11)	1.00	O(122)-Eu(1)-N(1)	65.34(8)
O(151)-H(151)	0.91(6)	C(13)-C(14)	1.531(5)	O(322)-Eu(1)-N(1)	141.10(8)
O(152)-C(15)	1.227(4)	C(13)-H(13B)	1.00(4)	O(5)-Eu(1)-N(1)	125.29(10)
O(221)-C(22)	1.242(4)	C(13)-H(13A)	0.98(4)	N(3)-Eu(1)-N(1)	106.20(8)
O(222)-C(22)	1.277(4)	C(14)-C(15)	1.514(5)	N(4)-Eu(1)-N(1)	69.47(8)
O(251)-C(25)	1.213(4)	C(14)-H(14B)	0.99	O(222)-Eu(1)-N(2)	65.39(8)
O(252)-C(25)	1.331(4)	C(14)-H(14A)	0.99	O(422)-Eu(1)-N(2)	141.58(8)
O(252)-H(252)	0.85(6)	C(21)-C(23)	1.532(5)	O(122)-Eu(1)-N(2)	73.13(9)
O(321)-C(32)	1.275(4)	C(21)-C(22)	1.537(4)	O(322)-Eu(1)-N(2)	131.54(8)
O(321)-H(321)	0.56(7)	C(21)-H(21)	0.98(4)	O(5)-Eu(1)-N(2)	125.97(11)
O(322)-C(32)	1.248(4)	C(23)-C(24)	1.527(5)	N(3)-Eu(1)-N(2)	68.63(8)
O(351)-C(35)	1.193(5)	C(23)-H(23B)	0.98(4)	N(4)-Eu(1)-N(2)	105.62(8)
O(352)-C(35)	1.319(4)	C(23)-H(23A)	0.94(4)	N(1)-Eu(1)-N(2)	67.98(9)
O(352)-H(352)	0.91(6)	C(24)-C(25)	1.511(5)	O(222)-Eu(1)-H(5D)	75.7(12)
O(421)-C(42)	1.230(4)	C(24)-H(24B)	0.93(4)	O(422)-Eu(1)-H(5D)	69.9(12)
O(422)-C(42)	1.287(4)	C(24)-H(24A)	0.93(4)	O(122)-Eu(1)-H(5D)	81.2(12)
O(451)-C(45)	1.214(5)	C(31)-C(33)	1.532(4)	O(322)-Eu(1)-H(5D)	63.5(12)
O(452)-C(45)	1.304(5)	C(31)-C(32)	1.539(4)	O(5)-Eu(1)-H(5D)	11.4(11)
O(452)-H(452)	0.77(9)	C(31)-H(31A)	0.93(4)	N(3)-Eu(1)-H(5D)	121.2(12)
O(1SA)-O(1SB)	0.58(2)	C(33)-C(34)	1.539(5)	N(4)-Eu(1)-H(5D)	119.2(11)
O(2SA)-O(2SB)	1.701(15)	C(33)-H(33B)	0.99(4)	N(1)-Eu(1)-H(5D)	132.0(12)
O(3SB)-O(3SA)	0.677(11)	C(33)-H(33A)	1.02(4)	N(2)-Eu(1)-H(5D)	134.8(11)
O(3SB)-O(3SC)	0.915(12)	C(34)-C(35)	1.515(5)	Eu(1)-O(5)-H(5D)	119.0(53)
O(3SA)-O(3SC)	1.52(2)	C(34)-H(34A)	0.95(5)	Eu(1)-O(5)-H(5C)	118.7(66)
N(1)-C(1)	1.488(5)	C(34)-H(34B)	0.96(6)	H(5D)-O(5)-H(5C)	98.3(76)
N(1)-C(11)	1.494(4)	C(41)-C(42)	1.540(4)	O(12B)-O(12A)-O(12C)	153.5(19)
N(1)-C(8)	1.501(4)	C(41)-C(43)	1.542(4)	O(12B)-O(12A)-C(12)	83.6(9)
N(2)-C(3)	1.489(4)	C(41)-H(41)	0.98(4)	O(12C)-O(12A)-C(12)	82.5(14)
N(2)-C(2)	1.497(4)	C(43)-C(44)	1.523(5)	O(12A)-O(12B)-O(12C)	12.9(9)
N(2)-C(21)	1.507(4)	C(43)-H(43B)	0.96(4)	O(12A)-O(12B)-C(12)	67.8(8)
N(3)-C(5)	1.483(4)	C(43)-H(43A)	0.95(4)	O(12C)-O(12B)-C(12)	61.6(7)
N(3)-C(4)	1.501(4)	C(44)-C(45)	1.510(5)	O(12A)-O(12C)-O(12B)	13.7(10)
N(3)-C(31)	1.503(4)	C(44)-H(44A)	0.98(5)	O(12A)-O(12C)-C(12)	70.1(14)
N(4)-C(7)	1.496(4)	C(44)-H(44B)	0.98(4)	O(12B)-O(12C)-C(12)	63.6(8)
N(4)-C(41)	1.500(4)			C(12)-O(122)-Eu(1)	125.7(2)
N(4)-C(6)	1.501(4)	O(222)-Eu(1)-O(422)	145.19(8)	C(15)-O(151)-H(151)	110.9(34)
C(1)-C(2)	1.520(5)	O(222)-Eu(1)-O(122)	84.31(8)	C(22)-O(222)-Eu(1)	126.7(2)
C(1)-H(1A)	0.99	O(422)-Eu(1)-O(122)	85.84(8)	C(25)-O(252)-H(252)	112.5(38)
C(1)-H(1B)	0.99	O(222)-Eu(1)-O(322)	85.83(8)	C(32)-O(321)-H(321)	119.5(93)

C(32)-O(322)-Eu(1)	124.1(2)	N(4)-C(6)-C(5)	112.3(3)	C(24)-C(23)-H(23A)	106.6(23)
C(35)-O(352)-H(352)	113.1(38)	N(4)-C(6)-H(6A)	110.5(21)	C(21)-C(23)-H(23A)	111.5(24)
C(42)-O(422)-Eu(1)	124.6(2)	C(5)-C(6)-H(6A)	107.6(21)	H(23B)-C(23)-H(23A)	106.6(32)
C(45)-O(452)-H(452)	107.8(68)	N(4)-C(6)-H(6B)	110.8(21)	C(25)-C(24)-C(23)	114.5(3)
O(3SA)-O(3SB)-O(3SC)	146.0(19)	C(5)-C(6)-H(6B)	111.2(21)	C(25)-C(24)-H(24B)	106.0(25)
O(3SB)-O(3SA)-O(3SC)	19.6(11)	H(6A)-C(6)-H(6B)	104.1(29)	C(23)-C(24)-H(24B)	109.6(25)
O(3SB)-O(3SC)-O(3SA)	14.4(8)	N(4)-C(7)-C(8)	114.6(3)	C(25)-C(24)-H(24A)	109.0(25)
C(1)-N(1)-C(11)	112.3(3)	N(4)-C(7)-H(7B)	104.7(21)	C(23)-C(24)-H(24A)	111.2(25)
C(1)-N(1)-C(8)	109.0(3)	C(8)-C(7)-H(7B)	110.0(21)	H(24B)-C(24)-H(24A)	106.0(35)
C(11)-N(1)-C(8)	109.8(3)	N(4)-C(7)-H(7A)	112.1(21)	O(251)-C(25)-O(252)	123.5(3)
C(1)-N(1)-Eu(1)	110.0(2)	C(8)-C(7)-H(7A)	108.5(21)	O(251)-C(25)-C(24)	124.9(3)
C(11)-N(1)-Eu(1)	107.1(2)	H(7B)-C(7)-H(7A)	106.6(29)	O(252)-C(25)-C(24)	111.7(3)
C(8)-N(1)-Eu(1)	108.7(2)	N(1)-C(8)-C(7)	112.3(3)	N(3)-C(31)-C(33)	115.1(3)
C(3)-N(2)-C(2)	108.8(3)	N(1)-C(8)-H(8B)	110.1(23)	N(3)-C(31)-C(32)	108.4(2)
C(3)-N(2)-C(21)	111.8(3)	C(7)-C(8)-H(8B)	107.3(23)	C(33)-C(31)-C(32)	115.6(3)
C(2)-N(2)-C(21)	109.4(2)	N(1)-C(8)-H(8A)	107.8(24)	N(3)-C(31)-H(31A)	108.0(23)
C(3)-N(2)-Eu(1)	110.2(2)	C(7)-C(8)-H(8A)	107.2(24)	C(33)-C(31)-H(31A)	103.8(23)
C(2)-N(2)-Eu(1)	111.4(2)	H(8B)-C(8)-H(8A)	112.1(33)	C(32)-C(31)-H(31A)	105.1(23)
C(21)-N(2)-Eu(1)	105.2(2)	N(1)-C(11)-C(12)	109.2(3)	O(322)-C(32)-O(321)	124.2(3)
C(5)-N(3)-C(4)	107.8(2)	N(1)-C(11)-C(13)	115.9(3)	O(322)-C(32)-C(31)	118.3(3)
C(5)-N(3)-C(31)	112.9(2)	C(12)-C(11)-C(13)	113.1(3)	O(321)-C(32)-C(31)	117.4(3)
C(4)-N(3)-C(31)	109.3(2)	N(1)-C(11)-H(11)	105.9(2)	C(31)-C(33)-C(34)	112.7(3)
C(5)-N(3)-Eu(1)	109.7(2)	C(12)-C(11)-H(11)	105.9(2)	C(31)-C(33)-H(33B)	108.8(23)
C(4)-N(3)-Eu(1)	110.4(2)	C(13)-C(11)-H(11)	105.9(2)	C(34)-C(33)-H(33B)	113.7(23)
C(31)-N(3)-Eu(1)	106.8(2)	O(122)-C(12)-O(12A)	120.7(4)	C(31)-C(33)-H(33A)	108.4(24)
C(7)-N(4)-C(41)	112.6(2)	O(122)-C(12)-O(12B)	123.2(4)	C(34)-C(33)-H(33A)	107.3(24)
C(7)-N(4)-C(6)	107.9(2)	O(12A)-C(12)-O(12B)	28.6(3)	H(33B)-C(33)-H(33A)	105.6(33)
C(41)-N(4)-C(6)	108.6(2)	O(122)-C(12)-O(12C)	120.9(6)	C(35)-C(34)-C(33)	114.3(3)
C(7)-N(4)-Eu(1)	109.4(2)	O(12A)-C(12)-O(12C)	27.3(6)	C(35)-C(34)-H(34A)	107.1(31)
C(41)-N(4)-Eu(1)	107.4(2)	O(12B)-C(12)-O(12C)	54.8(7)	C(33)-C(34)-H(34A)	112.4(30)
C(6)-N(4)-Eu(1)	110.9(2)	O(122)-C(12)-C(11)	117.9(3)	C(35)-C(34)-H(34B)	106.9(33)
N(1)-C(1)-C(2)	114.2(3)	O(12A)-C(12)-C(11)	120.9(4)	C(33)-C(34)-H(34B)	111.4(34)
N(1)-C(1)-H(1A)	108.7(2)	O(12B)-C(12)-C(11)	114.3(4)	H(34A)-C(34)-H(34B)	104.0(44)
C(2)-C(1)-H(1A)	108.7(2)	O(12C)-C(12)-C(11)	109.9(7)	O(351)-C(35)-O(352)	123.5(4)
N(1)-C(1)-H(1B)	108.7(2)	C(14)-C(13)-C(11)	112.3(3)	O(351)-C(35)-C(34)	122.7(3)
C(2)-C(1)-H(1B)	108.7(2)	C(14)-C(13)-H(13B)	112.3(25)	O(352)-C(35)-C(34)	113.8(3)
H(1A)-C(1)-H(1B)	107.6	C(11)-C(13)-H(13B)	108.9(25)	N(4)-C(41)-C(42)	112.2(3)
N(2)-C(2)-C(1)	111.5(3)	C(14)-C(13)-H(13A)	109.2(24)	N(4)-C(41)-C(43)	114.3(3)
N(2)-C(2)-H(2A)	109.8(26)	C(11)-C(13)-H(13A)	107.9(24)	C(42)-C(41)-C(43)	112.7(3)
C(1)-C(2)-H(2A)	111.2(26)	H(13B)-C(13)-H(13A)	106.0(34)	N(4)-C(41)-H(41)	106.5(23)
N(2)-C(2)-H(2B)	109.3(26)	C(15)-C(14)-C(13)	108.8(3)	C(42)-C(41)-H(41)	103.9(22)
C(1)-C(2)-H(2B)	107.2(26)	C(15)-C(14)-H(14B)	109.9(2)	C(43)-C(41)-H(41)	106.2(22)
H(2A)-C(2)-H(2B)	107.8(35)	C(13)-C(14)-H(14B)	109.9(2)	O(421)-C(42)-O(422)	124.9(3)
N(2)-C(3)-C(4)	114.3(3)	C(15)-C(14)-H(14A)	109.9(2)	O(421)-C(42)-C(41)	117.8(3)
N(2)-C(3)-H(3B)	108.7(2)	C(13)-C(14)-H(14A)	109.9(2)	O(422)-C(42)-C(41)	117.2(3)
C(4)-C(3)-H(3B)	108.7(2)	H(14B)-C(14)-H(14A)	108.3	C(44)-C(43)-C(41)	114.3(3)
N(2)-C(3)-H(3A)	108.7(2)	O(152)-C(15)-O(151)	123.2(3)	C(44)-C(43)-H(43B)	106.1(24)
C(4)-C(3)-H(3A)	108.7(2)	O(152)-C(15)-C(14)	123.3(3)	C(41)-C(43)-H(43B)	109.7(24)
H(3B)-C(3)-H(3A)	107.6	O(151)-C(15)-C(14)	113.4(3)	C(44)-C(43)-H(43A)	111.9(26)
N(3)-C(4)-C(3)	112.7(3)	N(2)-C(21)-C(23)	115.0(3)	C(41)-C(43)-H(43A)	107.2(26)
N(3)-C(4)-H(4B)	111.5(21)	N(2)-C(21)-C(22)	108.7(2)	H(43B)-C(43)-H(43A)	107.6(35)
C(3)-C(4)-H(4B)	105.0(21)	C(23)-C(21)-C(22)	113.7(3)	C(45)-C(44)-C(43)	113.6(3)
N(3)-C(4)-H(4A)	110.5(22)	N(2)-C(21)-H(21)	103.5(23)	C(45)-C(44)-H(44A)	109.9(27)
C(3)-C(4)-H(4A)	111.6(22)	C(23)-C(21)-H(21)	107.8(23)	C(43)-C(44)-H(44A)	110.0(26)
H(4B)-C(4)-H(4A)	105.1(30)	C(22)-C(21)-H(21)	107.3(23)	C(45)-C(44)-H(44B)	107.6(25)
N(3)-C(5)-C(6)	114.3(3)	O(221)-C(22)-O(222)	125.1(3)	C(43)-C(44)-H(44B)	107.6(25)
N(3)-C(5)-H(5B)	112.0(21)	O(221)-C(22)-C(21)	118.6(3)	H(44A)-C(44)-H(44B)	107.8(36)
C(6)-C(5)-H(5B)	106.8(21)	O(222)-C(22)-C(21)	116.3(3)	O(451)-C(45)-O(452)	123.4(4)
N(3)-C(5)-H(5A)	111.3(21)	C(24)-C(23)-C(21)	113.3(3)	O(451)-C(45)-C(44)	123.9(3)
C(6)-C(5)-H(5A)	107.4(21)	C(24)-C(23)-H(23B)	108.3(22)	O(452)-C(45)-C(44)	112.8(3)
H(5B)-C(5)-H(5A)	104.5(29)	C(21)-C(23)-H(23B)	110.3(22)		

© 2000 American Chemical Society, J. Am. Chem. Soc., Woods ja994492v Supporting Info Page 9

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 97srv139. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Eu(1)	12(1)	11(1)	13(1)	2(1)	5(1)	3(1)
O(5)	24(2)	17(1)	48(2)	6(1)	18(2)	9(1)
O(122)	22(1)	16(1)	21(1)	-1(1)	13(1)	0(1)
O(151)	20(1)	24(1)	20(1)	2(1)	3(1)	1(1)
O(152)	27(1)	27(1)	27(1)	8(1)	7(1)	9(1)
O(221)	19(1)	25(1)	26(1)	14(1)	4(1)	0(1)
O(222)	16(1)	20(1)	15(1)	6(1)	5(1)	5(1)
O(251)	40(2)	22(1)	30(1)	8(1)	12(1)	7(1)
O(252)	34(2)	21(1)	29(1)	2(1)	13(1)	12(1)
O(321)	29(2)	17(1)	25(1)	1(1)	-10(1)	6(1)
O(322)	15(1)	14(1)	19(1)	3(1)	3(1)	7(1)
O(351)	58(2)	31(2)	106(3)	38(2)	59(2)	24(2)
O(352)	47(2)	23(1)	58(2)	20(1)	34(2)	23(1)
O(421)	45(2)	29(1)	28(1)	14(1)	15(1)	28(1)
O(422)	24(1)	14(1)	18(1)	4(1)	9(1)	10(1)
O(451)	55(2)	26(2)	35(2)	4(1)	-3(1)	19(1)
O(452)	53(2)	48(2)	36(2)	-8(2)	-16(2)	31(2)
N(1)	16(1)	14(1)	17(1)	1(1)	7(1)	1(1)
N(2)	14(1)	20(1)	15(1)	5(1)	5(1)	4(1)
N(3)	14(1)	12(1)	15(1)	4(1)	3(1)	6(1)
N(4)	15(1)	13(1)	15(1)	5(1)	6(1)	5(1)
C(1)	17(2)	22(2)	23(2)	4(1)	7(1)	2(1)
C(2)	17(2)	28(2)	19(2)	5(1)	4(1)	2(1)
C(3)	18(2)	27(2)	16(2)	6(1)	4(1)	9(1)
C(4)	19(2)	19(2)	18(2)	7(1)	6(1)	12(1)
C(5)	17(2)	16(2)	18(2)	4(1)	8(1)	8(1)
C(6)	21(2)	15(2)	15(2)	3(1)	7(1)	10(1)
C(7)	17(2)	20(2)	17(2)	6(1)	8(1)	8(1)
C(8)	17(2)	17(2)	21(2)	7(1)	10(1)	2(1)
C(11)	19(2)	16(2)	20(2)	1(1)	8(1)	1(1)
C(12)	34(2)	22(2)	24(2)	-3(2)	20(2)	-2(2)
C(13)	19(2)	18(2)	31(2)	4(2)	7(2)	2(1)
C(14)	23(2)	20(2)	38(2)	2(2)	8(2)	5(2)
C(15)	21(2)	16(2)	28(2)	2(1)	5(1)	7(1)
C(21)	14(1)	17(2)	15(2)	4(1)	5(1)	4(1)
C(22)	16(2)	17(2)	15(2)	2(1)	5(1)	4(1)
C(23)	19(2)	22(2)	18(2)	6(1)	5(1)	11(1)
C(24)	24(2)	20(2)	18(2)	7(1)	6(1)	10(1)
C(25)	24(2)	21(2)	16(2)	4(1)	1(1)	8(1)
C(31)	16(2)	13(1)	18(2)	4(1)	4(1)	6(1)
C(32)	13(1)	16(2)	18(2)	5(1)	4(1)	6(1)
C(33)	21(2)	12(2)	28(2)	5(1)	10(1)	8(1)
C(34)	23(2)	13(2)	49(2)	8(2)	17(2)	5(1)
C(35)	22(2)	19(2)	28(2)	5(1)	9(1)	6(1)
C(41)	19(2)	13(1)	15(2)	3(1)	6(1)	8(1)
C(42)	18(2)	13(1)	21(2)	5(1)	7(1)	6(1)
C(43)	22(2)	19(2)	19(2)	8(1)	10(1)	9(1)
C(44)	37(2)	27(2)	19(2)	11(2)	12(2)	19(2)
C(45)	35(2)	30(2)	17(2)	7(1)	8(2)	19(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 97srv139.

	x	y	z	U(eq)
H(5D)	1313(67)	2873(52)	2657(37)	39(19)
H(5C)	2015(100)	3752(80)	3077(56)	117(33)
H(151)	11783(67)	9708(50)	4193(36)	56(16)
H(252)	6316(65)	4528(51)	7502(36)	55(16)
H(321)	315(102)	-310(76)	250(56)	103(34)
H(352)	2288(70)	-4471(55)	711(39)	68(18)
H(452)	753(106)	614(79)	-2382(60)	125(36)
H(1A)	9215(4)	4814(3)	3632(2)	28
H(1B)	8333(4)	3507(3)	2948(2)	28
H(2A)	7840(49)	4209(38)	4620(29)	28(11)
H(2B)	8762(54)	3416(39)	4390(29)	34(12)
H(3B)	7197(4)	1272(3)	3898(2)	25
H(3A)	7406(4)	1745(3)	3072(2)	25
H(4B)	5614(42)	-172(32)	2599(23)	12(9)
H(4A)	4540(45)	94(34)	3161(25)	18(9)
H(5B)	5100(41)	-15(33)	1070(24)	12(9)
H(5A)	6288(42)	1172(30)	1677(22)	7(8)
H(6A)	5428(43)	1337(32)	312(24)	16(9)
H(6B)	3760(41)	904(30)	383(22)	5(8)
H(7B)	7231(42)	2919(32)	1603(23)	12(9)
H(7A)	6970(42)	3512(32)	849(24)	14(9)
H(8B)	8286(47)	4996(34)	2147(25)	19(10)
H(8A)	6561(48)	4964(36)	1859(27)	24(10)
H(11)	6402(4)	5831(3)	3102(2)	25
H(13B)	9255(50)	6504(37)	4422(29)	28(11)
H(13A)	9227(47)	6572(35)	3457(27)	22(10)
H(14B)	8031(4)	7922(3)	3564(3)	36
H(14A)	7943(4)	7857(3)	4532(3)	36
H(21)	5786(45)	3171(36)	4873(26)	20(10)
H(23B)	7830(46)	2536(33)	5407(24)	16(9)
H(23A)	6534(44)	1284(36)	5141(25)	18(10)
H(24B)	6976(47)	2127(35)	6601(26)	21(10)
H(24A)	5363(51)	1931(37)	6152(27)	24(10)
H(31A)	2338(43)	-321(32)	2177(25)	14(9)
H(33B)	2684(46)	-1498(35)	636(27)	22(10)
H(33A)	3498(50)	-1593(37)	1565(28)	28(11)
H(34A)	813(59)	-2255(44)	1767(34)	45(14)
H(34B)	214(67)	-2566(49)	779(37)	57(16)
H(41)	2972(45)	2241(34)	304(25)	17(9)
H(43B)	5123(47)	2738(36)	-382(26)	22(10)
H(43A)	5219(50)	4000(39)	-41(28)	28(11)
H(44A)	2533(53)	3233(40)	-947(29)	34(12)
H(44B)	3719(50)	3198(38)	-1494(29)	30(11)

Table 6. Selected torsion angles [°] for 97srv139.

N(1)-C(1)-C(2)-N(2)	59.5(4)
N(2)-C(3)-C(4)-N(3)	58.4(4)
N(3)-C(5)-C(6)-N(4)	58.7(4)
N(4)-C(7)-C(8)-N(1)	60.9(4)
N(1)-C(11)-C(12)-O(122)	-38.5(5)
N(2)-C(21)-C(22)-O(222)	-39.7(4)
N(3)-C(31)-C(32)-O(322)	-40.6(4)
N(4)-C(41)-C(42)-O(422)	-17.5(4)

Table 1. Crystal data and structure refinement for 98srv107.

Identification code	98srv107	
Empirical formula	C28 H49 Gd N4 O20	
Formula weight	918.96	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P(-1)	
Unit cell dimensions	a = 9.6460(5) Å	α= 102.652(4)°.
	b = 12.6915(7) Å	β= 101.192(4)°.
	c = 16.2000(11) Å	γ = 110.446(3)°.
Volume	1731.9(2) $Å^3$	
Z	2	
Density (calculated)	1.762 Mg/m^3	
Absorption coefficient	2.007 mm^{-1}	
F(000)	938	
Crystal size	0.34 x 0.32 x 0.18 mm^3	
Theta range for data collection	1.35 to 27.50°.	
Index ranges	-12<=h<=12, -16<=k<=16, -13<=l<=21	
Reflections collected	14872	
Independent reflections	7843 [R(int) = 0.0251]	
Absorption correction	Multiscan - SADABS	
Max. and min. transmission	0.610200 and 0.490919	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7843 / 0 / 651	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0211, wR2 = 0.0511	
R indices (all data)	R1 = 0.0242, wR2 = 0.0523	
Extinction coefficient	none	
Largest diff. peak and hole	0.656 and -0.714 $e.Å^{-3}$	

© 2000 American Chemical Society, J. Am. Chem. Soc., Woods ja994492v Supporting Info Page 13

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 98srv107. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Gd(1)	806(1)	-7765(1)	2335(1)	11(1)
O(5)	3017(2)	-8109(2)	2045(2)	28(1)
O(121)	1991(2)	-9421(2)	4368(1)	28(1)
O(122)	1205(2)	-9092(1)	3097(1)	18(1)
O(151)	2317(3)	-5815(2)	6268(1)	40(1)
O(152)	3802(3)	-6310(2)	7201(1)	48(1)
O(22A)	-1636(5)	-11099(3)	40(2)	19(1)
O(22B)	-2157(6)	-10901(4)	-60(3)	14(1)
O(22C)	-1326(11)	-11326(8)	243(6)	24(2)
O(222)	-45(2)	-9382(1)	1015(1)	22(1)
O(251)	-5817(2)	-14221(2)	-315(1)	25(1)
O(252)	-5855(2)	-14076(2)	1073(1)	25(1)
O(321)	1460(2)	-5793(2)	375(1)	25(1)
O(322)	1753(2)	-6607(1)	1454(1)	16(1)
O(352)	-1132(2)	-8810(2)	-2265(1)	29(1)
O(351)	-2678(2)	-9471(2)	-1454(1)	33(1)
O(421)	4284(2)	-4548(2)	4555(1)	27(1)
O(422)	3028(2)	-6319(1)	3524(1)	16(1)
O(452)	2765(2)	-1238(2)	4237(2)	37(1)
O(451)	4633(3)	-612(2)	3626(2)	58(1)
N(1)	-5(2)	-7593(2)	3822(1)	14(1)
N(2)	-2007(2)	-9445(2)	2043(1)	17(1)
N(3)	-1390(2)	-7547(2)	1167(1)	16(1)
N(4)	625(2)	-5708(2)	2923(1)	13(1)
C(1)	-1688(2)	-8373(2)	3607(1)	16(1)
C(2)	-2221(3)	-9571(2)	2914(2)	18(1)
C(3)	-3228(2)	-9112(2)	1605(2)	20(1)
C(4)	-2878(3)	-8631(2)	854(2)	22(1)
C(5)	-1693(3)	-6507(2)	1583(2)	19(1)
C(6)	-244(3)	-5438(2)	2185(1)	17(1)
C(7)	-238(2)	-5769(2)	3594(1)	16(1)

C(8)	227(3)	-6352(2)	4258(1)	16(1)
C(11)	1024(2)	-7930(2)	4435(1)	15(1)
C(12)	1421(2)	-8908(2)	3932(1)	17(1)
C(13)	456(3)	-8195(2)	5222(2)	19(1)
C(14)	1751(3)	-7875(2)	6065(2)	25(1)
C(15)	2644(3)	-6559(2)	6512(2)	25(1)
C(21)	-2060(3)	-10578(2)	1487(2)	20(1)
C(22)	-1232(3)	-10322(2)	791(2)	31(1)
C(23)	-3662(3)	-11614(2)	1101(2)	23(1)
C(24)	-3558(3)	-12818(2)	882(2)	28(1)
C(25)	-5175(3)	-13786(2)	484(2)	21(1)
C(31)	-760(2)	-7391(2)	404(1)	15(1)
C(32)	954(2)	-6515(2)	769(1)	16(1)
C(33)	-1719(3)	-7091(2)	-306(2)	19(1)
C(34)	-1394(3)	-7361(2)	-1197(2)	20(1)
C(35)	-1826(3)	-8657(2)	-1642(2)	21(1)
C(41)	2264(2)	-4778(2)	3297(1)	16(1)
C(42)	3254(2)	-5263(2)	3832(1)	16(1)
C(43)	2426(3)	-3536(2)	3767(2)	21(1)
C(44)	3905(3)	-2552(2)	3755(2)	31(1)
C(45)	3817(3)	-1363(2)	3866(2)	25(1)
O(1WA)	5010(4)	-4153(3)	8197(2)	30(1)
O(1WB)	4657(7)	-4022(6)	8058(4)	20(1)
O(2WA)	-4005(7)	-6685(5)	3517(5)	30(1)
O(2WB)	-3421(9)	-6303(7)	4071(5)	42(2)
O(2WC)	-4051(6)	-6877(5)	3133(4)	27(1)
O(3WA)	5147(9)	-1421(7)	6922(5)	90(2)
O(3WB)	4797(8)	-1784(6)	5791(4)	76(2)

Table 3. Bond lengths [Å] and angles [°] for 98srv107.

Gd(1)-O(322)	2.3492(15)
Gd(1)-O(222)	2.383(2)
Gd(1)-O(122)	2.385(2)
Gd(1)-O(422)	2.4028(15)
Gd(1)-O(5)	2.432(2)
Gd(1)-N(4)	2.655(2)
Gd(1)-N(1)	2.662(2)
Gd(1)-N(2)	2.674(2)
Gd(1)-N(3)	2.689(2)
O(5)-H(5D)	0.75(6)
O(5)-H(5C)	0.68(5)
O(121)-C(12)	1.235(3)
O(122)-C(12)	1.282(3)
O(151)-C(15)	1.213(3)
O(152)-C(15)	1.307(3)
O(152)-H(152)	1.03(7)
O(22A)-O(22C)	0.587(9)
O(22A)-O(22B)	0.645(5)
O(22A)-C(22)	1.275(4)
O(22B)-O(22C)	1.199(11)
O(22B)-C(22)	1.363(6)
O(22C)-C(22)	1.346(9)
O(222)-C(22)	1.250(3)
O(251)-C(25)	1.225(3)
O(252)-C(25)	1.305(3)
O(252)-H(252)	0.86(4)
O(321)-C(32)	1.244(3)
O(322)-C(32)	1.275(3)
O(352)-C(35)	1.330(3)
O(352)-H(352)	0.83(5)
O(351)-C(35)	1.216(3)
O(421)-C(42)	1.280(3)
O(422)-C(42)	1.246(3)
O(452)-C(45)	1.313(3)

O(452)-H(452)	0.98(5)
O(451)-C(45)	1.198(3)
N(1)-C(8)	1.495(3)
N(1)-C(1)	1.497(3)
N(1)-C(11)	1.501(3)
N(2)-C(3)	1.492(3)
N(2)-C(21)	1.498(3)
N(2)-C(2)	1.500(3)
N(3)-C(5)	1.496(3)
N(3)-C(4)	1.498(3)
N(3)-C(31)	1.500(3)
N(4)-C(7)	1.491(3)
N(4)-C(6)	1.497(3)
N(4)-C(41)	1.507(3)
C(1)-C(2)	1.522(3)
C(1)-H(1B)	0.95(3)
C(1)-H(1A)	0.95(2)
C(2)-H(2B)	1.00(3)
C(2)-H(2A)	1.00(3)
C(3)-C(4)	1.520(3)
C(3)-H(3A)	0.94(3)
C(3)-H(3B)	0.95(3)
C(4)-H(4B)	0.93(3)
C(4)-H(4A)	1.00(3)
C(5)-C(6)	1.520(3)
C(5)-H(5B)	0.95(3)
C(5)-H(5A)	1.05(3)
C(6)-H(6B)	0.98(3)
C(6)-H(6A)	0.99(3)
C(7)-C(8)	1.516(3)
C(7)-H(7A)	0.98(2)
C(7)-H(7B)	0.99(3)
C(8)-H(8A)	1.01(3)
C(8)-H(8B)	1.02(3)
C(11)-C(12)	1.538(3)
C(11)-C(13)	1.538(3)

C(11)-H(11)	0.98(3)
C(13)-C(14)	1.527(3)
C(13)-H(13A)	0.99(3)
C(13)-H(13B)	1.02(3)
C(14)-C(15)	1.510(4)
C(14)-H(14A)	1.04(3)
C(14)-H(14B)	0.97(3)
C(21)-C(22)	1.529(3)
C(21)-C(23)	1.534(3)
C(21)-H(21)	0.95(2)
C(23)-C(24)	1.535(3)
C(23)-H(23A)	0.99(3)
C(23)-H(23B)	0.98(3)
C(24)-C(25)	1.511(3)
C(24)-H(24A)	0.97(2)
C(24)-H(24B)	0.98(3)
C(31)-C(33)	1.532(3)
C(31)-C(32)	1.539(3)
C(31)-H(31)	0.97(3)
C(33)-C(34)	1.528(3)
C(33)-H(33B)	0.95(3)
C(33)-H(33A)	0.94(3)
C(34)-C(35)	1.512(3)
C(34)-H(34A)	0.95(3)
C(34)-H(34B)	0.93(3)
C(41)-C(43)	1.531(3)
C(41)-C(42)	1.538(3)
C(41)-H(41)	0.99(3)
C(43)-C(44)	1.540(3)
C(43)-H(43B)	1.02(3)
C(43)-H(43A)	0.99(3)
C(44)-C(45)	1.515(3)
C(44)-H(42B)	1.01(4)
C(44)-H(42A)	0.92(4)
O(2WA)-O(2WC)	0.604(6)
O(2WA)-O(2WB)	0.883(8)

O(2WB)-O(2WC)	1.434(9)
O(3WA)-O(3WB)	1.722(9)
O(322)-Gd(1)-O(222)	84.22(5)
O(322)-Gd(1)-O(122)	144.86(5)
O(222)-Gd(1)-O(122)	85.82(6)
O(322)-Gd(1)-O(422)	85.68(5)
O(222)-Gd(1)-O(422)	144.47(5)
O(122)-Gd(1)-O(422)	83.14(5)
O(322)-Gd(1)-O(5)	72.57(6)
O(222)-Gd(1)-O(5)	70.33(7)
O(122)-Gd(1)-O(5)	72.34(6)
O(422)-Gd(1)-O(5)	74.14(6)
O(322)-Gd(1)-N(4)	72.59(5)
O(222)-Gd(1)-N(4)	140.73(6)
O(122)-Gd(1)-N(4)	130.66(5)
O(422)-Gd(1)-N(4)	66.02(5)
O(5)-Gd(1)-N(4)	128.11(6)
O(322)-Gd(1)-N(1)	140.92(5)
O(222)-Gd(1)-N(1)	131.61(5)
O(122)-Gd(1)-N(1)	65.28(5)
O(422)-Gd(1)-N(1)	72.43(5)
O(5)-Gd(1)-N(1)	128.11(6)
N(4)-Gd(1)-N(1)	69.03(5)
O(322)-Gd(1)-N(2)	130.09(5)
O(222)-Gd(1)-N(2)	65.47(5)
O(122)-Gd(1)-N(2)	74.17(6)
O(422)-Gd(1)-N(2)	141.16(5)
O(5)-Gd(1)-N(2)	125.48(6)
N(4)-Gd(1)-N(2)	106.36(5)
N(1)-Gd(1)-N(2)	69.56(5)
O(322)-Gd(1)-N(3)	65.51(5)
O(222)-Gd(1)-N(3)	72.95(6)
O(122)-Gd(1)-N(3)	141.63(5)
O(422)-Gd(1)-N(3)	131.78(5)
O(5)-Gd(1)-N(3)	125.97(6)

N(4)-Gd(1)-N(3)	68.72(5)
N(1)-Gd(1)-N(3)	105.89(5)
N(2)-Gd(1)-N(3)	68.03(5)
Gd(1)-O(5)-H(5D)	122.4(39)
Gd(1)-O(5)-H(5C)	118.4(42)
H(5D)-O(5)-H(5C)	102.2(52)
C(12)-O(122)-Gd(1)	124.52(13)
C(15)-O(152)-H(152)	106.8(36)
O(22C)-O(22A)-O(22B)	153.7(13)
O(22C)-O(22A)-C(22)	83.9(10)
O(22B)-O(22A)-C(22)	83.6(6)
O(22A)-O(22B)-O(22C)	12.5(6)
O(22A)-O(22B)-C(22)	68.4(6)
O(22C)-O(22B)-C(22)	63.0(5)
O(22A)-O(22C)-O(22B)	13.8(7)
O(22A)-O(22C)-C(22)	70.4(10)
O(22B)-O(22C)-C(22)	64.5(5)
C(22)-O(222)-Gd(1)	125.88(14)
C(25)-O(252)-H(252)	114.6(24)
C(32)-O(322)-Gd(1)	126.64(13)
C(35)-O(352)-H(352)	109.8(31)
C(42)-O(422)-Gd(1)	124.31(13)
C(45)-O(452)-H(452)	113.2(30)
C(8)-N(1)-C(1)	107.9(2)
C(8)-N(1)-C(11)	108.7(2)
C(1)-N(1)-C(11)	112.8(2)
C(8)-N(1)-Gd(1)	110.87(12)
C(1)-N(1)-Gd(1)	109.20(12)
C(11)-N(1)-Gd(1)	107.41(11)
C(3)-N(2)-C(21)	112.2(2)
C(3)-N(2)-C(2)	108.8(2)
C(21)-N(2)-C(2)	109.5(2)
C(3)-N(2)-Gd(1)	110.29(12)
C(21)-N(2)-Gd(1)	107.13(12)
C(2)-N(2)-Gd(1)	108.81(12)
C(5)-N(3)-C(4)	108.4(2)

C(5)-N(3)-C(31)	111.8(2)
C(4)-N(3)-C(31)	109.8(2)
C(5)-N(3)-Gd(1)	110.20(12)
C(4)-N(3)-Gd(1)	111.33(13)
C(31)-N(3)-Gd(1)	105.36(12)
C(7)-N(4)-C(6)	107.5(2)
C(7)-N(4)-C(41)	112.7(2)
C(6)-N(4)-C(41)	109.7(2)
C(7)-N(4)-Gd(1)	109.45(12)
C(6)-N(4)-Gd(1)	110.83(12)
C(41)-N(4)-Gd(1)	106.69(11)
N(1)-C(1)-C(2)	114.5(2)
N(1)-C(1)-H(1B)	105.9(16)
C(2)-C(1)-H(1B)	110.2(16)
N(1)-C(1)-H(1A)	111.3(15)
C(2)-C(1)-H(1A)	108.5(16)
H(1B)-C(1)-H(1A)	106.2(21)
N(2)-C(2)-C(1)	111.8(2)
N(2)-C(2)-H(2B)	108.8(15)
C(1)-C(2)-H(2B)	108.4(16)
N(2)-C(2)-H(2A)	110.9(14)
C(1)-C(2)-H(2A)	106.7(15)
H(2B)-C(2)-H(2A)	110.2(22)
N(2)-C(3)-C(4)	113.4(2)
N(2)-C(3)-H(3A)	110.2(17)
C(4)-C(3)-H(3A)	110.3(16)
N(2)-C(3)-H(3B)	107.8(15)
C(4)-C(3)-H(3B)	108.8(16)
H(3A)-C(3)-H(3B)	106.0(22)
N(3)-C(4)-C(3)	111.8(2)
N(3)-C(4)-H(4B)	108.8(19)
C(3)-C(4)-H(4B)	112.0(19)
N(3)-C(4)-H(4A)	110.0(15)
C(3)-C(4)-H(4A)	109.3(14)
H(4B)-C(4)-H(4A)	104.8(23)
N(3)-C(5)-C(6)	114.0(2)

N(3)-C(5)-H(5B)	112.3(17)
C(6)-C(5)-H(5B)	107.1(18)
N(3)-C(5)-H(5A)	109.4(15)
C(6)-C(5)-H(5A)	111.0(15)
H(5B)-C(5)-H(5A)	102.6(22)
N(4)-C(6)-C(5)	112.7(2)
N(4)-C(6)-H(6B)	111.6(15)
C(5)-C(6)-H(6B)	106.9(15)
N(4)-C(6)-H(6A)	107.2(15)
C(5)-C(6)-H(6A)	112.3(15)
H(6B)-C(6)-H(6A)	106.1(22)
N(4)-C(7)-C(8)	114.1(2)
N(4)-C(7)-H(7A)	107.7(14)
C(8)-C(7)-H(7A)	108.3(14)
N(4)-C(7)-H(7B)	113.0(15)
C(8)-C(7)-H(7B)	109.7(15)
H(7A)-C(7)-H(7B)	103.4(20)
N(1)-C(8)-C(7)	112.3(2)
N(1)-C(8)-H(8A)	110.4(16)
C(7)-C(8)-H(8A)	109.6(16)
N(1)-C(8)-H(8B)	109.7(16)
C(7)-C(8)-H(8B)	106.8(15)
H(8A)-C(8)-H(8B)	107.9(21)
N(1)-C(11)-C(12)	112.0(2)
N(1)-C(11)-C(13)	114.4(2)
C(12)-C(11)-C(13)	112.9(2)
N(1)-C(11)-H(11)	104.8(15)
C(12)-C(11)-H(11)	104.0(14)
C(13)-C(11)-H(11)	107.8(14)
O(121)-C(12)-O(122)	124.8(2)
O(121)-C(12)-C(11)	117.5(2)
O(122)-C(12)-C(11)	117.5(2)
C(14)-C(13)-C(11)	114.3(2)
C(14)-C(13)-H(13A)	107.2(17)
C(11)-C(13)-H(13A)	109.0(17)
C(14)-C(13)-H(13B)	109.0(16)

C(11)-C(13)-H(13B)	109.7(15)
H(13A)-C(13)-H(13B)	107.3(23)
C(15)-C(14)-C(13)	113.7(2)
C(15)-C(14)-H(14A)	110.0(18)
C(13)-C(14)-H(14A)	110.2(18)
C(15)-C(14)-H(14B)	108.3(19)
C(13)-C(14)-H(14B)	109.0(19)
H(14A)-C(14)-H(14B)	105.2(25)
O(151)-C(15)-O(152)	123.6(3)
O(151)-C(15)-C(14)	124.0(2)
O(152)-C(15)-C(14)	112.4(2)
N(2)-C(21)-C(22)	109.2(2)
N(2)-C(21)-C(23)	115.8(2)
C(22)-C(21)-C(23)	113.5(2)
N(2)-C(21)-H(21)	105.3(14)
C(22)-C(21)-H(21)	105.5(13)
C(23)-C(21)-H(21)	106.6(14)
O(222)-C(22)-O(22A)	120.6(2)
O(222)-C(22)-O(22C)	120.8(4)
O(22A)-C(22)-O(22C)	25.7(4)
O(222)-C(22)-O(22B)	123.6(3)
O(22A)-C(22)-O(22B)	28.0(2)
O(22C)-C(22)-O(22B)	52.6(5)
O(222)-C(22)-C(21)	117.9(2)
O(22A)-C(22)-C(21)	121.1(2)
O(22C)-C(22)-C(21)	111.3(4)
O(22B)-C(22)-C(21)	113.9(3)
C(21)-C(23)-C(24)	112.2(2)
C(21)-C(23)-H(23A)	111.2(18)
C(24)-C(23)-H(23A)	109.7(18)
C(21)-C(23)-H(23B)	107.3(19)
C(24)-C(23)-H(23B)	107.9(20)
H(23A)-C(23)-H(23B)	108.3(25)
C(25)-C(24)-C(23)	108.9(2)
C(25)-C(24)-H(24A)	109.0(14)
C(23)-C(24)-H(24A)	113.4(14)

C(25)-C(24)-H(24B)	108.3(20)
C(23)-C(24)-H(24B)	113.3(20)
H(24A)-C(24)-H(24B)	103.5(23)
O(251)-C(25)-O(252)	123.0(2)
O(251)-C(25)-C(24)	123.3(2)
O(252)-C(25)-C(24)	113.6(2)
N(3)-C(31)-C(33)	115.4(2)
N(3)-C(31)-C(32)	108.8(2)
C(33)-C(31)-C(32)	113.5(2)
N(3)-C(31)-H(31)	105.1(16)
C(33)-C(31)-H(31)	107.3(16)
C(32)-C(31)-H(31)	106.0(16)
O(321)-C(32)-O(322)	125.2(2)
O(321)-C(32)-C(31)	118.5(2)
O(322)-C(32)-C(31)	116.3(2)
C(34)-C(33)-C(31)	113.4(2)
C(34)-C(33)-H(33B)	107.8(15)
C(31)-C(33)-H(33B)	110.3(16)
C(34)-C(33)-H(33A)	108.1(18)
C(31)-C(33)-H(33A)	106.4(18)
H(33B)-C(33)-H(33A)	110.8(24)
C(35)-C(34)-C(33)	114.5(2)
C(35)-C(34)-H(34A)	105.4(18)
C(33)-C(34)-H(34A)	111.1(17)
C(35)-C(34)-H(34B)	106.7(18)
C(33)-C(34)-H(34B)	111.9(17)
H(34A)-C(34)-H(34B)	106.8(25)
O(351)-C(35)-O(352)	123.3(2)
O(351)-C(35)-C(34)	125.0(2)
O(352)-C(35)-C(34)	111.7(2)
N(4)-C(41)-C(43)	115.0(2)
N(4)-C(41)-C(42)	108.5(2)
C(43)-C(41)-C(42)	115.6(2)
N(4)-C(41)-H(41)	109.2(16)
C(43)-C(41)-H(41)	103.0(17)
C(42)-C(41)-H(41)	104.7(16)

O(422)-C(42)-O(421)	124.1(2)
O(422)-C(42)-C(41)	118.1(2)
O(421)-C(42)-C(41)	117.8(2)
C(41)-C(43)-C(44)	112.8(2)
C(41)-C(43)-H(43B)	108.2(16)
C(44)-C(43)-H(43B)	107.4(15)
C(41)-C(43)-H(43A)	108.5(18)
C(44)-C(43)-H(43A)	112.4(18)
H(43B)-C(43)-H(43A)	107.3(23)
C(45)-C(44)-C(43)	114.1(2)
C(45)-C(44)-H(42B)	107.3(23)
C(43)-C(44)-H(42B)	111.3(23)
C(45)-C(44)-H(42A)	108.9(24)
C(43)-C(44)-H(42A)	112.2(25)
H(42B)-C(44)-H(42A)	102.4(30)
O(451)-C(45)-O(452)	123.5(2)
O(451)-C(45)-C(44)	122.4(2)
O(452)-C(45)-C(44)	114.2(2)
O(2WC)-O(2WA)-O(2WB)	148.9(12)
O(2WA)-O(2WB)-O(2WC)	12.6(5)
O(2WA)-O(2WC)-O(2WB)	18.6(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 98srv107. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Gd(1)	11(1)	10(1)	12(1)	2(1)	5(1)	4(1)
O(5)	24(1)	18(1)	45(1)	7(1)	19(1)	10(1)
O(121)	44(1)	28(1)	27(1)	13(1)	14(1)	27(1)
O(122)	25(1)	15(1)	18(1)	5(1)	9(1)	10(1)
O(151)	52(1)	25(1)	33(1)	5(1)	-5(1)	19(1)
O(152)	52(1)	44(1)	35(1)	-6(1)	-15(1)	29(1)
O(222)	21(1)	16(1)	21(1)	0(1)	12(1)	1(1)
O(251)	24(1)	25(1)	24(1)	7(1)	6(1)	10(1)
O(252)	20(1)	25(1)	21(1)	3(1)	4(1)	3(1)
O(321)	21(1)	25(1)	24(1)	13(1)	4(1)	1(1)
O(322)	13(1)	18(1)	17(1)	6(1)	5(1)	5(1)
O(352)	34(1)	23(1)	31(1)	2(1)	14(1)	12(1)
O(351)	39(1)	23(1)	31(1)	8(1)	13(1)	6(1)
O(421)	27(1)	16(1)	25(1)	-1(1)	-9(1)	6(1)
O(422)	14(1)	13(1)	21(1)	4(1)	3(1)	6(1)
O(452)	48(1)	24(1)	58(1)	19(1)	34(1)	23(1)
O(451)	58(2)	31(1)	114(2)	39(1)	60(2)	24(1)
N(1)	17(1)	12(1)	14(1)	3(1)	5(1)	7(1)
N(2)	17(1)	15(1)	15(1)	2(1)	7(1)	3(1)
N(3)	12(1)	18(1)	15(1)	4(1)	5(1)	3(1)
N(4)	12(1)	13(1)	15(1)	4(1)	3(1)	6(1)
C(1)	15(1)	18(1)	17(1)	4(1)	7(1)	6(1)
C(2)	18(1)	16(1)	19(1)	5(1)	9(1)	3(1)
C(3)	13(1)	22(1)	20(1)	5(1)	5(1)	2(1)
C(4)	14(1)	25(1)	17(1)	5(1)	3(1)	0(1)
C(5)	16(1)	25(1)	17(1)	6(1)	4(1)	11(1)
C(6)	20(1)	18(1)	16(1)	7(1)	7(1)	11(1)
C(7)	18(1)	14(1)	16(1)	3(1)	6(1)	9(1)
C(8)	20(1)	13(1)	14(1)	2(1)	5(1)	8(1)
C(11)	18(1)	14(1)	15(1)	5(1)	6(1)	8(1)
C(12)	17(1)	11(1)	22(1)	5(1)	8(1)	5(1)

C(13)	24(1)	19(1)	19(1)	8(1)	10(1)	10(1)
C(14)	36(1)	27(1)	19(1)	11(1)	9(1)	18(1)
C(15)	33(1)	30(1)	18(1)	6(1)	8(1)	19(1)
C(21)	19(1)	15(1)	21(1)	1(1)	10(1)	2(1)
C(22)	37(1)	19(1)	26(1)	-2(1)	21(1)	0(1)
C(23)	17(1)	17(1)	28(1)	4(1)	7(1)	0(1)
C(24)	20(1)	20(1)	37(1)	2(1)	7(1)	3(1)
C(25)	20(1)	17(1)	27(1)	4(1)	6(1)	9(1)
C(31)	14(1)	17(1)	14(1)	4(1)	4(1)	5(1)
C(32)	15(1)	15(1)	16(1)	4(1)	6(1)	5(1)
C(33)	19(1)	20(1)	17(1)	5(1)	4(1)	8(1)
C(34)	24(1)	20(1)	16(1)	7(1)	5(1)	8(1)
C(35)	23(1)	22(1)	17(1)	6(1)	1(1)	8(1)
C(41)	14(1)	13(1)	20(1)	4(1)	3(1)	5(1)
C(42)	13(1)	15(1)	19(1)	5(1)	3(1)	5(1)
C(43)	21(1)	12(1)	28(1)	3(1)	8(1)	7(1)
C(44)	24(1)	15(1)	55(2)	8(1)	19(1)	7(1)
C(45)	23(1)	19(1)	30(1)	5(1)	10(1)	6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 98srv107.

	x	y	z	U(eq)
H(5D)	3814(64)	-7793(50)	2369(34)	85(18)
H(5C)	2949(58)	-8675(48)	1916(32)	78(17)
H(152)	4264(77)	-5406(62)	7500(43)	144(24)
H(252)	-6763(46)	-14650(36)	855(24)	54(11)
H(352)	-1341(53)	-9522(43)	-2475(29)	76(14)
H(452)	2529(61)	-563(49)	4166(33)	101(17)
H(1B)	-2235(31)	-7942(24)	3405(17)	18(6)
H(1A)	-1952(29)	-8501(23)	4122(17)	14(6)
H(2B)	-1593(32)	-9992(26)	3134(18)	23(7)
H(2A)	-3337(30)	-10018(23)	2854(16)	14(6)
H(3A)	-4192(32)	-9757(25)	1402(17)	20(7)
H(3B)	-3314(29)	-8525(24)	2040(17)	14(6)
H(4B)	-2829(34)	-9192(28)	395(20)	30(8)
H(4A)	-3754(30)	-8448(23)	579(17)	17(6)
H(5B)	-2193(33)	-6250(26)	1156(18)	24(7)
H(5A)	-2509(32)	-6766(25)	1922(18)	22(7)
H(6B)	-577(30)	-4810(24)	2411(17)	17(6)
H(6A)	485(30)	-5119(24)	1860(17)	18(6)
H(7A)	-1338(28)	-6225(22)	3276(15)	9(5)
H(7B)	-188(30)	-4992(25)	3910(17)	20(7)
H(8A)	1346(33)	-5860(26)	4625(18)	22(7)
H(8B)	-444(32)	-6352(25)	4671(18)	22(7)
H(11)	2014(29)	-7234(23)	4673(16)	14(6)
H(13A)	-158(34)	-7737(27)	5366(19)	29(7)
H(13B)	-256(33)	-9066(27)	5049(18)	25(7)
H(14A)	2506(37)	-8264(29)	5930(20)	37(8)
H(14B)	1307(36)	-8223(29)	6483(21)	35(8)
H(21)	-1435(26)	-10809(21)	1873(15)	4(5)
H(23A)	-4277(36)	-11545(28)	569(20)	33(8)
H(23B)	-4199(38)	-11579(30)	1552(21)	38(8)

H(24A)	-3028(26)	-12959(20)	1390(15)	3(5)
H(24B)	-2963(40)	-12907(31)	461(22)	43(9)
H(31)	-767(31)	-8152(26)	125(18)	21(7)
H(33B)	-1519(30)	-6271(25)	-116(17)	17(6)
H(33A)	-2767(36)	-7566(28)	-389(19)	29(7)
H(34A)	-1966(35)	-7122(27)	-1611(20)	30(8)
H(34B)	-357(34)	-6963(26)	-1146(18)	22(7)
H(41)	2710(32)	-4662(26)	2805(18)	24(7)
H(43B)	1504(31)	-3416(24)	3442(17)	20(7)
H(43A)	2363(35)	-3495(28)	4377(21)	34(8)
H(42B)	4838(47)	-2431(36)	4239(26)	59(11)
H(42A)	4182(44)	-2757(35)	3248(26)	56(11)

Table 6. Selected torsion angles [°] for 98srv107.

-61.45	(0.24)	N1 - C1 - C2 - N2
-59.59	(0.26)	N2 - C3 - C4 - N3
-58.06	(0.23)	N3 - C5 - C6 - N4
-58.94	(0.23)	N4 - C7 - C8 - N1
17.49	(0.26)	N1 - C11 - C12 - O122
37.58	(0.33)	N2 - C21 - C22 - O222
39.45	(0.24)	N3 - C31 - C32 - O322
40.61	(0.24)	N4 - C41 - C42 - O422

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for 98srv123.

Identification code	98srv123	
Empirical formula	$(C28\ H42\ N4\ O20\ Tb)^{-}.(H30)^{+}.2(H20)$	
Formula weight	920.63	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.62890(10) Å	α= 102.7389(8)°.
	b = 12.6877(2) Å	β= 101.2348(9)°.
	c = 16.2170(2) Å	γ = 110.5812(4)°.
Volume	1726.76(4) $Å^3$	
Z	2	
Density (calculated)	1.771 g/cm^3	
Absorption coefficient	2.141 mm^{-1}	
Absorption correction	Semi-empirical - Sadabs	
Max. and min. transmission	0.677155 and 0.419893	
F(000)	940	
Crystal size	0.10 x 0.20 x 0.25 mm^3	
Experimental device	Siemens SMART-CCD	
Experimental methods	ω scans	
θ range for data collection	1.35 to 27.53°.	
Index ranges	-11<=h<=12, -16<=k<=16, -21<=l<=20	
Reflections collected	Total	13969
	Observed	6646 [I > 2σ(I)]
	Unique	7856
	Calculation of cell	481
Independent reflections	7856 [R(int) = 0.0381]	
Completeness to θ = 27.53°	98.5 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7856 / 0 / 610	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2σ(I)]	R1 = 0.0442, wR2 = 0.1057	
R indices (all data)	R1 = 0.0601, wR2 = 0.1177	
Largest diff. peak and hole	2.683 and -2.362 $e.Å^{-3}$	

© 2000 American Chemical Society, J. Am. Chem. Soc., Woods ja994492v Supporting Info Page 31

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 98srv123. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tb(1)	795(1)	-7763(1)	2339(1)	16(1)
O(5)	3017(5)	-8097(4)	2060(3)	32(1)
O(121)	1981(5)	-9419(4)	4361(3)	31(1)
O(122)	1200(4)	-9082(3)	3090(2)	22(1)
O(151)	2335(6)	-5805(4)	6262(3)	43(1)
O(152)	3797(7)	-6313(5)	7196(3)	56(2)
O(22A)	-1634(11)	-11104(7)	37(5)	21(2)
O(22B)	-2130(16)	-10915(11)	-49(8)	20(3)
O(22C)	-1310(20)	-11349(16)	269(12)	19(4)
O(222)	-36(4)	-9377(3)	1027(2)	25(1)
O(251)	-5832(5)	-14229(4)	-315(3)	31(1)
O(252)	-5846(5)	-14073(4)	1073(2)	28(1)
O(321)	1463(4)	-5803(3)	382(2)	27(1)
O(322)	1746(4)	-6615(3)	1465(2)	20(1)
O(352)	-1141(5)	-8818(4)	-2266(3)	32(1)
O(351)	-2684(5)	-9483(4)	-1460(3)	36(1)
O(421)	4283(5)	-4547(3)	4560(3)	31(1)
O(422)	3010(4)	-6323(3)	3524(2)	19(1)
O(451)	4625(7)	-607(4)	3621(5)	63(2)
O(452)	2777(6)	-1231(4)	4249(4)	44(1)
N(1)	-17(5)	-7595(3)	3820(3)	17(1)
N(2)	-2013(5)	-9452(4)	2044(3)	21(1)
N(3)	-1403(5)	-7554(4)	1166(3)	19(1)
N(4)	609(5)	-5714(3)	2922(3)	15(1)
C(1)	-1700(6)	-8374(4)	3604(3)	20(1)
C(2)	-2239(6)	-9573(4)	2918(3)	21(1)
C(3)	-3233(6)	-9127(5)	1600(4)	24(1)
C(4)	-2904(6)	-8642(5)	852(4)	25(1)
C(5)	-1710(6)	-6522(5)	1582(3)	24(1)
C(6)	-255(6)	-5446(4)	2178(3)	19(1)
C(7)	-247(6)	-5768(4)	3590(3)	19(1)

C(8)	206(6)	-6345(4)	4252(3)	21(1)
C(11)	1026(6)	-7922(4)	4438(3)	18(1)
C(12)	1413(6)	-8896(4)	3932(3)	20(1)
C(13)	447(6)	-8186(5)	5226(3)	22(1)
C(14)	1748(7)	-7873(5)	6062(4)	26(1)
C(15)	2653(7)	-6556(5)	6508(4)	30(1)
C(21)	-2067(7)	-10584(4)	1487(4)	26(1)
C(22)	-1232(7)	-10316(5)	799(4)	34(1)
C(23)	-3652(7)	-11620(5)	1098(4)	29(1)
C(24)	-3555(7)	-12824(5)	887(5)	34(1)
C(25)	-5179(7)	-13794(5)	488(4)	28(1)
C(31)	-762(6)	-7399(4)	411(3)	20(1)
C(32)	956(6)	-6523(4)	775(3)	20(1)
C(33)	-1724(7)	-7099(5)	-308(3)	22(1)
C(34)	-1399(7)	-7370(5)	-1199(3)	23(1)
C(35)	-1834(6)	-8670(5)	-1641(3)	23(1)
C(41)	2251(6)	-4775(4)	3300(3)	20(1)
C(42)	3238(6)	-5266(4)	3835(3)	20(1)
C(43)	2408(6)	-3537(4)	3764(4)	24(1)
C(44)	3904(7)	-2550(5)	3760(5)	34(1)
C(45)	3823(7)	-1346(5)	3870(4)	30(1)
O(1WA)	5015(10)	-4154(7)	8200(5)	33(2)
O(1WB)	4690(17)	-4024(12)	8075(9)	28(3)
O(2WA)	-4004(14)	-6656(11)	3559(10)	39(3)
O(2WB)	-3420(30)	-6280(20)	4075(16)	46(5)
O(2WC)	-4072(16)	-6864(12)	3173(10)	32(3)
O(3WA)	5130(20)	-1426(18)	6927(13)	120(6)
O(3WB)	4800(20)	-1782(16)	5790(12)	108(5)

Table 3. Bond lengths [Å] and angles [°] for 98srv123

Tb(1)-O(322)	2.335(3)	O(452)-C(45)	1.312(7)
Tb(1)-O(122)	2.368(4)	O(452)-H(452)	0.68(9)
Tb(1)-O(222)	2.371(3)	N(1)-C(1)	1.492(6)
Tb(1)-O(422)	2.386(3)	N(1)-C(8)	1.505(6)
Tb(1)-O(5)	2.427(4)	N(1)-C(11)	1.507(6)
Tb(1)-N(4)	2.644(4)	N(2)-C(3)	1.487(7)
Tb(1)-N(1)	2.654(4)	N(2)-C(21)	1.495(6)
Tb(1)-N(2)	2.665(4)	N(2)-C(2)	1.508(6)
Tb(1)-N(3)	2.686(4)	N(3)-C(5)	1.490(7)
O(5)-H(5D)	0.64(9)	N(3)-C(31)	1.496(6)
O(5)-H(5C)	0.61(8)	N(3)-C(4)	1.501(6)
O(121)-C(12)	1.238(6)	N(4)-C(7)	1.483(6)
O(122)-C(12)	1.296(6)	N(4)-C(6)	1.500(6)
O(151)-C(15)	1.218(7)	N(4)-C(41)	1.507(6)
O(152)-C(15)	1.298(7)	C(1)-C(2)	1.516(7)
O(152)-H(152)	0.94(10)	C(1)-H(1A)	1.03(6)
O(22A)-O(22B)	0.611(12)	C(1)-H(1B)	0.90(6)
O(22A)-O(22C)	0.638(18)	C(2)-H(2A)	1.05(6)
O(22A)-C(22)	1.292(9)	C(2)-H(2B)	1.05(6)
O(22B)-O(22C)	1.21(2)	C(3)-C(4)	1.515(8)
O(22B)-C(22)	1.353(14)	C(3)-H(3A)	0.99(7)
O(22C)-C(22)	1.366(18)	C(3)-H(3B)	0.84(7)
O(222)-C(22)	1.249(7)	C(4)-H(4A)	0.75(7)
O(251)-C(25)	1.231(7)	C(4)-H(4B)	0.98(7)
O(252)-C(25)	1.289(7)	C(5)-C(6)	1.518(7)
O(252)-H(252)	0.92(8)	C(5)-H(5A)	0.85(7)
O(321)-C(32)	1.242(6)	C(5)-H(5B)	1.08(6)
O(322)-C(32)	1.276(6)	C(6)-H(6A)	0.91(6)
O(352)-C(35)	1.331(7)	C(6)-H(6B)	0.98(6)
O(352)-H(352)	0.71(8)	C(7)-C(8)	1.506(7)
O(351)-C(35)	1.207(7)	C(7)-H(7A)	0.98(6)
O(421)-C(42)	1.284(6)	C(7)-H(7B)	0.97(6)
O(422)-C(42)	1.247(6)	C(8)-H(8A)	1.07(6)
O(451)-C(45)	1.191(7)	C(8)-H(8B)	0.98(6)

C(11)-C(12)	1.529(6)	C(45)-H(452)	1.50(10)
C(11)-C(13)	1.546(7)	O(2WA)-O(2WC)	0.604(15)
C(11)-H(11)	1.04(6)	O(2WA)-O(2WB)	0.83(2)
C(13)-C(14)	1.522(7)	O(2WB)-O(2WC)	1.39(3)
C(13)-H(13A)	0.98(6)	O(3WA)-O(3WB)	1.73(3)
C(13)-H(13B)	1.09(6)		
C(14)-C(15)	1.507(8)	O(322)-Tb(1)-O(122)	144.33(12)
C(14)-H(14A)	1.09(7)	O(322)-Tb(1)-O(222)	84.08(12)
C(14)-H(14B)	1.00(7)	O(122)-Tb(1)-O(222)	85.38(13)
C(21)-C(23)	1.518(7)	O(322)-Tb(1)-O(422)	85.78(12)
C(21)-C(22)	1.527(7)	O(122)-Tb(1)-O(422)	83.04(12)
C(21)-H(21)	1.01(7)	O(222)-Tb(1)-O(422)	144.00(12)
C(23)-C(24)	1.531(8)	O(322)-Tb(1)-O(5)	72.46(14)
C(23)-H(23A)	1.14(7)	O(122)-Tb(1)-O(5)	71.91(14)
C(23)-H(23B)	1.02(7)	O(222)-Tb(1)-O(5)	70.16(14)
C(24)-C(25)	1.510(8)	O(422)-Tb(1)-O(5)	73.84(14)
C(24)-H(24A)	0.97(8)	O(322)-Tb(1)-N(4)	72.76(12)
C(24)-H(24B)	1.02(8)	O(122)-Tb(1)-N(4)	131.03(12)
C(31)-C(32)	1.536(7)	O(222)-Tb(1)-N(4)	140.94(13)
C(31)-C(33)	1.545(7)	O(422)-Tb(1)-N(4)	66.25(12)
C(31)-H(31)	0.77(6)	O(5)-Tb(1)-N(4)	128.06(13)
C(33)-C(34)	1.528(7)	O(322)-Tb(1)-N(1)	141.17(12)
C(33)-H(33A)	0.93(7)	O(122)-Tb(1)-N(1)	65.54(12)
C(33)-H(33B)	0.95(7)	O(222)-Tb(1)-N(1)	131.71(12)
C(34)-C(35)	1.511(7)	O(422)-Tb(1)-N(1)	72.40(12)
C(34)-H(34A)	0.91(7)	O(5)-Tb(1)-N(1)	127.81(15)
C(34)-H(34B)	0.90(7)	N(4)-Tb(1)-N(1)	69.15(12)
C(41)-C(43)	1.524(7)	O(322)-Tb(1)-N(2)	130.28(12)
C(41)-C(42)	1.542(7)	O(122)-Tb(1)-N(2)	74.10(13)
C(41)-H(41)	0.99(6)	O(222)-Tb(1)-N(2)	65.65(12)
C(43)-C(44)	1.543(8)	O(422)-Tb(1)-N(2)	141.07(12)
C(43)-H(43A)	1.06(6)	O(5)-Tb(1)-N(2)	125.39(14)
C(43)-H(43B)	1.05(6)	N(4)-Tb(1)-N(2)	106.51(13)
C(44)-C(45)	1.530(8)	N(1)-Tb(1)-N(2)	69.57(12)
C(44)-H(44A)	0.98(8)	O(322)-Tb(1)-N(3)	65.60(12)
C(44)-H(44B)	0.92(8)	O(122)-Tb(1)-N(3)	141.70(13)

O(222)-Tb(1)-N(3)	73.21(13)	C(21)-N(2)-Tb(1)	107.4(3)
O(422)-Tb(1)-N(3)	131.99(12)	C(2)-N(2)-Tb(1)	109.0(3)
O(5)-Tb(1)-N(3)	126.09(15)	C(5)-N(3)-C(31)	112.2(4)
N(4)-Tb(1)-N(3)	68.71(12)	C(5)-N(3)-C(4)	108.0(4)
N(1)-Tb(1)-N(3)	106.07(13)	C(31)-N(3)-C(4)	110.1(4)
N(2)-Tb(1)-N(3)	68.24(13)	C(5)-N(3)-Tb(1)	110.0(3)
Tb(1)-O(5)-H(5D)	117(8)	C(31)-N(3)-Tb(1)	105.0(3)
Tb(1)-O(5)-H(5C)	129(8)	C(4)-N(3)-Tb(1)	111.5(3)
H(5D)-O(5)-H(5C)	103(10)	C(7)-N(4)-C(6)	107.8(4)
C(12)-O(122)-Tb(1)	124.2(3)	C(7)-N(4)-C(41)	112.3(4)
C(15)-O(152)-H(152)	111(6)	C(6)-N(4)-C(41)	109.3(4)
O(22B)-O(22A)-O(22C)	150(3)	C(7)-N(4)-Tb(1)	109.7(3)
O(22B)-O(22A)-C(22)	82.2(15)	C(6)-N(4)-Tb(1)	110.8(3)
O(22C)-O(22A)-C(22)	82.7(19)	C(41)-N(4)-Tb(1)	106.9(3)
O(22A)-O(22B)-O(22C)	15.2(14)	N(1)-C(1)-C(2)	114.5(4)
O(22A)-O(22B)-C(22)	71.2(15)	N(1)-C(1)-H(1A)	107(3)
O(22C)-O(22B)-C(22)	64.2(10)	C(2)-C(1)-H(1A)	107(3)
O(22A)-O(22C)-O(22B)	14.5(14)	N(1)-C(1)-H(1B)	110(4)
O(22A)-O(22C)-C(22)	69.7(18)	C(2)-C(1)-H(1B)	108(4)
O(22B)-O(22C)-C(22)	63.0(10)	H(1A)-C(1)-H(1B)	111(5)
C(22)-O(222)-Tb(1)	125.6(3)	N(2)-C(2)-C(1)	111.6(4)
C(25)-O(252)-H(252)	106(4)	N(2)-C(2)-H(2A)	106(3)
C(32)-O(322)-Tb(1)	127.0(3)	C(1)-C(2)-H(2A)	111(3)
C(35)-O(352)-H(352)	116(7)	N(2)-C(2)-H(2B)	106(3)
C(42)-O(422)-Tb(1)	124.3(3)	C(1)-C(2)-H(2B)	107(3)
C(45)-O(452)-H(452)	92(8)	H(2A)-C(2)-H(2B)	115(5)
C(1)-N(1)-C(8)	107.4(4)	N(2)-C(3)-C(4)	114.6(4)
C(1)-N(1)-C(11)	113.2(4)	N(2)-C(3)-H(3A)	111(4)
C(8)-N(1)-C(11)	108.9(4)	C(4)-C(3)-H(3A)	112(4)
C(1)-N(1)-Tb(1)	109.4(3)	N(2)-C(3)-H(3B)	107(4)
C(8)-N(1)-Tb(1)	110.7(3)	C(4)-C(3)-H(3B)	109(4)
C(11)-N(1)-Tb(1)	107.5(3)	H(3A)-C(3)-H(3B)	102(6)
C(3)-N(2)-C(21)	111.8(4)	N(3)-C(4)-C(3)	111.5(4)
C(3)-N(2)-C(2)	108.7(4)	N(3)-C(4)-H(4A)	105(5)
C(21)-N(2)-C(2)	109.9(4)	C(3)-C(4)-H(4A)	111(5)
C(3)-N(2)-Tb(1)	110.0(3)	N(3)-C(4)-H(4B)	111(4)

C(3)-C(4)-H(4B)	114(4)	C(14)-C(13)-H(13A)	106(4)
H(4A)-C(4)-H(4B)	104(6)	C(11)-C(13)-H(13A)	112(4)
N(3)-C(5)-C(6)	113.8(4)	C(14)-C(13)-H(13B)	108(3)
N(3)-C(5)-H(5A)	105(4)	C(11)-C(13)-H(13B)	109(3)
C(6)-C(5)-H(5A)	117(4)	H(13A)-C(13)-H(13B)	108(5)
N(3)-C(5)-H(5B)	113(3)	C(15)-C(14)-C(13)	113.3(4)
C(6)-C(5)-H(5B)	109(3)	C(15)-C(14)-H(14A)	107(4)
H(5A)-C(5)-H(5B)	98(5)	C(13)-C(14)-H(14A)	110(3)
N(4)-C(6)-C(5)	112.2(4)	C(15)-C(14)-H(14B)	106(4)
N(4)-C(6)-H(6A)	110(4)	C(13)-C(14)-H(14B)	102(4)
C(5)-C(6)-H(6A)	103(4)	H(14A)-C(14)-H(14B)	118(5)
N(4)-C(6)-H(6B)	111(3)	O(151)-C(15)-O(152)	123.8(6)
C(5)-C(6)-H(6B)	108(3)	O(151)-C(15)-C(14)	124.1(5)
H(6A)-C(6)-H(6B)	112(5)	O(152)-C(15)-C(14)	112.0(5)
N(4)-C(7)-C(8)	114.5(4)	N(2)-C(21)-C(23)	116.3(4)
N(4)-C(7)-H(7A)	112(3)	N(2)-C(21)-C(22)	108.8(4)
C(8)-C(7)-H(7A)	114(4)	C(23)-C(21)-C(22)	113.5(5)
N(4)-C(7)-H(7B)	109(3)	N(2)-C(21)-H(21)	104(4)
C(8)-C(7)-H(7B)	110(3)	C(23)-C(21)-H(21)	111(4)
H(7A)-C(7)-H(7B)	96(5)	C(22)-C(21)-H(21)	102(4)
N(1)-C(8)-C(7)	112.5(4)	O(222)-C(22)-O(22A)	120.4(6)
N(1)-C(8)-H(8A)	116(3)	O(222)-C(22)-O(22B)	124.1(7)
C(7)-C(8)-H(8A)	105(3)	O(22A)-C(22)-O(22B)	26.6(5)
N(1)-C(8)-H(8B)	110(4)	O(222)-C(22)-O(22C)	120.9(9)
C(7)-C(8)-H(8B)	111(4)	O(22A)-C(22)-O(22C)	27.6(7)
H(8A)-C(8)-H(8B)	102(5)	O(22B)-C(22)-O(22C)	52.7(10)
N(1)-C(11)-C(12)	111.4(4)	O(222)-C(22)-C(21)	118.2(5)
N(1)-C(11)-C(13)	114.0(4)	O(22A)-C(22)-C(21)	120.9(6)
C(12)-C(11)-C(13)	113.3(4)	O(22B)-C(22)-C(21)	114.1(7)
N(1)-C(11)-H(11)	106(3)	O(22C)-C(22)-C(21)	109.3(9)
C(12)-C(11)-H(11)	103(3)	C(21)-C(23)-C(24)	112.9(5)
C(13)-C(11)-H(11)	108(3)	C(21)-C(23)-H(23A)	116(3)
O(121)-C(12)-O(122)	124.0(4)	C(24)-C(23)-H(23A)	110(3)
O(121)-C(12)-C(11)	117.9(4)	C(21)-C(23)-H(23B)	108(4)
O(122)-C(12)-C(11)	118.0(4)	C(24)-C(23)-H(23B)	110(4)
C(14)-C(13)-C(11)	113.8(4)	H(23A)-C(23)-H(23B)	100(5)

C(25)-C(24)-C(23)	109.0(5)	O(352)-C(35)-C(34)	111.2(5)
C(25)-C(24)-H(24A)	113(4)	N(4)-C(41)-C(43)	115.2(4)
C(23)-C(24)-H(24A)	111(4)	N(4)-C(41)-C(42)	107.9(4)
C(25)-C(24)-H(24B)	113(4)	C(43)-C(41)-C(42)	116.1(4)
C(23)-C(24)-H(24B)	114(4)	N(4)-C(41)-H(41)	113(4)
H(24A)-C(24)-H(24B)	96(6)	C(43)-C(41)-H(41)	101(3)
O(251)-C(25)-O(252)	123.3(5)	C(42)-C(41)-H(41)	103(3)
O(251)-C(25)-C(24)	123.3(6)	O(422)-C(42)-O(421)	123.9(5)
O(252)-C(25)-C(24)	113.3(5)	O(422)-C(42)-C(41)	118.2(4)
N(3)-C(31)-C(32)	109.3(4)	O(421)-C(42)-C(41)	117.8(4)
N(3)-C(31)-C(33)	115.3(4)	C(41)-C(43)-C(44)	112.5(4)
C(32)-C(31)-C(33)	113.3(4)	C(41)-C(43)-H(43A)	114(3)
N(3)-C(31)-H(31)	108(5)	C(44)-C(43)-H(43A)	107(4)
C(32)-C(31)-H(31)	105(5)	C(41)-C(43)-H(43B)	110(3)
C(33)-C(31)-H(31)	106(5)	C(44)-C(43)-H(43B)	111(4)
O(321)-C(32)-O(322)	125.7(5)	H(43A)-C(43)-H(43B)	102(5)
O(321)-C(32)-C(31)	118.5(4)	C(45)-C(44)-C(43)	114.1(5)
O(322)-C(32)-C(31)	115.8(4)	C(45)-C(44)-H(44A)	106(4)
C(34)-C(33)-C(31)	113.8(4)	C(43)-C(44)-H(44A)	113(4)
C(34)-C(33)-H(33A)	107(4)	C(45)-C(44)-H(44B)	99(5)
C(31)-C(33)-H(33A)	113(4)	C(43)-C(44)-H(44B)	115(5)
C(34)-C(33)-H(33B)	107(4)	H(44A)-C(44)-H(44B)	109(6)
C(31)-C(33)-H(33B)	106(4)	O(451)-C(45)-O(452)	124.4(5)
H(33A)-C(33)-H(33B)	111(5)	O(451)-C(45)-C(44)	122.4(6)
C(35)-C(34)-C(33)	114.3(4)	O(452)-C(45)-C(44)	113.1(5)
C(35)-C(34)-H(34A)	108(4)	O(451)-C(45)-H(452)	98(4)
C(33)-C(34)-H(34A)	106(4)	O(452)-C(45)-H(452)	27(4)
C(35)-C(34)-H(34B)	109(4)	C(44)-C(45)-H(452)	138(4)
C(33)-C(34)-H(34B)	112(4)	O(2WC)-O(2WA)-O(2WB)	148(3)
H(34A)-C(34)-H(34B)	109(6)	O(2WA)-O(2WB)-O(2WC)	13.2(13)
O(351)-C(35)-O(352)	123.3(5)	O(2WA)-O(2WC)-O(2WB)	18.4(18)
O(351)-C(35)-C(34)	125.5(5)		

© 2000 American Chemical Society, J. Am. Chem. Soc., Woods ja994492v Supporting Info Page 38

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 98srv123. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Tb(1)	18(1)	11(1)	14(1)	1(1)	5(1)	3(1)
O(5)	32(2)	18(2)	48(3)	6(2)	18(2)	11(2)
O(121)	46(3)	30(2)	32(2)	15(2)	15(2)	26(2)
O(122)	31(2)	15(2)	22(2)	3(1)	13(2)	11(2)
O(151)	55(3)	25(2)	36(2)	2(2)	-7(2)	16(2)
O(152)	70(4)	43(3)	38(3)	-8(2)	-18(3)	33(3)
O(222)	27(2)	15(2)	25(2)	-2(1)	14(2)	0(2)
O(251)	34(2)	30(2)	27(2)	8(2)	8(2)	14(2)
O(252)	28(2)	27(2)	18(2)	2(2)	0(2)	5(2)
O(321)	24(2)	25(2)	24(2)	12(2)	3(2)	0(2)
O(322)	17(2)	21(2)	18(2)	6(1)	4(1)	5(1)
O(352)	39(2)	22(2)	31(2)	-3(2)	14(2)	12(2)
O(351)	45(3)	23(2)	31(2)	6(2)	11(2)	6(2)
O(421)	31(2)	16(2)	28(2)	-2(2)	-9(2)	3(2)
O(422)	19(2)	15(2)	22(2)	5(1)	2(1)	7(1)
O(451)	63(4)	33(3)	119(5)	39(3)	60(4)	25(3)
O(452)	60(3)	25(2)	69(3)	23(2)	40(3)	25(2)
N(1)	23(2)	12(2)	14(2)	3(2)	7(2)	6(2)
N(2)	26(2)	18(2)	16(2)	2(2)	9(2)	5(2)
N(3)	16(2)	21(2)	14(2)	2(2)	3(2)	3(2)
N(4)	16(2)	12(2)	15(2)	3(2)	2(2)	4(2)
C(1)	22(3)	20(2)	20(2)	4(2)	10(2)	9(2)
C(2)	25(3)	16(2)	17(2)	2(2)	7(2)	3(2)
C(3)	18(3)	24(3)	22(3)	4(2)	5(2)	2(2)
C(4)	20(3)	25(3)	17(2)	0(2)	1(2)	-1(2)
C(5)	20(3)	33(3)	16(2)	4(2)	1(2)	13(2)
C(6)	25(3)	19(2)	16(2)	6(2)	4(2)	14(2)
C(7)	23(3)	16(2)	19(2)	5(2)	6(2)	9(2)
C(8)	28(3)	19(2)	16(2)	5(2)	8(2)	10(2)
C(11)	24(3)	13(2)	16(2)	4(2)	9(2)	8(2)
C(12)	22(3)	14(2)	25(3)	7(2)	7(2)	7(2)

C(13)	27(3)	22(2)	19(2)	8(2)	8(2)	10(2)
C(14)	36(3)	23(3)	21(3)	8(2)	5(2)	17(2)
C(15)	43(3)	32(3)	20(3)	7(2)	8(2)	21(3)
C(21)	27(3)	16(2)	26(3)	-2(2)	13(2)	2(2)
C(22)	41(3)	20(3)	26(3)	-4(2)	19(3)	-1(2)
C(23)	24(3)	22(3)	33(3)	3(2)	10(2)	5(2)
C(24)	30(3)	22(3)	43(4)	2(2)	12(3)	5(2)
C(25)	33(3)	17(2)	29(3)	4(2)	6(2)	9(2)
C(31)	23(3)	16(2)	17(2)	3(2)	5(2)	6(2)
C(32)	21(2)	17(2)	18(2)	3(2)	5(2)	5(2)
C(33)	27(3)	21(2)	17(2)	7(2)	6(2)	8(2)
C(34)	26(3)	22(2)	18(2)	5(2)	5(2)	8(2)
C(35)	24(3)	22(2)	17(2)	3(2)	-2(2)	7(2)
C(41)	21(2)	13(2)	23(2)	7(2)	5(2)	5(2)
C(42)	18(2)	14(2)	23(2)	7(2)	4(2)	4(2)
C(43)	25(3)	13(2)	31(3)	4(2)	8(2)	7(2)
C(44)	28(3)	19(3)	54(4)	6(3)	17(3)	10(2)
C(45)	29(3)	19(2)	35(3)	5(2)	9(2)	6(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 98srv123.

	x	y	z	U(eq)
H(5D)	3670(100)	-7820(80)	2370(60)	48
H(5C)	3050(100)	-8560(80)	1880(60)	48
H(152)	4160(110)	-5530(90)	7570(60)	84
H(252)	-6850(90)	-14610(70)	760(50)	42
H(352)	-1360(100)	-9410(70)	-2520(50)	48
H(452)	2780(110)	-770(80)	4100(60)	67
H(1A)	-2320(70)	-7940(50)	3350(40)	24
H(1B)	-1920(70)	-8500(50)	4100(40)	24
H(2A)	-1600(70)	-10040(50)	3110(40)	25
H(2B)	-3440(70)	-10010(50)	2800(40)	25
H(3A)	-4280(80)	-9790(60)	1410(40)	29
H(3B)	-3320(70)	-8610(60)	1990(40)	29
H(4A)	-2800(80)	-9080(60)	510(40)	30
H(4B)	-3760(80)	-8500(60)	530(40)	30
H(5A)	-2270(80)	-6430(60)	1150(40)	29
H(5B)	-2550(70)	-6740(50)	1940(40)	29
H(6A)	-630(70)	-4920(50)	2400(40)	23
H(6B)	400(70)	-5160(50)	1810(40)	23
H(7A)	-1370(70)	-6070(50)	3310(40)	23
H(7B)	-110(70)	-4970(50)	3890(40)	23
H(8A)	1360(70)	-5740(50)	4650(40)	25
H(8B)	-370(70)	-6330(50)	4690(40)	25
H(11)	2100(70)	-7190(50)	4690(40)	21
H(13A)	-160(70)	-7740(60)	5390(40)	29
H(13B)	-300(70)	-9130(60)	5040(40)	29
H(14A)	2580(80)	-8230(60)	5900(40)	33
H(14B)	1160(80)	-8170(60)	6470(40)	33
H(21)	-1330(80)	-10770(60)	1900(40)	31
H(23A)	-4470(80)	-11590(60)	500(40)	37
H(23B)	-4260(80)	-11570(60)	1540(40)	37