Table 8. Bond Angles(°) Involving Hydrogen

atom	atom	atom	angle	atom	atom	atom	angle
Pr(2)	O(8)	H(1)	109.5	Pr(2)	O(8)	H(2)	109.5
H(1)	O(8)	H(2)	109.5	C(57)	O(12)	H(59)	109.5
N(1)	C(1)	H(3)	108.8	N(1)	C(1)	H(4)	108.8
C(2)	C(1)	H(3)	108.8	C(2)	C(1)	H(4)	108.8
H(3)	C(1)	H(4)	109.5	N(2)	C(2)	H(5)	108.7
N(2)	C(2)	H(6)	108.7	C(1)	C(2)	H(5)	108.7
C(1)	C(2)	H(6)	108.7	H(5)	C(2)	H(6)	109.5
N(1)	C(3)	H(7)	109.0	N(1)	C(3)	H(8)	109.0
C(4)	C(3)	H(7)	109.0	C(4)	C(3)	H(8)	109.0
H(7)	C(3)	H(8)	109.5	C(4)	C(5)	H(9)	120.4
C(6)	C(5)	H(9)	120.4	C(5)	C(6)	H(10)	120.2
C(7)	C(6)	H(10)	120.2	C(6)	C(7)	H(11)	120.7
C(8)	C(7)	H(11)	120.7	N(3)	C(8)	H(12)	118.6
C(7)	C(8)	H(12)	118.6	N(1)	C(9)	H(13)	107.6
N(1)	C(9)	H(14)	107.6	C(10)	C(9)	H(13)	107.6
C(10)	C(9)	H(14)	107.6	H(13)	C(9)	H(14)	109.5
C(11)	C(12)	H(15)	119.0	C(13)	C(12)	H(15)	119.0
C(12)	C(13)	H(16)	119.6	C(14)	C(13)	H(16)	119.6
C(13)	C(14)	H(17)	120.8	C(15)	C(14)	H(17)	120.9
C(10)	C(15)	H(18)	118.8	C(14)	C(15)	H(18)	118.8
N(2)	C(16)	H(19)	108.9	N(2)	C(16)	H(20)	108.9
C(17)	C(16)	H(19)	108.9	C(17)	C(16)	H(20)	108.9
H(19)	C(16)	H(20)	109.5	C(17)	C(18)	H(21)	120.7
C(19)	C(18)	H(21)	120.7	C(18)	C(19)	H(22)	120.6

Table 8. Bond Angles(°) Involving Hydrogen (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(20)	C(19)	H(22)	120.6	C(19)	C(20)	H(23)	120.4
C(21)	C(20)	H(23)	120.4	N(4)	C(21)	H(24)	118.6
C(20)	C(21)	H(24)	118.6	N(2)	C(22)	H(25)	108.2
N(2)	C(22)	H(26)	108.2	C(23)	C(22)	H(25)	108.2
C(23)	C(22)	H(26)	108.2	H(25)	C(22)	H(26)	109.5
C(24)	C(25)	H(27)	119.1	C(26)	C(25)	H(27)	119.1
C(25)	C(26)	H(28)	119.7	C(27)	C(26)	H(28)	119.7
C(26)	C(27)	H(29)	120.7	C(28)	C(27)	H(29)	120.7
C(23)	C(28)	H(30)	119.3	C(27)	C(28)	H(30)	119.3
N(5)	C(29)	H(31)	108.8	N(5)	C(29)	H(32)	108.8
C(30)	C(29)	H(31)	108.8	C(30)	C(29)	H(32)	108.8
H(31)	C(29)	H(32)	109.5	N(6)	C(30)	H(33)	108.6
N(6)	C(30)	H(34)	108.6	C(29)	C(30)	H(33)	108.6
C(29)	C(30)	H(34)	108.6	H(33)	C(30)	H(34)	109.5
N(5)	C(31)	H(35)	108.1	N(5)	C(31)	H(36)	108.1
C(32)	C(31)	H(35)	108.1	C(32)	C(31)	H(36)	108.1
H(35)	C(31)	H(36)	109.5	C(32)	C(33)	H(37)	120.3
C(34)	C(33)	H(37)	120.3	C(33)	C(34)	H(38)	120.1
C(35)	C(34)	H(38)	120.1	C(34)	C(35)	H(39)	121.2
C(36)	C(35)	H(39)	121.2	N(7)	C(36)	H(40)	118.2
C(35)	C(36)	H(40)	118.2	N(5)	C(37)	H(41)	108.9
N(5)	C(37)	H(42)	108.9	C(38)	C(37)	H(41)	108.9
C(38)	C(37)	H(42)	108.9	H(41)	C(37)	H(42)	109.5
C(39)	C(40)	H(43)	120.0	C(41)	C(40)	H(43)	120.0

Table 8. Bond Angles(°) Involving Hydrogen (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(40)	C(41)	H(44)	119.6	C(42)	C(41)	H(44)	119.6
C(41)	C(42)	H(45)	120.5	C(43)	C(42)	H(45)	120.5
C(38)	C(43)	H(46)	119.3	C(42)	C(43)	H(46)	119.3
N(6)	C(44)	H(47)	107.9	N(6)	C(44)	H(48)	107.9
C(45)	C(44)	H(47)	107.9	C(45)	C(44)	H(48)	107.9
H(47)	C(44)	H(48)	109.5	C(45)	C(46)	H(49)	120.4
C(47)	C(46)	H(49)	120.4	C(46)	C(47)	H(50)	120.5
C(48)	C(47)	H(50)	120.5	C(47)	C(48)	H(51)	120.6
C(49)	C(48)	H(51)	120.5	N(8)	C(49)	H(52)	118.8
C(48)	C(49)	H(52)	118.8	N(6)	C(50)	H(53)	108.8
N(6)	C(50)	H(54)	108.8	C(51)	C(50)	H(53)	108.8
C(51)	C(50)	H(54)	108.8	H(53)	C(50)	H(54)	109.5
C(52)	C(53)	H(55)	120.0	C(54)	C(53)	H(55)	120.0
C(53)	C(54)	H(56)	119.3	C(55)	C(54)	H(56)	119.3
C(54)	C(55)	H(57)	120.8	C(56)	C(55)	H(57)	120.8
C(51)	C(56)	H(58)	119.4	C(55)	C(56)	H(58)	119.4
O(12)	C(57)	H(60)	109.5	O(12)	C(57)	H(61)	109.5
O(12)	C(57)	H(62)	109.5	H(60)	C(57)	H(61)	109.5
H(60)	C(57)	H(62)	109.5	H(61)	C(57)	H(62)	109.5

Table 9. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Pr(1)	O(1)	C(11)	C(10)	4.8(5)	Pr(1)	O(1)	C(11)	C(12)	-174.9(2)
Pr(1)	O(2)	C(24)	C(23)	50.9(3)	Pr(1)	O(2)	C(24)	C(25)	-127.7(3)
Pr(1)	O(3)	Pr(2)	O(4)	5.45(8)	Pr(1)	O(3)	Pr(2)	O(5)	-121.22(8)
Pr(1)	O(3)	Pr(2)	O(6)	162.77(8)	Pr(1)	O(3)	Pr(2)	O(8)	-71.86(8)
Pr(1)	O(3)	Pr(2)	N(5)	132.39(10)	Pr(1)	O(3)	Pr(2)	N(6)	71.95(9)
Pr(1)	O(3)	Pr(2)	N(7)	-159.70(10)	Pr(1)	O(3)	Pr(2)	N(8)	8.9(2)
Pr(1)	O(3)	C(39)	C(38)	-108.2(2)	Pr(1)	O(3)	C(39)	C(40)	72.5(3)
Pr(1)	O(4)	Pr(2)	O(3)	-5.17(7)	Pr(1)	O(4)	Pr(2)	O(5)	126.55(8)
Pr(1)	O(4)	Pr(2)	O(6)	-158.75(9)	Pr(1)	O(4)	Pr(2)	O(8)	78.91(8)
Pr(1)	O(4)	Pr(2)	N(5)	-62.42(9)	Pr(1)	O(4)	Pr(2)	N(6)	-117.94(9)
Pr(1)	O(4)	Pr(2)	N(7)	18.53(15)	Pr(1)	O(4)	Pr(2)	N(8)	176.61(9)
Pr(1)	O(4)	C(52)	C(51)	101.3(3)	Pr(1)	O(4)	C(52)	C(53)	-82.9(3)
Pr(1)	N(1)	C(1)	C(2)	52.8(3)	Pr(1)	N(1)	C(3)	C(4)	56.8(2)
Pr(1)	N(1)	C(9)	C(10)	67.1(3)	Pr(1)	N(2)	C(2)	C(1)	36.8(3)
Pr(1)	N(2)	C(16)	C(17)	49.9(3)	Pr(1)	N(2)	C(22)	C(23)	67.1(3)
Pr(1)	N(3)	C(4)	C(3)	-5.0(3)	Pr(1)	N(3)	C(4)	C(5)	175.5(2)
Pr(1)	N(3)	C(8)	C(7)	-173.9(2)	Pr(1)	N(4)	C(17)	C(16)	4.3(3)
Pr(1)	N(4)	C(17)	C(18)	-176.7(2)	Pr(1)	N(4)	C(21)	C(20)	178.9(2)
Pr(2)	O(3)	Pr(1)	O(1)	-83.13(9)	Pr(2)	O(3)	Pr(1)	O(2)	85.01(9)
Pr(2)	O(3)	Pr(1)	O(4)	-5.43(8)	Pr(2)	O(3)	Pr(1)	N(1)	-125.9(2)
Pr(2)	O(3)	Pr(1)	N(2)	151.09(8)	Pr(2)	O(3)	Pr(1)	N(3)	34.33(15)
Pr(2)	O(3)	Pr(1)	N(4)	-156.64(10)	Pr(2)	O(3)	C(39)	C(38)	68.3(3)
Pr(2)	O(3)	C(39)	C(40)	-110.9(3)	Pr(2)	O(4)	Pr(1)	O(1)	103.32(8)
Pr(2)	O(4)	Pr(1)	O(2)	-74.11(7)	Pr(2)	O(4)	Pr(1)	O(3)	5.11(7)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Pr(2)	O(4)	Pr(1)	N(1)	162.61(7)	Pr(2)	O(4)	Pr(1)	N(2)	-91.8(2)
Pr(2)	O(4)	Pr(1)	N(3)	-150.22(9)	Pr(2)	O(4)	Pr(1)	N(4)	49.17(13)
Pr(2)	O(4)	C(52)	C(51)	-68.9(3)	Pr(2)	O(4)	C(52)	C(53)	107.0(3)
Pr(2)	O(5)	N(9)	O(6)	3.8(3)	Pr(2)	O(5)	N(9)	O(7)	-177.4(3)
Pr(2)	O(6)	N(9)	O(5)	-3.8(3)	Pr(2)	O(6)	N(9)	O(7)	177.4(3)
Pr(2)	N(5)	C(29)	C(30)	55.2(3)	Pr(2)	N(5)	C(31)	C(32)	-39.6(3)
Pr(2)	N(5)	C(37)	C(38)	69.5(2)	Pr(2)	N(6)	C(30)	C(29)	32.5(3)
Pr(2)	N(6)	C(44)	C(45)	43.4(3)	Pr(2)	N(6)	C(50)	C(51)	-59.3(3)
Pr(2)	N(7)	C(32)	C(31)	-20.9(3)	Pr(2)	N(7)	C(32)	C(33)	164.3(2)
Pr(2)	N(7)	C(36)	C(35)	-165.9(2)	Pr(2)	N(8)	C(45)	C(44)	-6.9(3)
Pr(2)	N(8)	C(45)	C(46)	170.4(2)	Pr(2)	N(8)	C(49)	C(48)	-169.9(2)
O(1)	Pr(1)	O(2)	C(24)	141.9(3)	O(1)	Pr(1)	O(3)	C(39)	93.8(2)
O(1)	Pr(1)	O(4)	C(52)	-67.4(2)	O(1)	Pr(1)	N(1)	C(1)	-161.4(2)
O(1)	Pr(1)	N(1)	C(3)	79.3(2)	O(1)	Pr(1)	N(1)	C(9)	-39.8(2)
O(1)	Pr(1)	N(2)	C(2)	39.0(2)	O(1)	Pr(1)	N(2)	C(16)	-79.8(2)
O(1)	Pr(1)	N(2)	C(22)	159.14(15)	O(1)	Pr(1)	N(3)	C(4)	-32.4(2)
O(1)	Pr(1)	N(3)	C(8)	142.7(2)	O(1)	Pr(1)	N(4)	C(17)	155.3(2)
O(1)	Pr(1)	N(4)	C(21)	-23.8(2)	O(1)	C(11)	C(10)	C(9)	8.7(4)
O(1)	C(11)	C(10)	C(15)	-175.4(3)	O(1)	C(11)	C(12)	C(13)	177.4(3)
O(2)	Pr(1)	O(1)	C(11)	149.2(3)	O(2)	Pr(1)	O(3)	C(39)	-98.0(2)
O(2)	Pr(1)	O(4)	C(52)	115.1(2)	O(2)	Pr(1)	N(1)	C(1)	29.0(2)
O(2)	Pr(1)	N(1)	C(3)	-90.3(2)	O(2)	Pr(1)	N(1)	C(9)	150.6(2)
O(2)	Pr(1)	N(2)	C(2)	-142.1(2)	O(2)	Pr(1)	N(2)	C(16)	99.2(2)
O(2)	Pr(1)	N(2)	C(22)	-21.92(15)	O(2)	Pr(1)	N(3)	C(4)	162.1(2)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(2)	Pr(1)	N(3)	C(8)	-22.8(2)	O(2)	Pr(1)	N(4)	C(17)	-35.8(2)
O(2)	Pr(1)	N(4)	C(21)	145.2(2)	O(2)	C(24)	C(23)	C(22)	3.7(4)
O(2)	C(24)	C(23)	C(28)	-175.0(2)	O(2)	C(24)	C(25)	C(26)	175.0(3)
O(3)	Pr(1)	O(1)	C(11)	-154.9(3)	O(3)	Pr(1)	O(2)	C(24)	84.4(2)
O(3)	Pr(1)	O(4)	C(52)	-165.6(2)	O(3)	Pr(1)	N(1)	C(1)	-115.5(2)
O(3)	Pr(1)	N(1)	C(3)	125.3(2)	O(3)	Pr(1)	N(1)	C(9)	6.2(3)
O(3)	Pr(1)	N(2)	C(2)	148.7(2)	O(3)	Pr(1)	N(2)	C(16)	29.9(2)
O(3)	Pr(1)	N(2)	C(22)	-91.2(2)	O(3)	Pr(1)	N(3)	C(4)	-146.4(2)
O(3)	Pr(1)	N(3)	C(8)	28.7(3)	O(3)	Pr(1)	N(4)	C(17)	-108.0(2)
O(3)	Pr(1)	N(4)	C(21)	72.9(2)	O(3)	Pr(2)	O(4)	C(52)	167.2(2)
O(3)	Pr(2)	O(5)	N(9)	-126.8(2)	O(3)	Pr(2)	O(6)	N(9)	117.4(2)
O(3)	Pr(2)	N(5)	C(29)	-140.4(2)	O(3)	Pr(2)	N(5)	C(31)	102.6(2)
O(3)	Pr(2)	N(5)	C(37)	-20.0(2)	O(3)	Pr(2)	N(6)	C(30)	60.4(2)
O(3)	Pr(2)	N(6)	C(44)	178.69(15)	O(3)	Pr(2)	N(6)	C(50)	-57.1(2)
O(3)	Pr(2)	N(7)	C(32)	-76.9(2)	O(3)	Pr(2)	N(7)	C(36)	88.0(2)
O(3)	Pr(2)	N(8)	C(45)	95.3(2)	O(3)	Pr(2)	N(8)	C(49)	-93.6(3)
O(3)	C(39)	C(38)	C(37)	-7.4(4)	O(3)	C(39)	C(38)	C(43)	174.9(3)
O(3)	C(39)	C(40)	C(41)	-177.1(3)	O(4)	Pr(1)	O(1)	C(11)	138.7(3)
O(4)	Pr(1)	O(2)	C(24)	152.3(2)	O(4)	Pr(1)	O(3)	C(39)	171.5(2)
O(4)	Pr(1)	N(1)	C(1)	134.5(2)	O(4)	Pr(1)	N(1)	C(3)	15.2(2)
O(4)	Pr(1)	N(1)	C(9)	-103.9(2)	O(4)	Pr(1)	N(2)	C(2)	-123.6(2)
O(4)	Pr(1)	N(2)	C(16)	117.6(2)	O(4)	Pr(1)	N(2)	C(22)	-3.5(3)
O(4)	Pr(1)	N(3)	C(4)	-109.6(2)	O(4)	Pr(1)	N(3)	C(8)	65.5(2)
O(4)	Pr(1)	N(4)	C(17)	-148.7(2)	O(4)	Pr(1)	N(4)	C(21)	32.2(3)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(4)	Pr(2)	O(3)	C(39)	-171.3(2)	O(4)	Pr(2)	O(5)	N(9)	132.65(15)
O(4)	Pr(2)	O(6)	N(9)	-102.7(2)	O(4)	Pr(2)	N(5)	C(29)	-85.0(2)
O(4)	Pr(2)	N(5)	C(31)	158.1(2)	O(4)	Pr(2)	N(5)	C(37)	35.5(2)
O(4)	Pr(2)	N(6)	C(30)	123.1(2)	O(4)	Pr(2)	N(6)	C(44)	-118.6(2)
O(4)	Pr(2)	N(6)	C(50)	5.6(2)	O(4)	Pr(2)	N(7)	C(32)	-99.6(2)
O(4)	Pr(2)	N(7)	C(36)	65.2(3)	O(4)	Pr(2)	N(8)	C(45)	98.5(2)
O(4)	Pr(2)	N(8)	C(49)	-90.4(2)	O(4)	C(52)	C(51)	C(50)	-1.4(4)
O(4)	C(52)	C(51)	C(56)	178.0(3)	O(4)	C(52)	C(53)	C(54)	-177.6(3)
O(5)	Pr(2)	O(3)	C(39)	62.1(2)	O(5)	Pr(2)	O(4)	C(52)	-61.1(2)
O(5)	Pr(2)	O(6)	N(9)	2.2(2)	O(5)	Pr(2)	N(5)	C(29)	87.6(2)
O(5)	Pr(2)	N(5)	C(31)	-29.3(2)	O(5)	Pr(2)	N(5)	C(37)	-152.0(2)
O(5)	Pr(2)	N(6)	C(30)	-108.9(2)	O(5)	Pr(2)	N(6)	C(44)	9.4(2)
O(5)	Pr(2)	N(6)	C(50)	133.5(2)	O(5)	Pr(2)	N(7)	C(32)	131.4(2)
O(5)	Pr(2)	N(7)	C(36)	-63.8(2)	O(5)	Pr(2)	N(8)	C(45)	-120.4(2)
O(5)	Pr(2)	N(8)	C(49)	50.7(2)	O(6)	Pr(2)	O(3)	C(39)	-14.0(3)
O(6)	Pr(2)	O(4)	C(52)	13.6(3)	O(6)	Pr(2)	O(5)	N(9)	-2.2(2)
O(6)	Pr(2)	N(5)	C(29)	59.5(2)	O(6)	Pr(2)	N(5)	C(31)	-57.4(2)
O(6)	Pr(2)	N(5)	C(37)	179.9(2)	O(6)	Pr(2)	N(6)	C(30)	-78.7(2)
O(6)	Pr(2)	N(6)	C(44)	39.63(15)	O(6)	Pr(2)	N(6)	C(50)	163.8(2)
O(6)	Pr(2)	N(7)	C(32)	78.8(2)	O(6)	Pr(2)	N(7)	C(36)	-116.4(2)
O(6)	Pr(2)	N(8)	C(45)	-67.0(2)	O(6)	Pr(2)	N(8)	C(49)	104.1(2)
O(8)	Pr(2)	O(3)	C(39)	111.4(2)	O(8)	Pr(2)	O(4)	C(52)	-108.7(2)
O(8)	Pr(2)	O(5)	N(9)	-178.7(2)	O(8)	Pr(2)	O(6)	N(9)	6.1(2)
O(8)	Pr(2)	N(5)	C(29)	177.87(15)	O(8)	Pr(2)	N(5)	C(31)	61.0(2)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(8)	Pr(2)	N(5)	C(37)	-61.7(2)	O(8)	Pr(2)	N(6)	C(30)	151.9(2)
O(8)	Pr(2)	N(6)	C(44)	-89.8(2)	O(8)	Pr(2)	N(6)	C(50)	34.4(2)
O(8)	Pr(2)	N(7)	C(32)	-156.8(2)	O(8)	Pr(2)	N(7)	C(36)	8.1(2)
O(8)	Pr(2)	N(8)	C(45)	171.8(2)	O(8)	Pr(2)	N(8)	C(49)	-17.1(2)
N(1)	Pr(1)	O(1)	C(11)	9.4(3)	N(1)	Pr(1)	O(2)	C(24)	-82.7(2)
N(1)	Pr(1)	O(3)	C(39)	51.1(3)	N(1)	Pr(1)	O(4)	C(52)	-8.1(3)
N(1)	Pr(1)	N(2)	C(2)	-7.2(2)	N(1)	Pr(1)	N(2)	C(16)	-125.9(2)
N(1)	Pr(1)	N(2)	C(22)	113.0(2)	N(1)	Pr(1)	N(3)	C(4)	25.2(2)
N(1)	Pr(1)	N(3)	C(8)	-159.7(3)	N(1)	Pr(1)	N(4)	C(17)	83.3(2)
N(1)	Pr(1)	N(4)	C(21)	-95.8(2)	N(1)	C(1)	C(2)	N(2)	-63.0(3)
N(1)	C(3)	C(4)	N(3)	-36.5(3)	N(1)	C(3)	C(4)	C(5)	143.0(3)
N(1)	C(9)	C(10)	C(11)	-50.2(4)	N(1)	C(9)	C(10)	C(15)	133.8(3)
N(2)	Pr(1)	O(1)	C(11)	-34.9(4)	N(2)	Pr(1)	O(2)	C(24)	-34.4(2)
N(2)	Pr(1)	O(3)	C(39)	-31.9(2)	N(2)	Pr(1)	O(4)	C(52)	97.4(3)
N(2)	Pr(1)	N(1)	C(1)	-22.6(2)	N(2)	Pr(1)	N(1)	C(3)	-141.9(2)
N(2)	Pr(1)	N(1)	C(9)	99.0(2)	N(2)	Pr(1)	N(3)	C(4)	88.8(2)
N(2)	Pr(1)	N(3)	C(8)	-96.2(2)	N(2)	Pr(1)	N(4)	C(17)	15.9(2)
N(2)	Pr(1)	N(4)	C(21)	-163.2(2)	N(2)	C(16)	C(17)	N(4)	-38.1(3)
N(2)	C(16)	C(17)	C(18)	142.8(3)	N(2)	C(22)	C(23)	C(24)	-67.7(4)
N(2)	C(22)	C(23)	C(28)	111.0(3)	N(3)	Pr(1)	O(1)	C(11)	61.3(3)
N(3)	Pr(1)	O(2)	C(24)	-126.5(2)	N(3)	Pr(1)	O(3)	C(39)	-148.7(2)
N(3)	Pr(1)	O(4)	C(52)	39.0(2)	N(3)	Pr(1)	N(1)	C(1)	78.9(2)
N(3)	Pr(1)	N(1)	C(3)	-40.3(2)	N(3)	Pr(1)	N(1)	C(9)	-159.5(2)
N(3)	Pr(1)	N(2)	C(2)	-66.4(2)	N(3)	Pr(1)	N(2)	C(16)	174.8(2)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(3)	Pr(1)	N(2)	C(22)	53.7(2)	N(3)	Pr(1)	N(4)	C(17)	61.3(2)
N(3)	Pr(1)	N(4)	C(21)	-117.8(2)	N(3)	C(4)	C(5)	C(6)	-1.8(5)
N(3)	C(8)	C(7)	C(6)	-0.8(5)	N(4)	Pr(1)	O(1)	C(11)	-76.4(3)
N(4)	Pr(1)	O(2)	C(24)	11.3(2)	N(4)	Pr(1)	O(3)	C(39)	20.3(2)
N(4)	Pr(1)	O(4)	C(52)	-121.6(2)	N(4)	Pr(1)	N(1)	C(1)	-84.8(2)
N(4)	Pr(1)	N(1)	C(3)	155.9(2)	N(4)	Pr(1)	N(1)	C(9)	36.8(2)
N(4)	Pr(1)	N(2)	C(2)	85.8(2)	N(4)	Pr(1)	N(2)	C(16)	-33.0(2)
N(4)	Pr(1)	N(2)	C(22)	-154.1(2)	N(4)	Pr(1)	N(3)	C(4)	50.2(2)
N(4)	Pr(1)	N(3)	C(8)	-134.7(2)	N(4)	C(17)	C(18)	C(19)	-2.8(5)
N(4)	C(21)	C(20)	C(19)	-1.5(5)	N(5)	Pr(2)	O(3)	C(39)	-44.3(2)
N(5)	Pr(2)	O(4)	C(52)	110.0(2)	N(5)	Pr(2)	O(5)	N(9)	-38.5(2)
N(5)	Pr(2)	O(6)	N(9)	147.7(2)	N(5)	Pr(2)	N(6)	C(30)	-3.1(2)
N(5)	Pr(2)	N(6)	C(44)	115.1(2)	N(5)	Pr(2)	N(6)	C(50)	-120.7(2)
N(5)	Pr(2)	N(7)	C(32)	-0.1(2)	N(5)	Pr(2)	N(7)	C(36)	164.8(3)
N(5)	Pr(2)	N(8)	C(45)	-15.2(2)	N(5)	Pr(2)	N(8)	C(49)	155.9(2)
N(5)	C(29)	C(30)	N(6)	-62.6(3)	N(5)	C(31)	C(32)	N(7)	42.1(4)
N(5)	C(31)	C(32)	C(33)	-143.1(3)	N(5)	C(37)	C(38)	C(39)	-64.5(3)
N(5)	C(37)	C(38)	C(43)	113.1(3)	N(6)	Pr(2)	O(3)	C(39)	-104.8(2)
N(6)	Pr(2)	O(4)	C(52)	54.5(2)	N(6)	Pr(2)	O(5)	N(9)	38.5(2)
N(6)	Pr(2)	O(6)	N(9)	-142.5(2)	N(6)	Pr(2)	N(5)	C(29)	-25.9(2)
N(6)	Pr(2)	N(5)	C(31)	-142.8(2)	N(6)	Pr(2)	N(5)	C(37)	94.5(2)
N(6)	Pr(2)	N(7)	C(32)	20.3(3)	N(6)	Pr(2)	N(7)	C(36)	-174.9(2)
N(6)	Pr(2)	N(8)	C(45)	21.4(2)	N(6)	Pr(2)	N(8)	C(49)	-167.5(2)
N(6)	C(44)	C(45)	N(8)	-26.8(4)	N(6)	C(44)	C(45)	C(46)	155.8(3)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(6)	C(50)	C(51)	C(52)	73.4(3)	N(6)	C(50)	C(51)	C(56)	-106.0(3)
N(7)	Pr(2)	O(3)	C(39)	23.6(2)	N(7)	Pr(2)	O(4)	C(52)	-169.1(2)
N(7)	Pr(2)	O(5)	N(9)	-86.5(2)	N(7)	Pr(2)	O(6)	N(9)	79.0(2)
N(7)	Pr(2)	N(5)	C(29)	137.3(2)	N(7)	Pr(2)	N(5)	C(31)	20.4(2)
N(7)	Pr(2)	N(5)	C(37)	-102.2(2)	N(7)	Pr(2)	N(6)	C(30)	-23.1(2)
N(7)	Pr(2)	N(6)	C(44)	95.2(2)	N(7)	Pr(2)	N(6)	C(50)	-140.6(2)
N(7)	Pr(2)	N(8)	C(45)	-100.2(2)	N(7)	Pr(2)	N(8)	C(49)	70.9(2)
N(7)	C(32)	C(33)	C(34)	1.8(4)	N(7)	C(36)	C(35)	C(34)	1.8(5)
N(8)	Pr(2)	O(3)	C(39)	-167.8(2)	N(8)	Pr(2)	O(4)	C(52)	-11.0(2)
N(8)	Pr(2)	O(5)	N(9)	78.0(2)	N(8)	Pr(2)	O(6)	N(9)	-76.6(2)
N(8)	Pr(2)	N(5)	C(29)	9.4(2)	N(8)	Pr(2)	N(5)	C(31)	-107.5(2)
N(8)	Pr(2)	N(5)	C(37)	129.9(2)	N(8)	Pr(2)	N(6)	C(30)	-150.0(2)
N(8)	Pr(2)	N(6)	C(44)	-31.75(15)	N(8)	Pr(2)	N(6)	C(50)	92.4(2)
N(8)	Pr(2)	N(7)	C(32)	111.2(2)	N(8)	Pr(2)	N(7)	C(36)	-84.0(3)
N(8)	C(45)	C(46)	C(47)	0.1(5)	N(8)	C(49)	C(48)	C(47)	-0.3(5)
C(1)	N(1)	C(3)	C(4)	-62.0(3)	C(1)	N(1)	C(9)	C(10)	-170.8(2)
C(1)	C(2)	N(2)	C(16)	156.2(2)	C(1)	C(2)	N(2)	C(22)	-84.4(3)
C(2)	N(2)	C(16)	C(17)	-70.5(3)	C(2)	N(2)	C(22)	C(23)	-171.5(2)
C(2)	C(1)	N(1)	C(3)	169.4(3)	C(2)	C(1)	N(1)	C(9)	-71.6(3)
C(3)	N(1)	C(9)	C(10)	-50.7(3)	C(3)	C(4)	N(3)	C(8)	179.6(3)
C(3)	C(4)	C(5)	C(6)	178.7(3)	C(4)	N(3)	C(8)	C(7)	1.2(5)
C(4)	C(3)	N(1)	C(9)	179.0(2)	C(4)	C(5)	C(6)	C(7)	2.2(5)
C(5)	C(4)	N(3)	C(8)	0.1(4)	C(5)	C(6)	C(7)	C(8)	-0.9(5)
C(9)	C(10)	C(11)	C(12)	-171.5(3)	C(9)	C(10)	C(15)	C(14)	172.6(3)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(10)	C(11)	C(12)	C(13)	-2.4(4)	C(10)	C(15)	C(14)	C(13)	0.3(5)
C(11)	C(10)	C(15)	C(14)	-3.5(5)	C(11)	C(12)	C(13)	C(14)	-0.7(5)
C(12)	C(11)	C(10)	C(15)	4.4(4)	C(12)	C(13)	C(14)	C(15)	1.8(5)
C(16)	N(2)	C(22)	C(23)	-53.4(3)	C(16)	C(17)	N(4)	C(21)	-176.5(2)
C(16)	C(17)	C(18)	C(19)	176.1(3)	C(17)	N(4)	C(21)	C(20)	-0.2(4)
C(17)	C(16)	N(2)	C(22)	171.1(2)	C(17)	C(18)	C(19)	C(20)	0.9(5)
C(18)	C(17)	N(4)	C(21)	2.4(4)	C(18)	C(19)	C(20)	C(21)	1.1(5)
C(22)	C(23)	C(24)	C(25)	-177.7(2)	C(22)	C(23)	C(28)	C(27)	-179.9(3)
C(23)	C(24)	C(25)	C(26)	-3.7(4)	C(23)	C(28)	C(27)	C(26)	-1.4(5)
C(24)	C(23)	C(28)	C(27)	-1.1(4)	C(24)	C(25)	C(26)	C(27)	1.1(5)
C(25)	C(24)	C(23)	C(28)	3.6(4)	C(25)	C(26)	C(27)	C(28)	1.4(5)
C(29)	N(5)	C(31)	C(32)	-155.4(3)	C(29)	N(5)	C(37)	C(38)	-172.3(2)
C(29)	C(30)	N(6)	C(44)	-85.7(3)	C(29)	C(30)	N(6)	C(50)	153.9(2)
C(30)	N(6)	C(44)	C(45)	163.8(2)	C(30)	N(6)	C(50)	C(51)	179.7(2)
C(30)	C(29)	N(5)	C(31)	173.7(2)	C(30)	C(29)	N(5)	C(37)	-66.7(3)
C(31)	N(5)	C(37)	C(38)	-53.6(3)	C(31)	C(32)	N(7)	C(36)	173.9(3)
C(31)	C(32)	C(33)	C(34)	-172.7(3)	C(32)	N(7)	C(36)	C(35)	-0.9(5)
C(32)	C(31)	N(5)	C(37)	84.6(3)	C(32)	C(33)	C(34)	C(35)	-0.8(5)
C(33)	C(32)	N(7)	C(36)	-0.9(4)	C(33)	C(34)	C(35)	C(36)	-0.9(5)
C(37)	C(38)	C(39)	C(40)	171.8(3)	C(37)	C(38)	C(43)	C(42)	-174.3(3)
C(38)	C(39)	C(40)	C(41)	3.7(4)	C(38)	C(43)	C(42)	C(41)	1.6(5)
C(39)	C(38)	C(43)	C(42)	3.2(4)	C(39)	C(40)	C(41)	C(42)	1.2(5)
C(40)	C(39)	C(38)	C(43)	-5.8(4)	C(40)	C(41)	C(42)	C(43)	-3.9(5)
C(44)	N(6)	C(50)	C(51)	62.3(3)	C(44)	C(45)	N(8)	C(49)	-178.4(3)

Table 9. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(44)	C(45)	C(46)	C(47)	177.3(3)	C(45)	N(8)	C(49)	C(48)	1.2(5)
C(45)	C(44)	N(6)	C(50)	-80.3(3)	C(45)	C(46)	C(47)	C(48)	0.9(6)
C(46)	C(45)	N(8)	C(49)	-1.1(4)	C(46)	C(47)	C(48)	C(49)	-0.7(6)
C(50)	C(51)	C(52)	C(53)	-177.3(3)	C(50)	C(51)	C(56)	C(55)	178.1(3)
C(51)	C(52)	C(53)	C(54)	-1.7(4)	C(51)	C(56)	C(55)	C(54)	0.1(5)
C(52)	C(51)	C(56)	C(55)	-1.3(5)	C(52)	C(53)	C(54)	C(55)	0.5(5)
C(53)	C(52)	C(51)	C(56)	2.1(4)	C(53)	C(54)	C(55)	C(56)	0.3(5)

Table 10. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O(5)	C(19)	3.468(4)	54501	O(6)	C(33)	3.403(3)	65602
O(7)	C(33)	3.562(4)	65602	O(8)	O(10)	2.686(3)	1
O(8)	O(9)	3.394(4)	1	O(8)	N(10)	3.455(4)	1
O(9)	O(12)	3.284(4)	1	O(9)	C(57)	3.334(6)	1
O(9)	C(53)	3.468(4)	1	O(9)	C(30)	3.482(4)	45501
O(10)	C(35)	3.263(4)	55602	O(10)	C(34)	3.286(5)	55602
O(10)	C(18)	3.305(4)	54501	O(10)	C(19)	3.424(5)	54501
O(11)	O(12)	2.851(4)	1	O(11)	C(2)	3.315(4)	54501
O(11)	C(44)	3.414(4)	45501	O(11)	C(18)	3.437(4)	54501
O(12)	C(46)	3.371(5)	45501	O(12)	C(1)	3.372(4)	54501
O(12)	C(44)	3.404(4)	45501	O(12)	N(10)	3.441(4)	1
O(12)	C(9)	3.477(4)	54501	O(12)	C(2)	3.524(4)	54501
C(3)	C(5)	3.530(4)	56502	C(6)	C(14)	3.560(5)	56502
C(14)	C(47)	3.555(5)	56501	C(20)	C(48)	3.574(5)	56501
C(31)	C(33)	3.561(4)	65602	C(41)	C(41)	3.417(7)	56602
O(5)	H(22)	2.60	54501	O(6)	H(37)	2.78	65602
O(7)	H(37)	2.60	65602	O(7)	H(29)	2.95	55602
O(9)	H(59)	2.51	1	O(9)	H(33)	2.62	45501
O(9)	H(55)	2.64	1	O(9)	H(2)	2.65	1
O(9)	H(12)	2.93	1	O(9)	H(60)	2.94	1
O(10)	H(2)	1.89	1	O(10)	H(39)	2.63	55602
O(10)	H(38)	2.67	55602	O(10)	H(52)	2.87	1
O(10)	H(21)	2.93	54501	O(11)	H(59)	1.93	1
O(11)	H(6)	2.57	54501	O(11)	H(48)	2.58	45501

Table 10. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(11)	H(38)	2.86	55602	O(12)	H(49)	2.49	45501
O(12)	H(3)	2.57	54501	O(12)	H(13)	2.71	54501
O(12)	H(47)	2.76	45501	N(9)	H(37)	2.90	65602
N(10)	H(59)	2.52	1	N(10)	H(2)	2.61	1
C(5)	H(8)	2.79	56502	C(6)	H(16)	2.97	45501
C(6)	H(8)	2.99	56502	C(11)	H(10)	3.00	56502
C(12)	H(10)	2.78	56502	C(13)	H(10)	2.70	56502
C(13)	H(50)	2.98	56501	C(14)	H(50)	2.78	56501
C(14)	H(10)	2.80	56502	C(15)	H(10)	2.99	56502
C(18)	H(44)	2.88	56602	C(27)	H(46)	2.76	45501
C(28)	H(45)	2.82	56602	C(28)	H(46)	2.93	45501
C(33)	H(35)	2.66	65602	C(34)	H(35)	2.77	65602
C(34)	H(21)	2.88	56602	C(41)	H(44)	2.78	56602
C(54)	H(7)	2.86	56502	C(55)	H(7)	2.90	56502
C(57)	H(18)	2.90	56502	H(8)	H(9)	2.53	56502
H(11)	H(33)	2.46	45501	H(11)	H(54)	2.57	45501
H(17)	H(58)	2.30	66502	H(18)	H(61)	2.42	56502
H(18)	H(60)	2.59	56502	H(20)	H(45)	2.44	56602
H(21)	H(38)	2.43	56602	H(21)	H(44)	2.60	56602
H(29)	H(46)	2.57	45501	H(44)	H(44)	2.39	56602
H(47)	H(59)	2.58	65501	H(56)	H(62)	2.60	1

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ±4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	x,	y,	z	(2)	-x,	-y,	-z

Table 11. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
N(3)	0.004(2)
C(4)	0.004(3)
C(5)	-0.012(3)
C(6)	0.011(3)
C(7)	0.002(3)
C(8)	-0.010(3)
Additional Atoms	**Distance**
Pr(1)	0.221
C(3)	0.011

Plane number 2

Atoms defining plane	Distance
N(4)	-0.005(2)
C(17)	0.015(3)
C(18)	-0.012(3)
C(19)	-0.004(3)
C(20)	0.012(3)
C(21)	-0.004(3)
Additional Atoms	**Distance**
Pr(1)	-0.083
C(16)	0.095

Plane number 3

Atoms defining plane	Distance
C(10)	0.022(3)
C(11)	-0.019(3)
C(12)	0.004(3)
C(13)	0.015(3)
C(14)	-0.012(3)
C(15)	-0.010(3)
Additional Atoms	**Distance**
Pr(1)	-0.269
O(1)	-0.081
C(9)	0.193

Plane number 4

Atoms defining plane	Distance
C(23)	-0.013(3)
C(24)	0.020(3)
C(25)	-0.015(3)
C(26)	-0.006(3)
C(27)	0.016(3)
C(28)	-0.003(3)

Additional Atoms	Distance
Pr(1)	1.585
O(2)	0.111
C(22)	-0.031
H(1)	0.103

Plane number 5

Atoms defining plane	Distance
N(7)	-0.001(2)
C(32)	0.009(3)
C(33)	-0.009(3)
C(34)	0.000(3)
C(35)	0.010(3)
C(36)	-0.009(3)

Additional Atoms	Distance
Pr(2)	-0.590
C(31)	0.162

Plane number 6

Atoms defining plane	Distance
N(8)	0.005(2)
C(45)	-0.004(3)
C(46)	-0.003(3)
C(47)	0.008(4)
C(48)	-0.002(4)
C(49)	-0.006(3)

Additional Atoms	Distance
Pr(2)	0.388
C(44)	0.046

Plane number 7

Atoms defining plane	Distance
C(38)	0.027(3)
C(39)	-0.028(3)
C(40)	0.010(3)
C(41)	0.023(3)
C(42)	-0.025(3)
C(43)	-0.006(3)

Additional Atoms	Distance
O(3)	-0.101
C(37)	0.172

Plane number 8

Atoms defining plane	Distance
C(51)	0.009(3)
C(52)	-0.010(3)
C(53)	0.006(3)
C(54)	0.002(3)
C(55)	-0.005(3)
C(56)	-0.002(3)

Additional Atoms	Distance
O(4)	0.042
C(50)	0.053

Plane number 9

Atoms defining plane	Distance
O(5)	-0.001(2)
O(6)	-0.002(2)
O(7)	-0.003(3)
N(9)	0.006(3)

Additional Atoms	Distance
Pr(2)	0.144

Plane number 10

Atoms defining plane	Distance
O(9)	-0.009(4)
O(10)	-0.005(3)
O(11)	-0.010(4)
N(10)	0.019(3)

Additional Atoms	Distance
H(2)	0.370
H(59)	0.616

$[Pr_2(L1)_2(NO_3)(H_2O)]\,NO_3 \bullet CH_3OH$

Summary

plane	mean deviation	χ^2
1	0.0070	36.9
2	0.0088	70.4
3	0.0137	168.6
4	0.0122	137.4
5	0.0063	37.7
6	0.0046	15.1
7	0.0197	335.7
8	0.0056	28.4
9	0.0029	6.4
10	0.0106	46.7

Dihedral angles between planes (°)

plane	1	2	3	4	5	6	7	8	9
2	78.5								
3	111.8	69.5							
4	79.0	74.9	35.8						
5	41.2	40.9	101.5	86.1					
6	73.1	10.5	64.7	65.3	39.9				
7	61.0	23.9	92.0	88.2	20.0	27.4			
8	58.9	25.3	92.7	87.6	17.9	27.9	2.2		
9	58.5	125.1	154.5	122.1	85.5	125.3	101.2	99.8	
10	9.4	85.6	109.4	74.8	50.0	79.2	69.7	67.5	56.8

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{57}H_{66}Gd_2N_{10}O_{14}$
Formula Weight	1429.71
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.20 X 0.25 X 0.35 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 12.9850(7) Å b = 21.5181(15) Å c = 22.1460(2) Å β = 106.9883(2)°
	V = 5917.9(4) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.605 g/cm^3
F_{000}	2872.00
μ(MoKα)	23.01 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku/ADSC CCD
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Aperture	94 mm x 94 mm
Data Images	768 exposures of 30.0 seconds
ϕ oscillation Range (χ=-90)	0.0 - 189.9°

ω oscillation Range (χ=-90)	-23.0 - 17.8°
Detector Position	39.226(4) mm
Detector Swing Angle	-10.0°
$2\theta_{max}$	60.1°
No. of Reflections Measured	Total: 54984 Unique: 14195 (R_{int} = 0.043)
Corrections	Lorentz-polarization Absorption/decay/scaling (corr. factors: 0.6275 - 1.0000)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo^2\| - \|Fc^2\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo^2)}$
p-factor	0.0000
Anomalous Dispersion	All non-hydrogen atoms
No. Observations	14195
No. Variables	748
Reflection/Parameter Ratio	18.98
Residuals (on F^2, all data): R; Rw	0.069 ; 0.066
Goodness of Fit Indicator	1.26
No. Observations (I>3σ(I))	8278
Residuals (on F, I>3σ(I)): R; Rw	0.037 ; 0.029
Max Shift/Error in Final Cycle	0.01
Maximum peak in Final Diff. Map	3.39 $e^-/\AA^3$ (near Gd)
Minimum peak in Final Diff. Map	-2.62 $e^-/\AA^3$ (near Gd)

$[Gd_2(L1)_2(NO_3)]\ NO_3 \bullet CH_3OH \bullet 3H_2O$

Table 2. Atomic coordinates and B_{eq}

atom	x	y	z	B_{eq}
Gd(1)	0.20933(2)	0.219494(11)	0.356219(10)	1.323(5)
Gd(2)	0.33720(2)	0.079078(11)	0.321536(10)	1.451(5)
O(1)	0.2800(3)	0.31462(13)	0.36380(13)	1.52(7)
O(2)	0.2502(2)	0.11458(13)	0.39356(12)	1.50(7)
O(3)	0.3859(2)	0.18449(14)	0.34134(13)	1.51(7)
O(4)	0.1927(2)	0.15222(14)	0.26874(12)	1.54(7)
O(5)	0.4245(3)	-0.02368(15)	0.32309(13)	2.10(8)
O(6)	0.3777(3)	-0.00106(14)	0.40743(13)	1.90(8)
O(7)	0.4587(3)	-0.0893(2)	0.40196(15)	3.24(10)
O(8)	0.4564(8)	0.0615(4)	0.0351(4)	14.7(3)
O(9)	0.3607(6)	0.1410(4)	-0.0041(3)	12.9(3)
O(10)	0.4860(5)	0.1493(3)	0.0826(3)	9.1(2)
O(11)	0.4555(4)	0.2833(2)	0.0551(2)	6.32(15)
O(12)	0.3891(6)	0.0237(3)	-0.0948(3)	13.2(3)
O(13)	0.6990(4)	0.1351(2)	0.1692(2)	5.88(14)
O(14)	0.2195(9)	-0.0063(4)	-0.2002(3)	20.6(4)
N(1)	0.0968(3)	0.2894(2)	0.41806(15)	1.60(9)
N(2)	0.0184(3)	0.1708(2)	0.3514(2)	1.58(9)
N(3)	0.2940(3)	0.2292(2)	0.47276(15)	1.54(9)
N(4)	0.0464(3)	0.2679(2)	0.2703(2)	1.68(9)
N(5)	0.4801(3)	0.0871(2)	0.2615(2)	1.76(9)
N(6)	0.2615(3)	0.0409(2)	0.2006(2)	1.99(10)
N(7)	0.5395(3)	0.0839(2)	0.3945(2)	1.65(9)
N(8)	0.1931(3)	-0.0115(2)	0.2995(2)	1.97(9)

Table 2. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
N(9)	0.4219(3)	-0.0396(2)	0.3787(2)	2.12(10)
N(10)	0.4316(7)	0.1168(5)	0.0362(3)	7.0(3)
C(1)	-0.0199(4)	0.2739(2)	0.3961(2)	1.75(11)
C(2)	-0.0389(4)	0.2051(2)	0.3909(2)	1.93(11)
C(3)	0.1372(4)	0.2785(2)	0.4878(2)	1.97(11)
C(4)	0.2555(4)	0.2660(2)	0.5094(2)	1.78(11)
C(5)	0.3200(4)	0.2871(2)	0.5676(2)	2.34(12)
C(6)	0.4250(4)	0.2675(3)	0.5885(2)	2.64(13)
C(7)	0.4654(4)	0.2271(3)	0.5517(2)	2.41(12)
C(8)	0.3976(4)	0.2101(2)	0.4943(2)	2.03(11)
C(9)	0.1062(4)	0.3577(2)	0.4055(2)	1.70(11)
C(10)	0.2193(4)	0.3811(2)	0.4320(2)	1.88(11)
C(11)	0.3020(4)	0.3575(2)	0.4088(2)	1.51(10)
C(12)	0.4064(4)	0.3810(2)	0.4339(2)	1.96(11)
C(13)	0.4287(4)	0.4267(3)	0.4805(2)	2.80(13)
C(14)	0.3471(5)	0.4499(3)	0.5027(2)	3.12(14)
C(15)	0.2429(4)	0.4273(2)	0.4783(2)	2.51(12)
C(16)	-0.0451(4)	0.1740(2)	0.2835(2)	2.08(11)
C(17)	-0.0496(4)	0.2377(2)	0.2566(2)	1.66(11)
C(18)	-0.1446(4)	0.2633(2)	0.2205(2)	2.04(11)
C(19)	-0.1440(4)	0.3225(3)	0.1967(2)	2.61(13)
C(20)	-0.0471(4)	0.3547(2)	0.2094(2)	2.19(12)
C(21)	0.0464(4)	0.3255(2)	0.2455(2)	2.07(12)
C(22)	0.0271(4)	0.1039(2)	0.3691(2)	2.05(11)

Table 2. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
C(23)	0.1030(4)	0.0909(2)	0.4334(2)	1.76(11)
C(24)	0.2141(4)	0.0948(2)	0.4417(2)	1.59(11)
C(25)	0.2857(4)	0.0771(2)	0.4996(2)	1.78(10)
C(26)	0.2458(4)	0.0575(2)	0.5488(2)	2.41(12)
C(27)	0.1357(5)	0.0548(3)	0.5409(2)	2.73(13)
C(28)	0.0654(4)	0.0707(2)	0.4835(2)	2.46(12)
C(29)	0.4543(4)	0.0434(2)	0.2063(2)	2.14(12)
C(30)	0.3431(4)	0.0497(2)	0.1655(2)	2.26(12)
C(31)	0.5923(4)	0.0743(2)	0.2993(2)	2.08(11)
C(32)	0.6188(4)	0.0924(2)	0.3674(2)	1.84(11)
C(33)	0.7201(4)	0.1117(2)	0.4004(2)	2.25(12)
C(34)	0.7451(4)	0.1245(3)	0.4643(2)	2.69(13)
C(35)	0.6653(4)	0.1132(2)	0.4934(2)	2.51(12)
C(36)	0.5657(4)	0.0937(2)	0.4576(2)	2.00(11)
C(37)	0.4726(4)	0.1531(2)	0.2381(2)	1.96(11)
C(38)	0.5202(4)	0.1998(2)	0.2884(2)	1.91(11)
C(39)	0.4756(4)	0.2129(2)	0.3379(2)	1.45(10)
C(40)	0.5294(4)	0.2555(2)	0.3847(2)	2.07(12)
C(41)	0.6218(4)	0.2849(2)	0.3817(2)	2.56(12)
C(42)	0.6648(4)	0.2741(3)	0.3324(3)	2.77(13)
C(43)	0.6139(4)	0.2309(2)	0.2868(2)	2.43(12)
C(44)	0.2414(5)	-0.0266(2)	0.2021(2)	2.74(13)
C(45)	0.1786(4)	-0.0451(2)	0.2464(2)	2.19(12)
C(46)	0.1180(5)	-0.0986(2)	0.2353(2)	2.72(13)

Table 2. Atomic coordinates and B_{eq} (continued)

atom	x	y	z	B_{eq}
C(47)	0.0682(5)	-0.1181(3)	0.2796(3)	3.20(14)
C(48)	0.0845(4)	-0.0837(2)	0.3350(2)	2.66(13)
C(49)	0.1463(4)	-0.0316(2)	0.3422(2)	2.07(12)
C(50)	0.1572(4)	0.0715(2)	0.1657(2)	2.29(12)
C(51)	0.1748(4)	0.1398(2)	0.1588(2)	1.81(11)
C(52)	0.1976(4)	0.1781(2)	0.2127(2)	1.75(11)
C(53)	0.2294(4)	0.2388(2)	0.2088(2)	1.81(11)
C(54)	0.2391(4)	0.2622(2)	0.1522(2)	2.39(12)
C(55)	0.2160(4)	0.2255(3)	0.0983(2)	2.69(13)
C(56)	0.1836(4)	0.1650(3)	0.1023(2)	2.71(13)
C(57)	0.5441(8)	0.2850(4)	0.1092(3)	8.7(3)

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

$[Gd_2(L1)_2(NO_3)]\ NO_3 \bullet CH_3OH \bullet 3H_2O$

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Gd(1)	Gd(2)	3.6362(3)	Gd(1)	O(1)	2.230(3)
Gd(1)	O(2)	2.409(3)	Gd(1)	O(3)	2.524(3)
Gd(1)	O(4)	2.377(3)	Gd(1)	N(1)	2.728(3)
Gd(1)	N(2)	2.665(4)	Gd(1)	N(3)	2.501(3)
Gd(1)	N(4)	2.613(4)	Gd(2)	O(2)	2.336(3)
Gd(2)	O(3)	2.361(3)	Gd(2)	O(4)	2.467(3)
Gd(2)	O(5)	2.481(3)	Gd(2)	O(6)	2.507(3)
Gd(2)	N(5)	2.586(3)	Gd(2)	N(6)	2.697(4)
Gd(2)	N(7)	2.654(4)	Gd(2)	N(8)	2.647(4)
O(1)	C(11)	1.327(5)	O(2)	C(24)	1.352(4)
O(3)	C(39)	1.338(5)	O(4)	C(52)	1.378(5)
O(5)	N(9)	1.289(4)	O(6)	N(9)	1.280(4)
O(7)	N(9)	1.220(5)	O(8)	N(10)	1.235(9)
O(9)	N(10)	1.196(9)	O(10)	N(10)	1.273(8)
O(11)	C(57)	1.398(9)	N(1)	C(1)	1.487(6)
N(1)	C(3)	1.497(5)	N(1)	C(9)	1.508(6)
N(2)	C(2)	1.495(5)	N(2)	C(16)	1.491(5)
N(2)	C(22)	1.487(6)	N(3)	C(4)	1.331(5)
N(3)	C(8)	1.353(6)	N(4)	C(17)	1.358(6)
N(4)	C(21)	1.358(6)	N(5)	C(29)	1.501(6)
N(5)	C(31)	1.479(6)	N(5)	C(37)	1.504(6)
N(6)	C(30)	1.499(6)	N(6)	C(44)	1.478(6)
N(6)	C(50)	1.501(6)	N(7)	C(32)	1.347(5)
N(7)	C(36)	1.355(5)	N(8)	C(45)	1.346(5)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
N(8)	C(49)	1.336(5)	C(1)	C(2)	1.500(6)
C(3)	C(4)	1.494(6)	C(4)	C(5)	1.392(6)
C(5)	C(6)	1.372(7)	C(6)	C(7)	1.393(7)
C(7)	C(8)	1.368(6)	C(9)	C(10)	1.501(6)
C(10)	C(11)	1.414(6)	C(10)	C(15)	1.397(6)
C(11)	C(12)	1.400(6)	C(12)	C(13)	1.395(6)
C(13)	C(14)	1.385(7)	C(14)	C(15)	1.390(7)
C(16)	C(17)	1.490(6)	C(17)	C(18)	1.374(6)
C(18)	C(19)	1.379(7)	C(19)	C(20)	1.391(7)
C(20)	C(21)	1.392(7)	C(22)	C(23)	1.502(6)
C(23)	C(24)	1.403(6)	C(23)	C(28)	1.406(6)
C(24)	C(25)	1.399(6)	C(25)	C(26)	1.402(6)
C(26)	C(27)	1.389(7)	C(27)	C(28)	1.373(7)
C(29)	C(30)	1.468(7)	C(31)	C(32)	1.495(6)
C(32)	C(33)	1.370(6)	C(33)	C(34)	1.383(6)
C(34)	C(35)	1.392(6)	C(35)	C(36)	1.371(7)
C(37)	C(38)	1.493(6)	C(38)	C(39)	1.410(5)
C(38)	C(43)	1.398(6)	C(39)	C(40)	1.407(6)
C(40)	C(41)	1.375(6)	C(41)	C(42)	1.384(6)
C(42)	C(43)	1.389(7)	C(44)	C(45)	1.500(6)
C(45)	C(46)	1.375(7)	C(46)	C(47)	1.388(6)
C(47)	C(48)	1.395(6)	C(48)	C(49)	1.362(7)
C(50)	C(51)	1.503(7)	C(51)	C(52)	1.408(6)
C(51)	C(56)	1.398(6)	C(52)	C(53)	1.380(6)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(53)	C(54)	1.390(6)	C(54)	C(55)	1.389(6)
C(55)	C(56)	1.380(7)			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Gd(1)	O(2)	142.16(11)	O(1)	Gd(1)	O(3)	85.07(10)
O(1)	Gd(1)	O(4)	123.91(10)	O(1)	Gd(1)	N(1)	74.06(11)
O(1)	Gd(1)	N(2)	136.18(11)	O(1)	Gd(1)	N(3)	78.38(11)
O(1)	Gd(1)	N(4)	85.25(12)	O(2)	Gd(1)	O(3)	69.37(9)
O(2)	Gd(1)	O(4)	70.59(9)	O(2)	Gd(1)	N(1)	116.16(10)
O(2)	Gd(1)	N(2)	75.81(11)	O(2)	Gd(1)	N(3)	74.79(11)
O(2)	Gd(1)	N(4)	132.33(11)	O(3)	Gd(1)	O(4)	65.28(10)
O(3)	Gd(1)	N(1)	150.48(10)	O(3)	Gd(1)	N(2)	138.37(10)
O(3)	Gd(1)	N(3)	91.01(11)	O(3)	Gd(1)	N(4)	126.64(10)
O(4)	Gd(1)	N(1)	144.12(11)	O(4)	Gd(1)	N(2)	82.31(10)
O(4)	Gd(1)	N(3)	143.11(11)	O(4)	Gd(1)	N(4)	77.73(10)
N(1)	Gd(1)	N(2)	66.91(11)	N(1)	Gd(1)	N(3)	64.81(11)
N(1)	Gd(1)	N(4)	72.99(10)	N(2)	Gd(1)	N(3)	101.37(11)
N(2)	Gd(1)	N(4)	65.25(11)	N(3)	Gd(1)	N(4)	137.43(11)
O(2)	Gd(2)	O(3)	73.47(10)	O(2)	Gd(2)	O(4)	70.26(9)
O(2)	Gd(2)	O(5)	126.32(9)	O(2)	Gd(2)	O(6)	75.10(10)
O(2)	Gd(2)	N(5)	153.16(11)	O(2)	Gd(2)	N(6)	131.99(12)
O(2)	Gd(2)	N(7)	99.30(10)	O(2)	Gd(2)	N(8)	84.85(11)
O(3)	Gd(2)	O(4)	66.45(10)	O(3)	Gd(2)	O(5)	139.22(11)
O(3)	Gd(2)	O(6)	122.31(10)	O(3)	Gd(2)	N(5)	80.66(11)
O(3)	Gd(2)	N(6)	118.50(11)	O(3)	Gd(2)	N(7)	71.67(11)
O(3)	Gd(2)	N(8)	151.45(11)	O(4)	Gd(2)	O(5)	148.95(10)
O(4)	Gd(2)	O(6)	139.50(9)	O(4)	Gd(2)	N(5)	105.92(10)
O(4)	Gd(2)	N(6)	73.59(11)	O(4)	Gd(2)	N(7)	138.10(11)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O(4)	Gd(2)	N(8)	89.07(11)	O(5)	Gd(2)	O(6)	51.88(9)
O(5)	Gd(2)	N(5)	70.92(11)	O(5)	Gd(2)	N(6)	76.99(11)
O(5)	Gd(2)	N(7)	70.09(11)	O(5)	Gd(2)	N(8)	68.99(12)
O(6)	Gd(2)	N(5)	114.44(11)	O(6)	Gd(2)	N(6)	118.60(11)
O(6)	Gd(2)	N(7)	67.31(11)	O(6)	Gd(2)	N(8)	67.26(11)
N(5)	Gd(2)	N(6)	67.53(12)	N(5)	Gd(2)	N(7)	65.10(11)
N(5)	Gd(2)	N(8)	121.95(11)	N(6)	Gd(2)	N(7)	128.70(11)
N(6)	Gd(2)	N(8)	63.87(11)	N(7)	Gd(2)	N(8)	131.44(12)
Gd(1)	O(1)	C(11)	133.5(2)	Gd(1)	O(2)	Gd(2)	100.03(10)
Gd(1)	O(2)	C(24)	118.3(3)	Gd(2)	O(2)	C(24)	141.5(3)
Gd(1)	O(3)	Gd(2)	96.13(10)	Gd(1)	O(3)	C(39)	135.2(3)
Gd(2)	O(3)	C(39)	128.3(3)	Gd(1)	O(4)	Gd(2)	97.28(10)
Gd(1)	O(4)	C(52)	118.1(3)	Gd(2)	O(4)	C(52)	117.1(3)
Gd(2)	O(5)	N(9)	96.4(2)	Gd(2)	O(6)	N(9)	95.4(2)
Gd(1)	N(1)	C(1)	110.9(3)	Gd(1)	N(1)	C(3)	110.7(3)
Gd(1)	N(1)	C(9)	111.1(2)	C(1)	N(1)	C(3)	108.6(3)
C(1)	N(1)	C(9)	106.8(4)	C(3)	N(1)	C(9)	108.6(4)
Gd(1)	N(2)	C(2)	113.5(3)	Gd(1)	N(2)	C(16)	104.8(2)
Gd(1)	N(2)	C(22)	111.8(3)	C(2)	N(2)	C(16)	110.2(4)
C(2)	N(2)	C(22)	109.6(3)	C(16)	N(2)	C(22)	106.6(4)
Gd(1)	N(3)	C(4)	123.3(3)	Gd(1)	N(3)	C(8)	115.5(3)
C(4)	N(3)	C(8)	118.5(4)	Gd(1)	N(4)	C(17)	117.8(3)
Gd(1)	N(4)	C(21)	124.3(3)	C(17)	N(4)	C(21)	117.1(4)
Gd(2)	N(5)	C(29)	110.7(3)	Gd(2)	N(5)	C(31)	115.6(2)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Gd(2)	N(5)	C(37)	104.8(2)	C(29)	N(5)	C(31)	107.0(4)
C(29)	N(5)	C(37)	109.6(3)	C(31)	N(5)	C(37)	109.0(4)
Gd(2)	N(6)	C(30)	111.7(3)	Gd(2)	N(6)	C(44)	107.0(3)
Gd(2)	N(6)	C(50)	113.0(3)	C(30)	N(6)	C(44)	107.0(4)
C(30)	N(6)	C(50)	110.2(4)	C(44)	N(6)	C(50)	107.7(4)
Gd(2)	N(7)	C(32)	118.9(3)	Gd(2)	N(7)	C(36)	122.6(3)
C(32)	N(7)	C(36)	116.4(4)	Gd(2)	N(8)	C(45)	117.9(3)
Gd(2)	N(8)	C(49)	123.4(3)	C(45)	N(8)	C(49)	118.0(4)
O(5)	N(9)	O(6)	116.3(4)	O(5)	N(9)	O(7)	121.3(4)
O(6)	N(9)	O(7)	122.4(4)	O(8)	N(10)	O(9)	123.6(10)
O(8)	N(10)	O(10)	117.3(10)	O(9)	N(10)	O(10)	119.2(10)
N(1)	C(1)	C(2)	112.0(4)	N(2)	C(2)	C(1)	115.7(4)
N(1)	C(3)	C(4)	112.1(3)	N(3)	C(4)	C(3)	116.5(4)
N(3)	C(4)	C(5)	121.8(5)	C(3)	C(4)	C(5)	121.5(4)
C(4)	C(5)	C(6)	118.8(4)	C(5)	C(6)	C(7)	120.1(5)
C(6)	C(7)	C(8)	117.4(5)	N(3)	C(8)	C(7)	123.4(4)
N(1)	C(9)	C(10)	112.2(4)	C(9)	C(10)	C(11)	119.9(4)
C(9)	C(10)	C(15)	120.4(4)	C(11)	C(10)	C(15)	119.7(5)
O(1)	C(11)	C(10)	120.2(4)	O(1)	C(11)	C(12)	121.3(4)
C(10)	C(11)	C(12)	118.4(4)	C(11)	C(12)	C(13)	121.1(5)
C(12)	C(13)	C(14)	120.1(5)	C(13)	C(14)	C(15)	119.7(5)
C(10)	C(15)	C(14)	120.9(5)	N(2)	C(16)	C(17)	112.9(4)
N(4)	C(17)	C(16)	115.1(4)	N(4)	C(17)	C(18)	123.2(4)
C(16)	C(17)	C(18)	121.7(4)	C(17)	C(18)	C(19)	119.3(5)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle
C(18)	C(19)	C(20)	119.2(5)
N(4)	C(21)	C(20)	122.8(5)
C(22)	C(23)	C(24)	118.6(4)
C(24)	C(23)	C(28)	119.7(4)
O(2)	C(24)	C(25)	121.2(4)
C(24)	C(25)	C(26)	119.8(4)
C(26)	C(27)	C(28)	119.2(4)
N(5)	C(29)	C(30)	112.9(4)
N(5)	C(31)	C(32)	114.9(4)
N(7)	C(32)	C(33)	122.8(4)
C(32)	C(33)	C(34)	120.6(4)
C(34)	C(35)	C(36)	119.4(4)
N(5)	C(37)	C(38)	114.0(4)
C(37)	C(38)	C(43)	118.5(4)
O(3)	C(39)	C(38)	121.0(4)
C(38)	C(39)	C(40)	118.3(4)
C(40)	C(41)	C(42)	121.2(5)
C(38)	C(43)	C(42)	122.3(4)
N(8)	C(45)	C(44)	117.7(4)
C(44)	C(45)	C(46)	119.9(4)
C(46)	C(47)	C(48)	118.7(5)
N(8)	C(49)	C(48)	123.9(4)
C(50)	C(51)	C(52)	119.1(4)
C(52)	C(51)	C(56)	118.7(5)

atom	atom	atom	angle
C(19)	C(20)	C(21)	118.5(5)
N(2)	C(22)	C(23)	114.1(4)
C(22)	C(23)	C(28)	121.5(4)
O(2)	C(24)	C(23)	119.7(4)
C(23)	C(24)	C(25)	119.1(4)
C(25)	C(26)	C(27)	121.0(5)
C(23)	C(28)	C(27)	121.2(5)
N(6)	C(30)	C(29)	112.7(4)
N(7)	C(32)	C(31)	115.7(4)
C(31)	C(32)	C(33)	121.3(4)
C(33)	C(34)	C(35)	117.0(5)
N(7)	C(36)	C(35)	123.6(4)
C(37)	C(38)	C(39)	122.7(4)
C(39)	C(38)	C(43)	118.8(4)
O(3)	C(39)	C(40)	120.6(4)
C(39)	C(40)	C(41)	121.2(4)
C(41)	C(42)	C(43)	118.1(5)
N(6)	C(44)	C(45)	114.1(4)
N(8)	C(45)	C(46)	122.1(4)
C(45)	C(46)	C(47)	119.2(5)
C(47)	C(48)	C(49)	118.1(4)
N(6)	C(50)	C(51)	109.9(4)
C(50)	C(51)	C(56)	121.6(4)
O(4)	C(52)	C(51)	118.2(4)

Table 4. Bond Angles(°) (continued).

atom	atom	atom	angle	atom	atom	atom	angle
O(4)	C(52)	C(53)	122.1(4)	C(51)	C(52)	C(53)	119.5(4)
C(52)	C(53)	C(54)	120.4(4)	C(53)	C(54)	C(55)	121.1(5)
C(54)	C(55)	C(56)	118.2(4)	C(51)	C(56)	C(55)	122.0(5)

Table 5. Hydrogen atom coordinates and B_{iso}

atom	x	y	z	B_{iso}
H(1)	-0.0547	0.2908	0.4263	2.1
H(2)	-0.0517	0.2928	0.3546	2.1
H(3)	-0.1163	0.1981	0.3725	2.3
H(4)	-0.0155	0.1875	0.4335	2.3
H(5)	0.1222	0.3155	0.5096	2.4
H(6)	0.0993	0.2427	0.4985	2.4
H(7)	0.2910	0.3155	0.5932	2.8
H(8)	0.4717	0.2818	0.6293	3.2
H(9)	0.5395	0.2115	0.5664	2.9
H(10)	0.4255	0.1827	0.4674	2.4
H(11)	0.0831	0.3646	0.3598	2.0
H(12)	0.0591	0.3809	0.4248	2.0
H(13)	0.4647	0.3650	0.4185	2.3
H(14)	0.5023	0.4425	0.4976	3.4
H(15)	0.3627	0.4821	0.5354	3.7
H(16)	0.1851	0.4441	0.4939	3.0
H(17)	-0.0120	0.1461	0.2595	2.5
H(18)	-0.1188	0.1601	0.2792	2.5
H(19)	-0.2120	0.2398	0.2118	2.4
H(20)	-0.2111	0.3416	0.1711	3.1
H(21)	-0.0447	0.3970	0.1934	2.6
H(22)	0.1151	0.3476	0.2533	2.5
H(23)	-0.0446	0.0890	0.3682	2.5
H(24)	0.0523	0.0811	0.3378	2.5

Table 5. Hydrogen atom coordinates and B_{iso} (continued)

atom	x	y	z	B_{iso}
H(25)	0.3635	0.0784	0.5058	2.1
H(26)	0.2962	0.0454	0.5894	2.9
H(27)	0.1086	0.0417	0.5758	3.3
H(28)	-0.0123	0.0680	0.4775	3.0
H(29)	0.5034	0.0519	0.1811	2.6
H(30)	0.4650	0.0007	0.2223	2.6
H(31)	0.3305	0.0185	0.1319	2.7
H(32)	0.3341	0.0914	0.1467	2.7
H(33)	0.6052	0.0296	0.2973	2.5
H(34)	0.6405	0.0971	0.2805	2.5
H(35)	0.7754	0.1165	0.3786	2.7
H(36)	0.8159	0.1408	0.4880	3.2
H(37)	0.6803	0.1192	0.5390	3.0
H(38)	0.5103	0.0865	0.4788	2.4
H(39)	0.5104	0.1560	0.2058	2.4
H(40)	0.3964	0.1633	0.2192	2.4
H(41)	0.5006	0.2643	0.4200	2.5
H(42)	0.6578	0.3142	0.4152	3.1
H(43)	0.7293	0.2962	0.3298	3.3
H(44)	0.6447	0.2220	0.2523	2.9
H(45)	0.2012	-0.0399	0.1594	3.3
H(46)	0.3111	-0.0480	0.2151	3.3
H(47)	0.1100	-0.1226	0.1966	3.3
H(48)	0.0225	-0.1552	0.2721	3.8

Table 5. Hydrogen atom coordinates and B_{iso} (continued)

atom	x	y	z	B_{iso}
H(49)	0.0523	-0.0968	0.3679	3.2
H(50)	0.1571	-0.0073	0.3810	2.5
H(51)	0.1296	0.0527	0.1238	2.7
H(52)	0.1047	0.0655	0.1893	2.7
H(53)	0.2453	0.2656	0.2462	2.2
H(54)	0.2627	0.3052	0.1503	2.9
H(55)	0.2225	0.2423	0.0584	3.2
H(56)	0.1663	0.1388	0.0645	3.3
H(57)	0.4357	0.2436	0.0455	7.6
H(58)	0.5835	0.3240	0.1101	10.4
H(59)	0.5192	0.2822	0.1469	10.4
H(60)	0.5918	0.2498	0.1086	10.4
H(61)	0.3975	0.0410	-0.0567	16.6
H(62)	0.4379	-0.0126	-0.0842	16.6
H(63)	0.6307	0.1398	0.1415	6.7
H(64)	0.7173	0.0955	0.1701	6.7
H(65)	0.2811	0.0052	-0.1703	22.5
H(66)	0.1643	-0.0005	-0.1811	22.5

Table 6. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd(1)	0.01392(13)	0.01685(13)	0.02052(10)	-0.00169(12)	0.00666(9)	-0.00178(10)
Gd(2)	0.01757(14)	0.01822(13)	0.02123(10)	0.00074(12)	0.00862(10)	-0.00078(10)
O(1)	0.020(2)	0.014(2)	0.026(2)	-0.0058(15)	0.0092(14)	-0.0004(14)
O(2)	0.021(2)	0.017(2)	0.0230(15)	-0.0019(15)	0.0127(14)	-0.0002(13)
O(3)	0.014(2)	0.016(2)	0.028(2)	-0.0044(15)	0.0088(14)	-0.0021(14)
O(4)	0.019(2)	0.020(2)	0.0192(15)	0.001(2)	0.0054(14)	0.0000(13)
O(5)	0.036(2)	0.025(2)	0.025(2)	0.007(2)	0.019(2)	0.0046(15)
O(6)	0.026(2)	0.023(2)	0.027(2)	0.002(2)	0.014(2)	-0.0016(14)
O(7)	0.062(3)	0.025(2)	0.041(2)	0.024(2)	0.022(2)	0.013(2)
O(8)	0.295(13)	0.107(6)	0.162(7)	0.029(8)	0.076(8)	-0.028(6)
O(9)	0.094(6)	0.298(11)	0.087(4)	0.012(6)	0.009(4)	0.080(6)
O(10)	0.139(6)	0.154(7)	0.063(4)	-0.026(5)	0.046(4)	0.005(4)
O(11)	0.065(4)	0.096(4)	0.091(4)	0.039(3)	0.040(3)	0.031(3)
O(12)	0.214(9)	0.170(7)	0.124(5)	-0.086(7)	0.061(6)	-0.040(5)
O(13)	0.068(4)	0.082(4)	0.086(3)	-0.023(3)	0.040(3)	-0.011(3)
O(14)	0.389(15)	0.187(9)	0.148(6)	-0.048(9)	-0.010(8)	-0.087(6)
N(1)	0.014(2)	0.024(2)	0.024(2)	0.002(2)	0.007(2)	-0.001(2)
N(2)	0.016(2)	0.022(2)	0.023(2)	-0.001(2)	0.007(2)	0.004(2)
N(3)	0.019(2)	0.019(2)	0.020(2)	-0.001(2)	0.005(2)	0.002(2)
N(4)	0.019(2)	0.022(3)	0.024(2)	-0.001(2)	0.008(2)	-0.002(2)
N(5)	0.020(2)	0.023(2)	0.027(2)	0.005(2)	0.012(2)	0.000(2)
N(6)	0.028(3)	0.022(3)	0.025(2)	0.000(2)	0.008(2)	-0.005(2)
N(7)	0.015(2)	0.019(2)	0.030(2)	0.001(2)	0.008(2)	0.003(2)
N(8)	0.024(3)	0.017(2)	0.035(2)	-0.005(2)	0.010(2)	-0.006(2)

Table 6. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(9)	0.023(3)	0.026(3)	0.032(2)	-0.002(2)	0.009(2)	0.000(2)
N(10)	0.106(7)	0.126(8)	0.048(4)	-0.018(6)	0.046(5)	0.009(5)
C(1)	0.014(3)	0.024(3)	0.031(2)	0.001(2)	0.010(2)	-0.001(2)
C(2)	0.016(3)	0.030(3)	0.030(3)	-0.001(2)	0.013(2)	-0.002(2)
C(3)	0.024(3)	0.029(3)	0.024(2)	-0.001(3)	0.012(2)	-0.001(2)
C(4)	0.029(3)	0.031(3)	0.011(2)	-0.003(3)	0.011(2)	-0.001(2)
C(5)	0.034(3)	0.033(3)	0.025(2)	-0.003(3)	0.012(2)	-0.001(2)
C(6)	0.032(4)	0.038(4)	0.025(3)	-0.011(3)	0.000(2)	-0.001(2)
C(7)	0.022(3)	0.036(3)	0.029(3)	-0.005(3)	0.001(2)	0.003(2)
C(8)	0.025(3)	0.024(3)	0.027(2)	-0.003(3)	0.007(2)	0.003(2)
C(9)	0.026(3)	0.010(3)	0.036(3)	-0.003(2)	0.020(2)	-0.004(2)
C(10)	0.031(3)	0.015(3)	0.025(2)	-0.003(2)	0.009(2)	0.001(2)
C(11)	0.022(3)	0.012(3)	0.021(2)	-0.005(2)	0.003(2)	0.000(2)
C(12)	0.025(3)	0.017(3)	0.031(3)	-0.001(2)	0.005(2)	0.003(2)
C(13)	0.031(4)	0.024(3)	0.041(3)	-0.009(3)	-0.006(3)	0.002(3)
C(14)	0.056(5)	0.025(3)	0.033(3)	-0.016(3)	0.006(3)	-0.009(2)
C(15)	0.039(4)	0.022(3)	0.037(3)	-0.005(3)	0.017(3)	-0.009(2)
C(16)	0.011(3)	0.036(3)	0.030(3)	-0.006(3)	0.002(2)	-0.004(2)
C(17)	0.020(3)	0.022(3)	0.022(2)	-0.006(2)	0.007(2)	-0.002(2)
C(18)	0.013(3)	0.037(3)	0.026(2)	0.001(3)	0.002(2)	0.004(2)
C(19)	0.023(3)	0.034(3)	0.039(3)	0.007(3)	0.003(3)	0.005(3)
C(20)	0.029(3)	0.024(3)	0.033(3)	0.003(3)	0.012(2)	0.007(2)
C(21)	0.026(3)	0.028(3)	0.027(3)	-0.009(3)	0.012(2)	-0.004(2)
C(22)	0.023(3)	0.019(3)	0.038(3)	-0.011(2)	0.014(2)	-0.007(2)

Table 6. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(23)	0.021(3)	0.013(3)	0.034(3)	0.002(2)	0.010(2)	0.003(2)
C(24)	0.021(3)	0.013(3)	0.031(2)	-0.005(2)	0.015(2)	-0.002(2)
C(25)	0.022(3)	0.023(3)	0.022(2)	-0.001(3)	0.006(2)	0.000(2)
C(26)	0.036(4)	0.031(3)	0.026(3)	-0.001(3)	0.012(3)	0.002(2)
C(27)	0.039(4)	0.036(4)	0.036(3)	0.002(3)	0.023(3)	0.006(3)
C(28)	0.026(3)	0.024(3)	0.053(3)	0.000(3)	0.026(3)	0.006(3)
C(29)	0.029(3)	0.026(3)	0.032(3)	0.007(3)	0.018(2)	0.002(2)
C(30)	0.034(4)	0.031(3)	0.025(2)	0.004(3)	0.016(2)	-0.003(2)
C(31)	0.024(3)	0.027(3)	0.032(3)	0.005(3)	0.015(2)	0.005(2)
C(32)	0.021(3)	0.022(3)	0.029(2)	0.006(2)	0.011(2)	0.004(2)
C(33)	0.016(3)	0.030(3)	0.041(3)	-0.001(3)	0.012(2)	0.004(2)
C(34)	0.018(3)	0.046(4)	0.035(3)	-0.004(3)	0.003(2)	0.002(3)
C(35)	0.023(3)	0.028(3)	0.041(3)	-0.003(3)	0.005(3)	-0.001(3)
C(36)	0.023(3)	0.025(3)	0.027(2)	-0.002(3)	0.006(2)	0.002(2)
C(37)	0.023(3)	0.024(3)	0.033(3)	0.005(2)	0.018(2)	0.008(2)
C(38)	0.024(3)	0.025(3)	0.023(2)	-0.006(2)	0.005(2)	0.005(2)
C(39)	0.014(3)	0.020(3)	0.024(2)	0.000(2)	0.009(2)	0.006(2)
C(40)	0.018(3)	0.026(3)	0.035(3)	0.000(2)	0.009(2)	-0.002(2)
C(41)	0.024(3)	0.026(3)	0.045(3)	-0.008(3)	0.006(3)	-0.002(3)
C(42)	0.017(3)	0.032(3)	0.059(3)	-0.006(3)	0.016(3)	0.005(3)
C(43)	0.028(3)	0.032(3)	0.039(3)	0.003(3)	0.020(3)	0.013(3)
C(44)	0.048(4)	0.020(3)	0.037(3)	-0.006(3)	0.015(3)	-0.008(2)
C(45)	0.031(3)	0.017(3)	0.033(3)	-0.001(3)	0.005(2)	-0.004(2)
C(46)	0.037(4)	0.031(3)	0.035(3)	-0.006(3)	0.011(3)	-0.008(2)

Table 6. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(47)	0.046(4)	0.022(3)	0.051(3)	-0.016(3)	0.010(3)	-0.005(3)
C(48)	0.034(4)	0.023(3)	0.047(3)	-0.005(3)	0.017(3)	-0.002(3)
C(49)	0.024(3)	0.019(3)	0.038(3)	-0.002(2)	0.012(2)	-0.005(2)
C(50)	0.026(3)	0.037(3)	0.022(2)	0.001(3)	0.003(2)	-0.008(2)
C(51)	0.016(3)	0.025(3)	0.025(2)	0.005(2)	0.000(2)	-0.001(2)
C(52)	0.012(3)	0.033(3)	0.020(2)	0.007(2)	0.003(2)	0.002(2)
C(53)	0.016(3)	0.021(3)	0.032(3)	0.002(2)	0.007(2)	0.000(2)
C(54)	0.025(3)	0.026(3)	0.041(3)	0.004(3)	0.012(3)	0.011(2)
C(55)	0.033(4)	0.046(4)	0.025(3)	0.010(3)	0.010(2)	0.010(3)
C(56)	0.037(4)	0.043(4)	0.021(2)	0.008(3)	0.006(2)	-0.002(2)
C(57)	0.143(9)	0.141(9)	0.063(5)	0.086(8)	0.056(6)	0.024(5)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$