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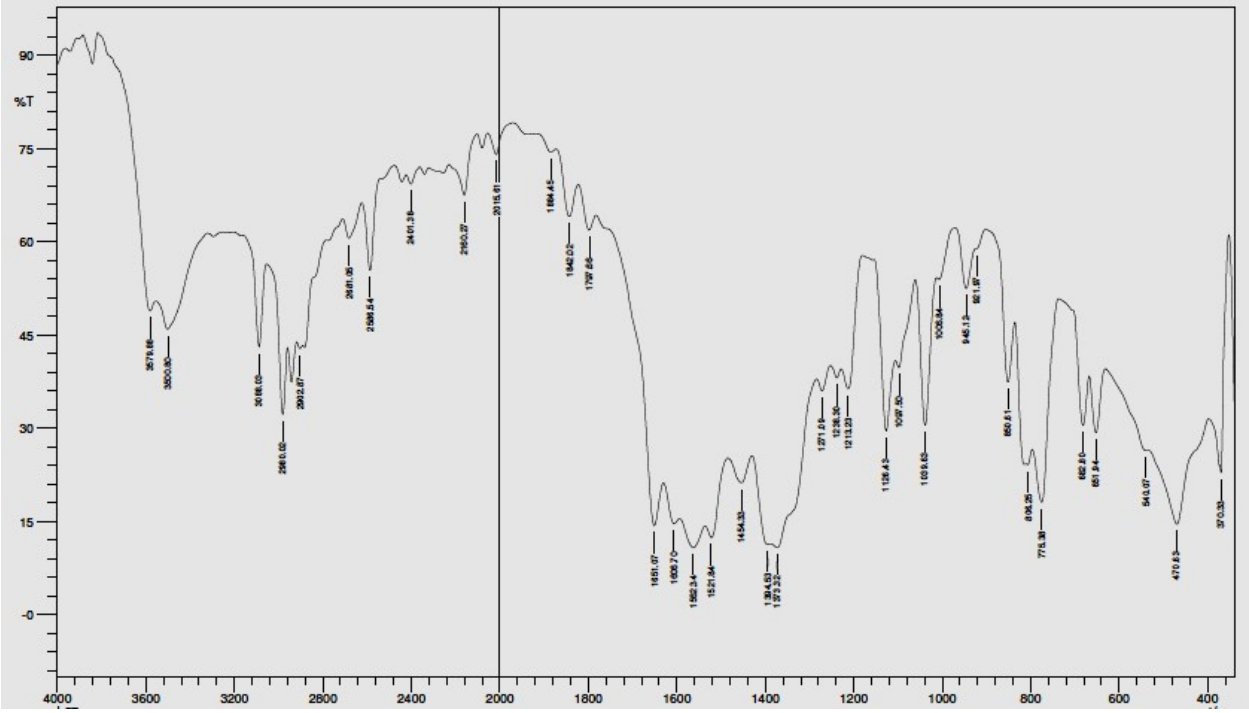
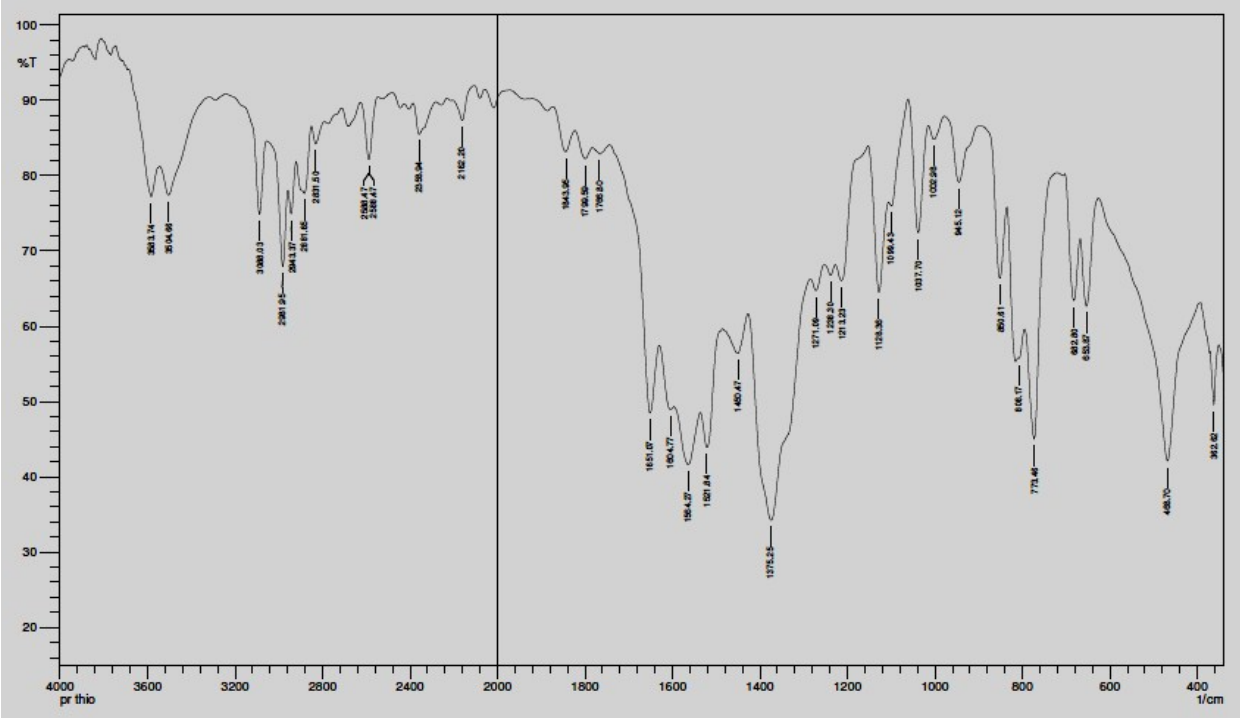
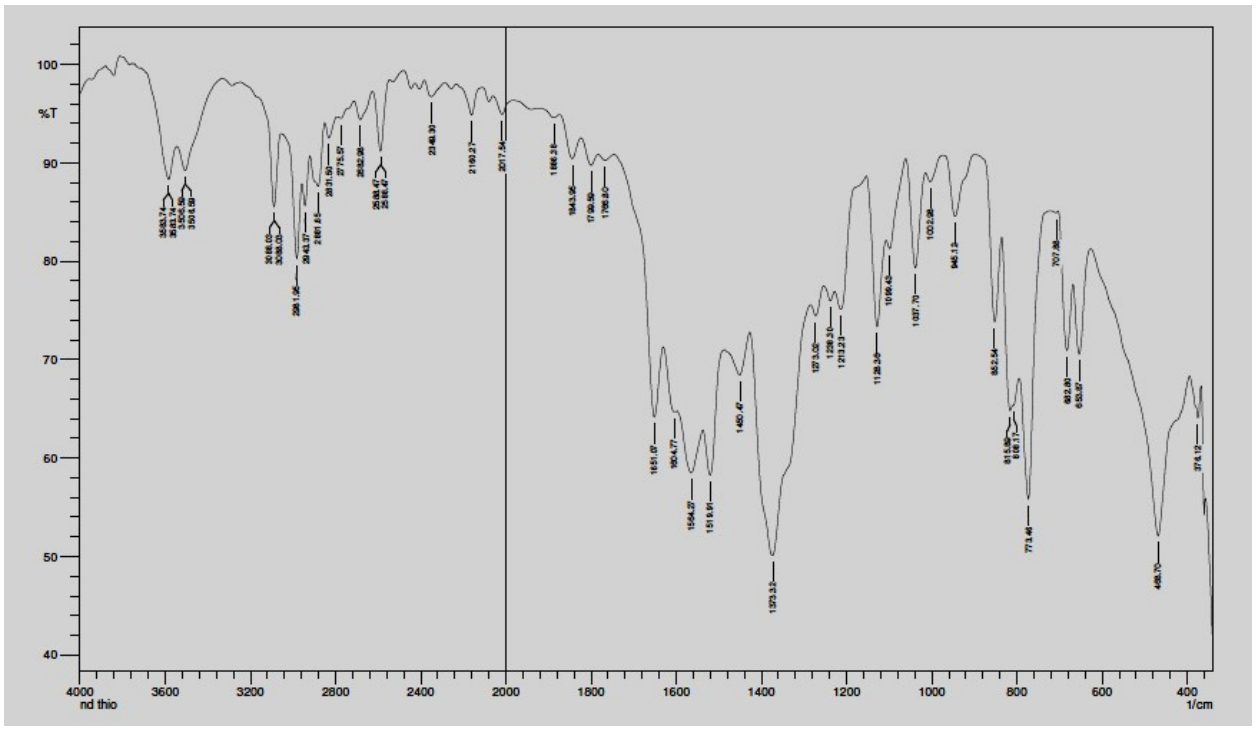


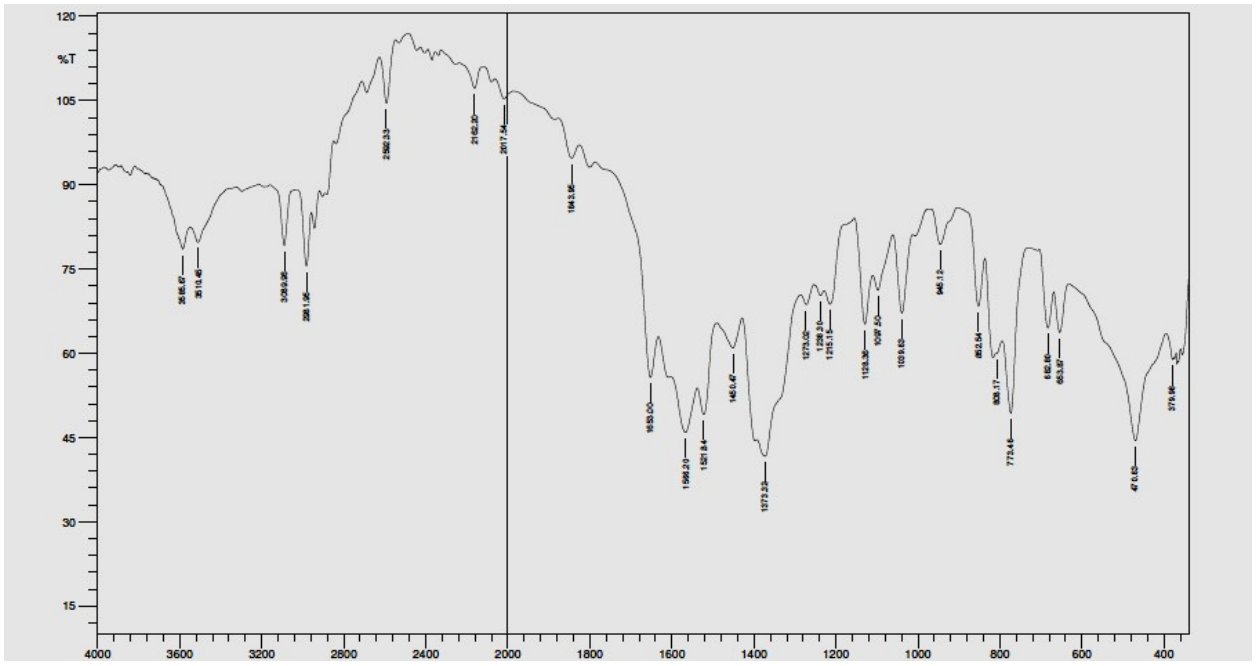
S1 (a) FT-IR spectrum of CP **1**



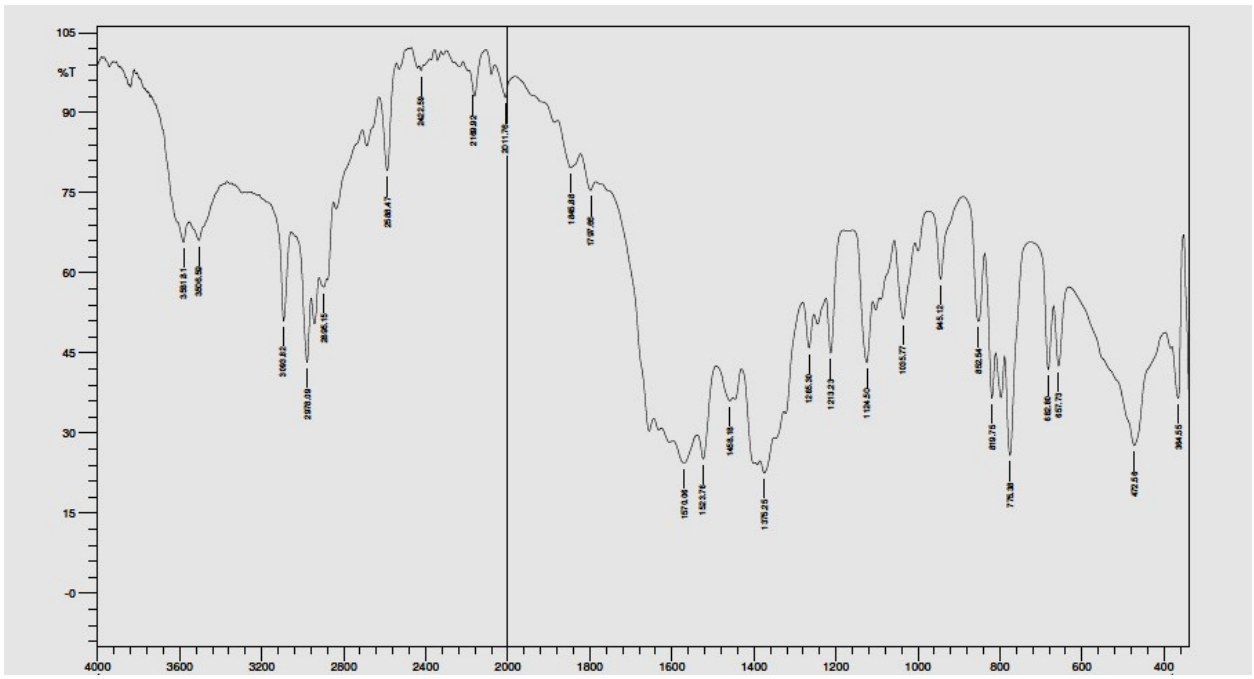
S1 (b) FT-IR spectrum of CP **2**



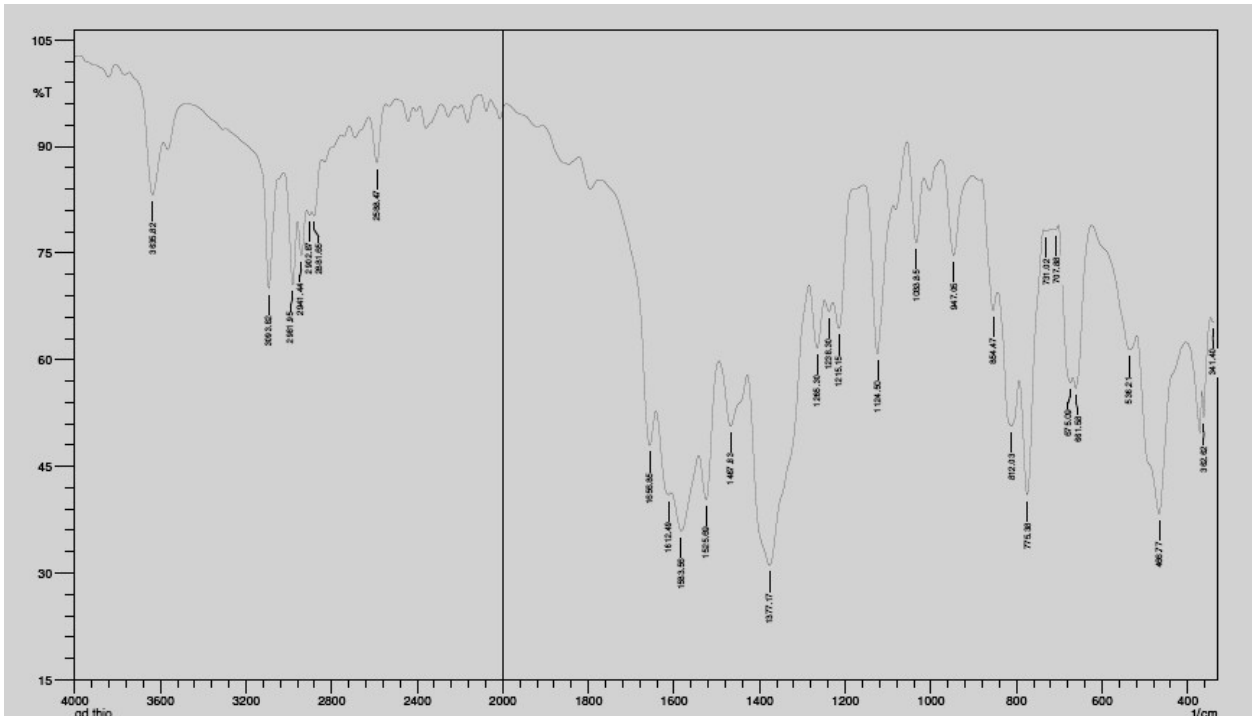
S1 (c) FT-IR spectrum of CP **3**



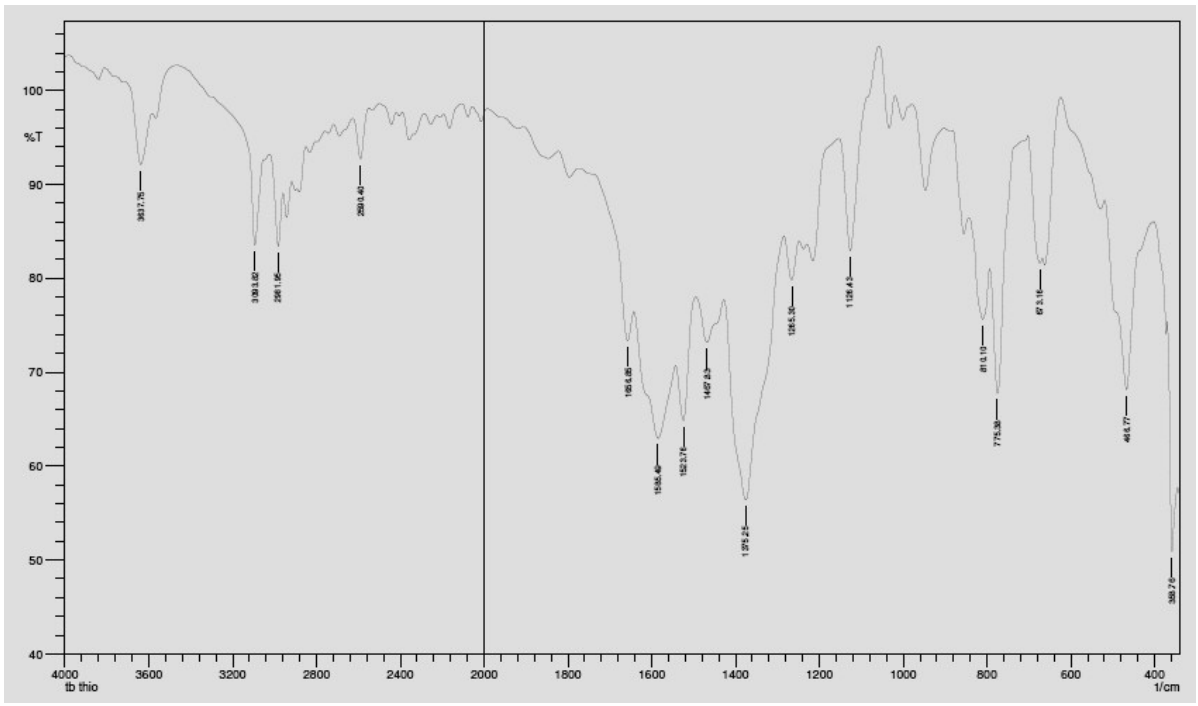
S1 (d) FT-IR spectrum of CP **4**



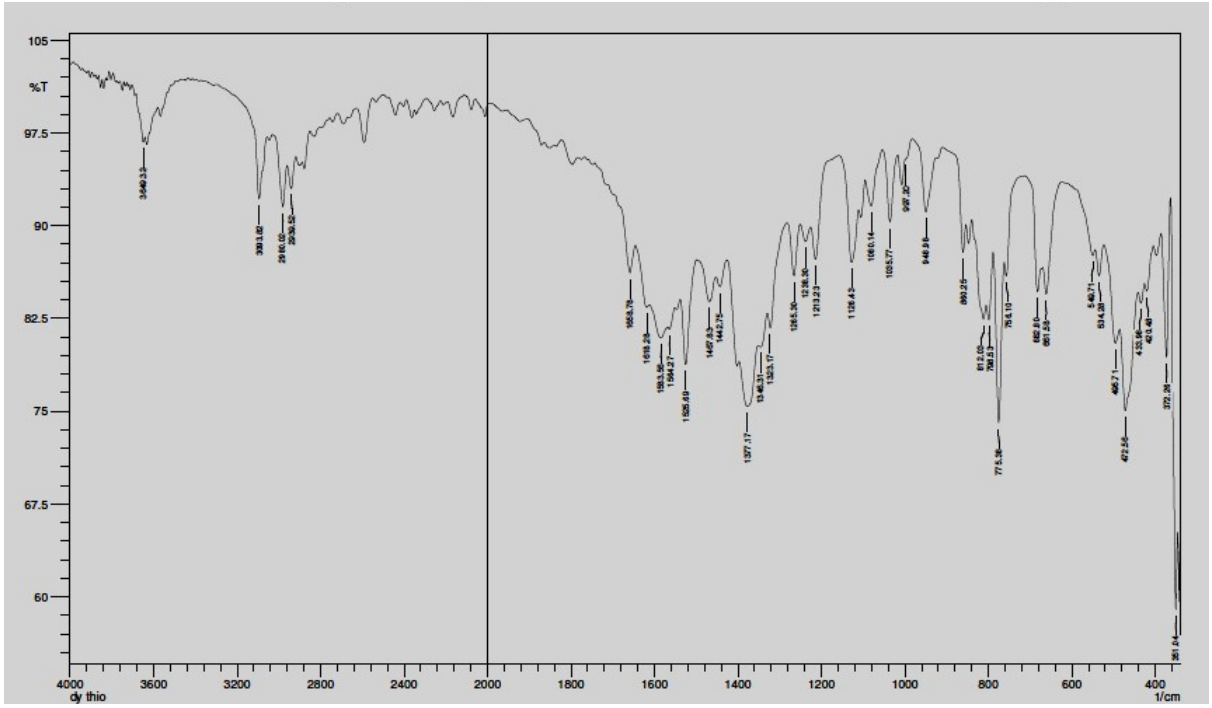
S1 (e) FT-IR spectrum of CP **5**



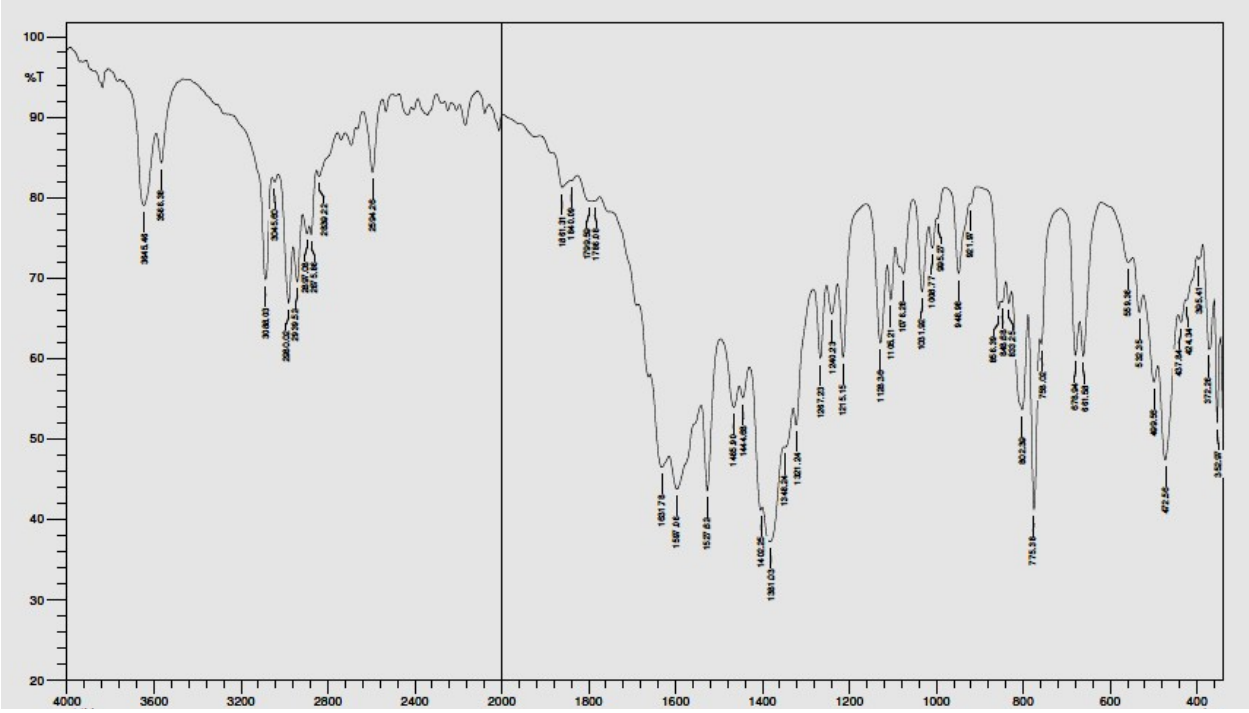
S1 (f) FT-IR spectrum of CP **6**



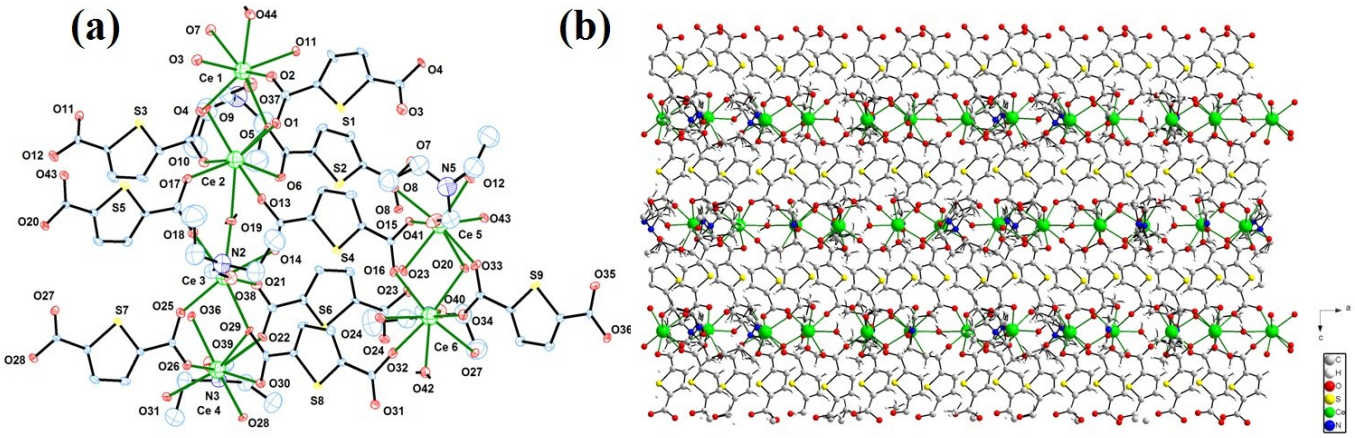
S1 (g) FT-IR spectrum of CP **7**



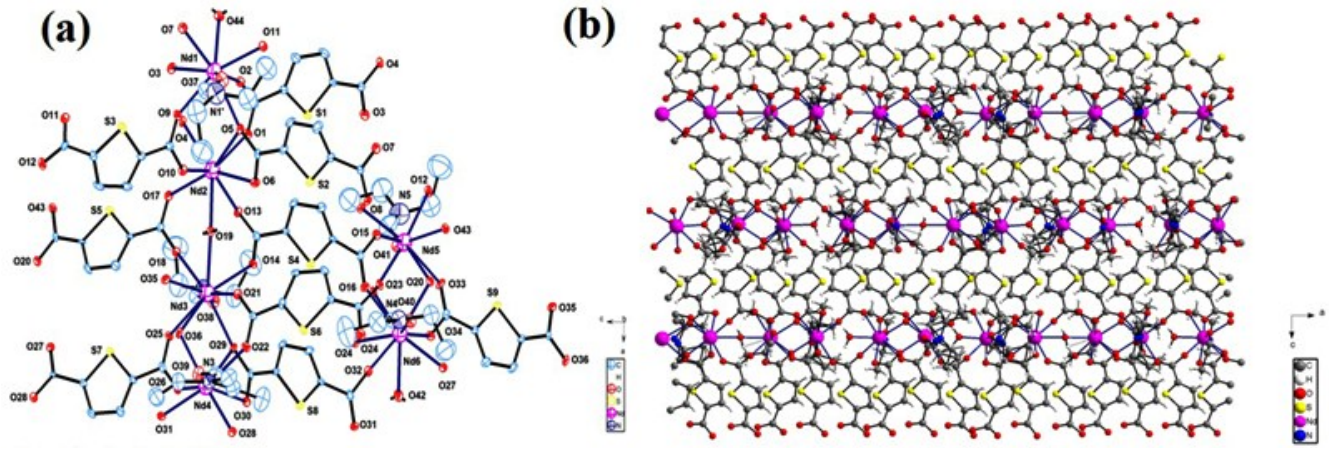
S1 (h) FT-IR spectrum of CP **8**



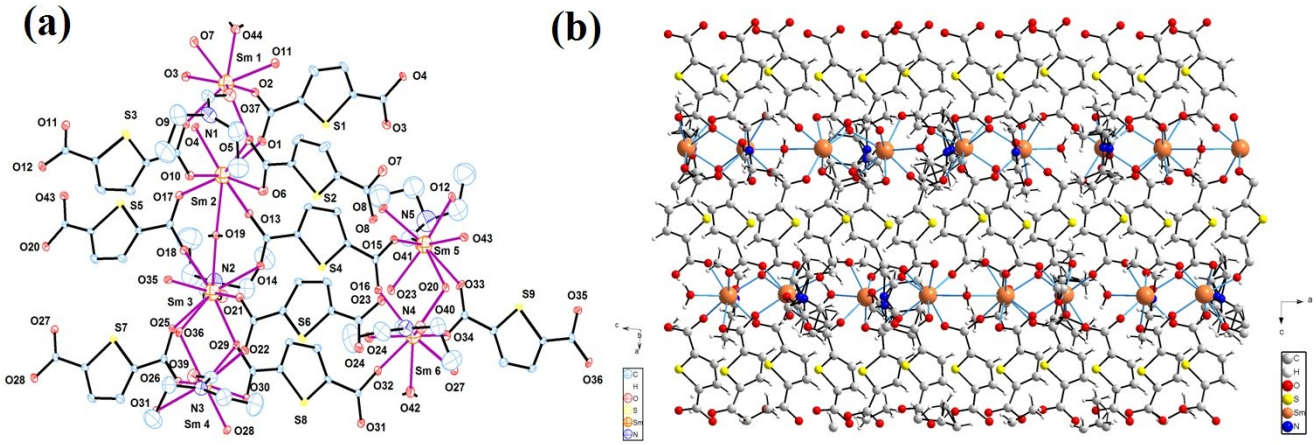
S1 (i) FT-IR spectrum of CP **9**



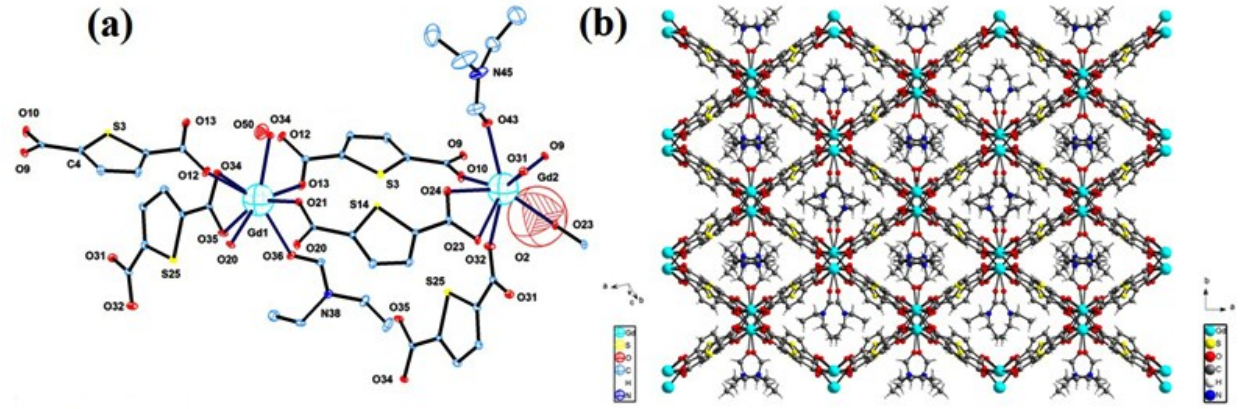
S 2. (a) ORTEP diagram of CP **1** (b) View of CP **1** along b-axis.



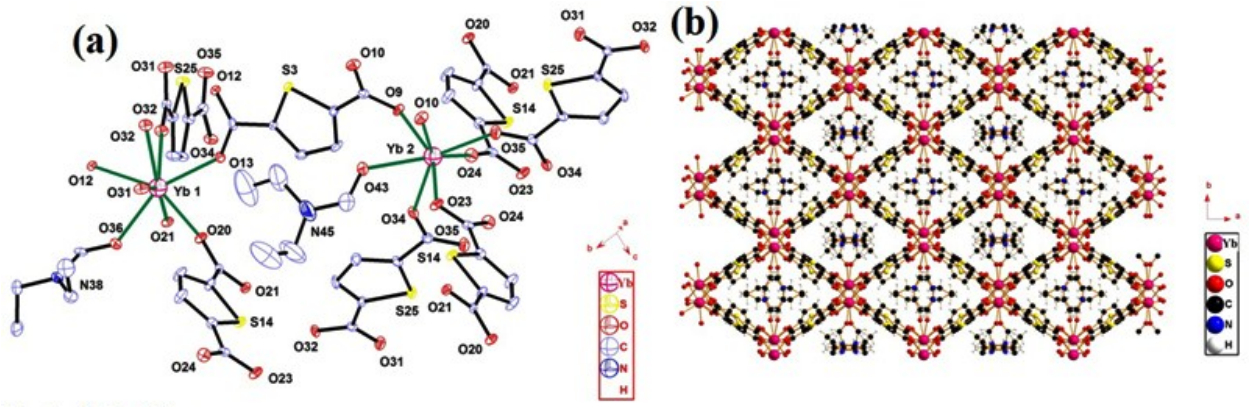
S 3. (a) ORTEP diagram of CP **3** (b) View of CP **3** along b-axis.



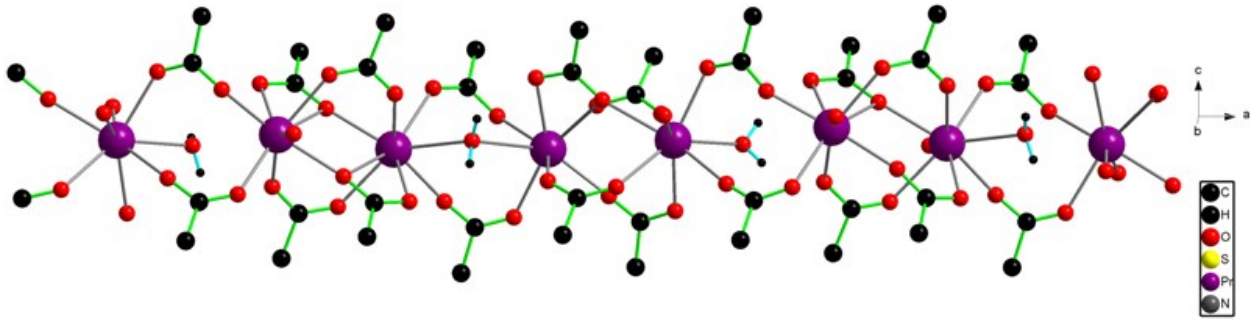
S 4. (a) ORTEP diagram of CP **4** (b) View of CP **4** along b-axis.



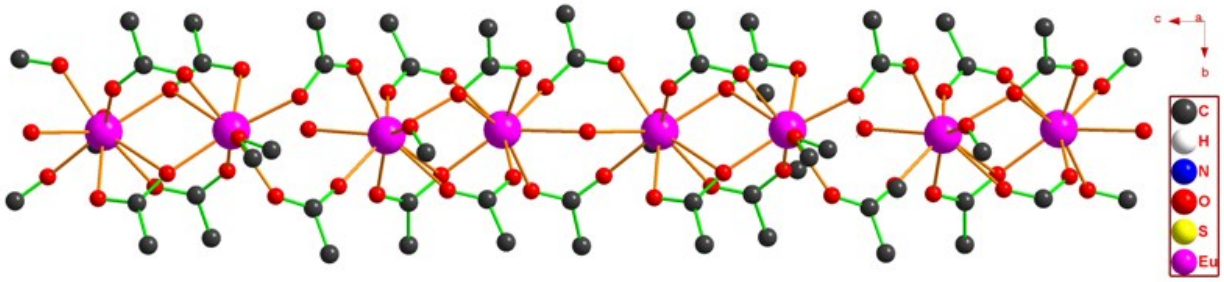
S 5. (a) ORTEP diagram of CP **6** (b) View of CP **6** along b-axis.



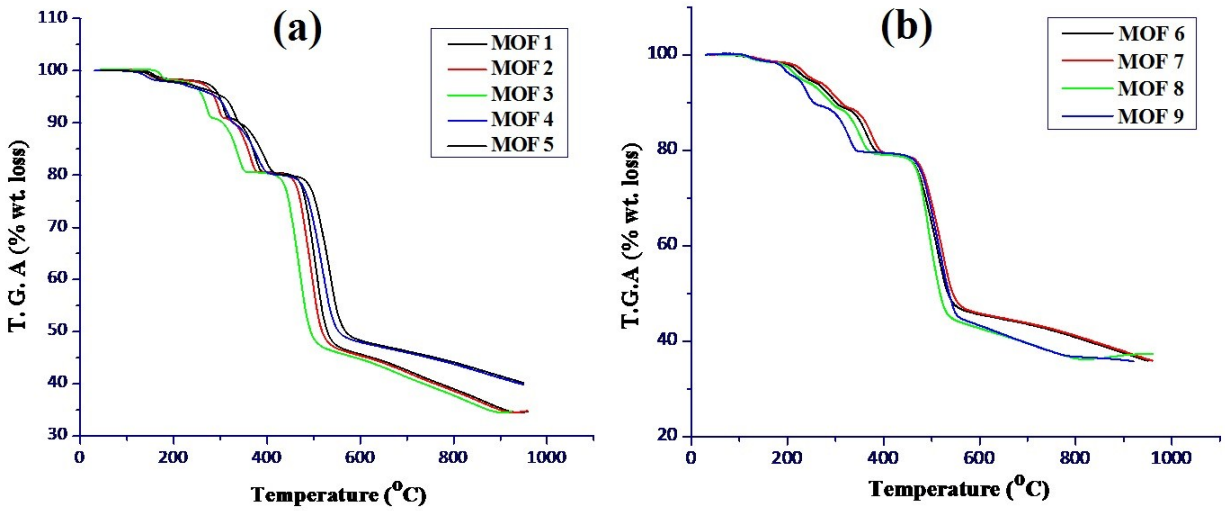
S 6. (a) ORTEP diagram of CP **9** (b) View of CP **9** along b-axis.



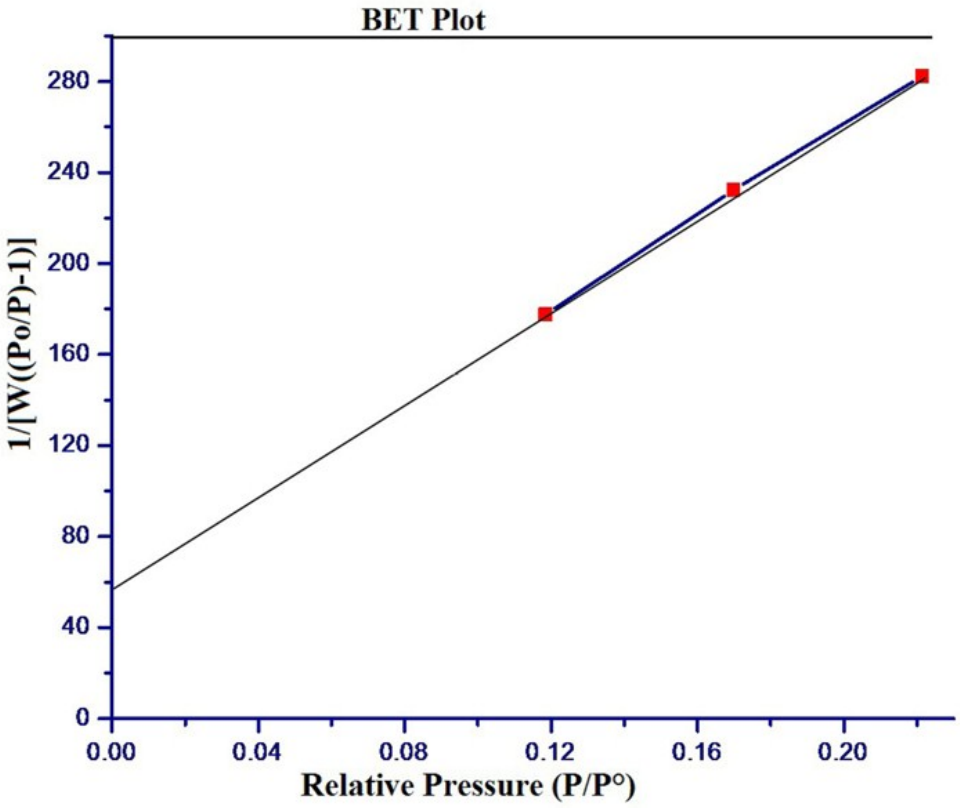
S 7. (a) The 1D rod shape SBU in CP **1.**



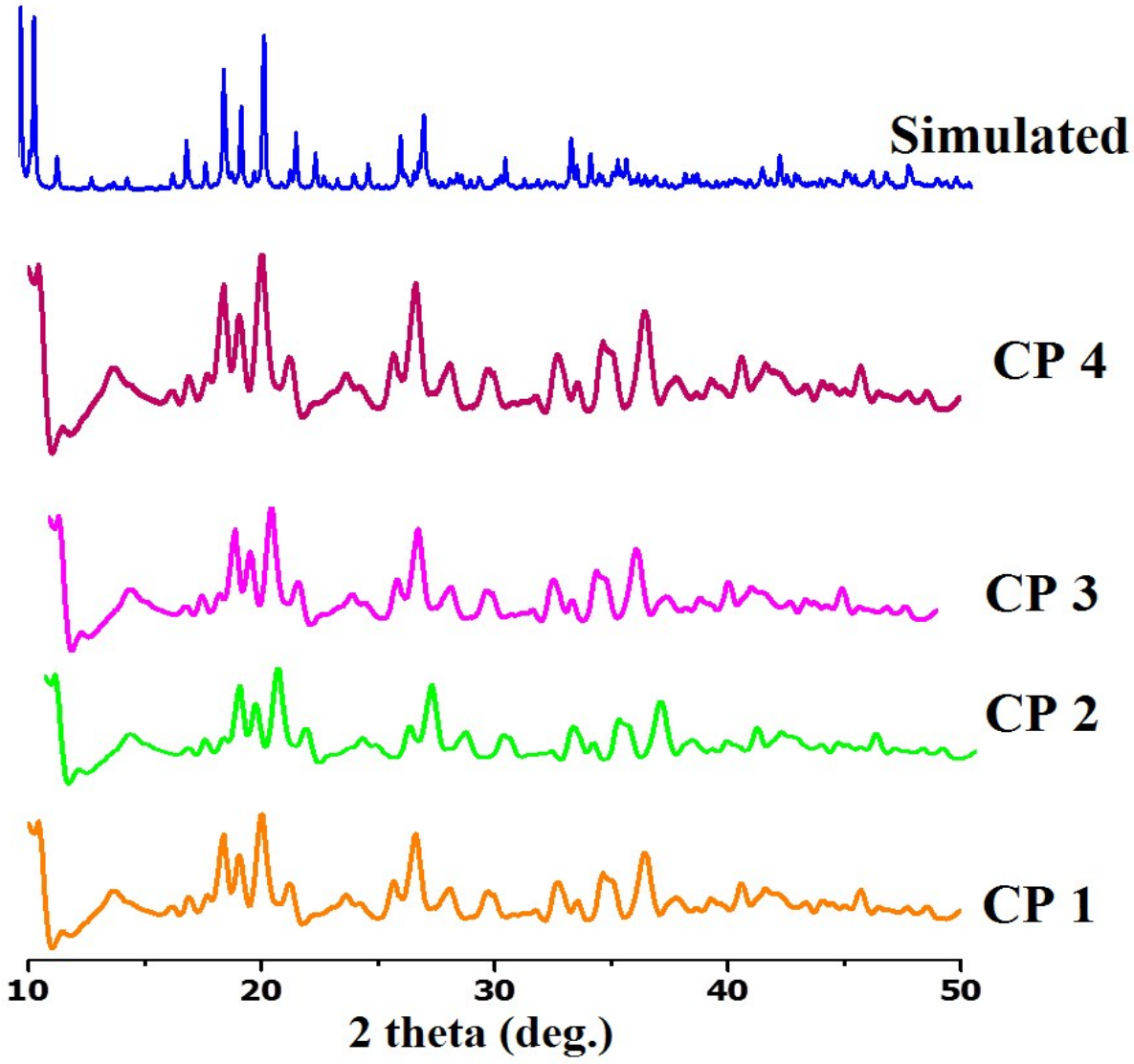
S 7. (b) The 1D rod shape SBU in CP **2.**



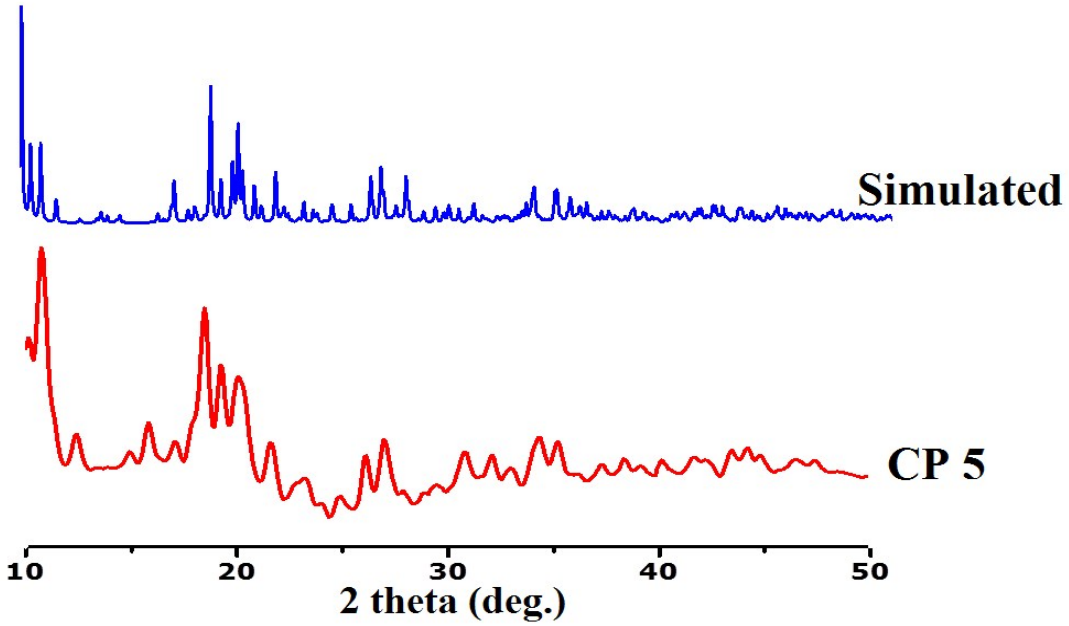
S 8 (a) T.G.A of CP **1-5** (b) T.G.A of CP **6-9.**



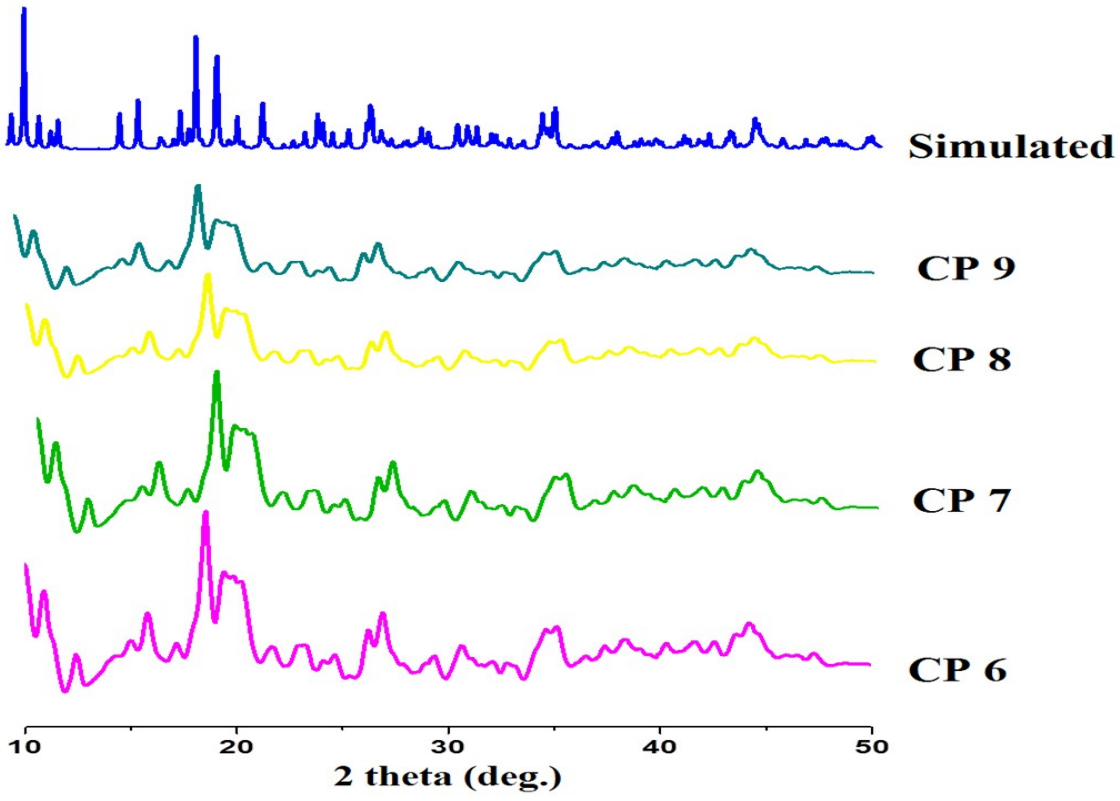
S9 (a). BET plot for CP **1.**



S10. (a) PXRD patterns of CPs **1** - **4**, compared with a simulated pattern.



S10. (b) PXRD pattern of CP **5**, compared with a simulated pattern.



S10. (c) PXRD patterns of CP **6 - 9**, compared with a simulated pattern.

Table S1. **Bond lengths [Å] and angles [°] for CPs 1-9.**

1

C(1)-O(1)	1.242(19)	C(32)-C(33)	1.39(2)
C(1)-O(2)	1.249(18)	C(32)-S(6)	1.700(17)
C(1)-C(2)	1.47(2)	C(33)-C(34)	1.42(2)
C(2)-C(3)	1.35(2)	C(33)-H(33)	0.9300
C(2)-S(1)	1.715(15)	C(34)-C(35)	1.35(2)
C(3)-C(4)	1.41(2)	C(34)-H(34)	0.9300
C(3)-H(3)	0.9300	C(35)-C(36)	1.47(2)
C(4)-C(5)	1.34(2)	C(35)-S(6)	1.709(14)
C(4)-H(4)	0.9300	C(36)-O(24)	1.26(2)
C(5)-C(6)	1.44(2)	C(36)-O(23)	1.265(18)
C(5)-S(1)	1.712(15)	C(36)-Ce(6)#2	3.065(15)
C(6)-O(3)	1.235(19)	C(37)-O(26)	1.23(2)
C(6)-O(4)	1.267(18)	C(37)-O(25)	1.27(2)
C(7)-O(6)	1.22(2)	C(37)-C(38)	1.49(2)
C(7)-O(5)	1.260(19)	C(38)-C(39)	1.36(2)
C(7)-C(8)	1.496(19)	C(38)-S(7)	1.711(16)
C(7)-Ce(2)	2.982(14)	C(39)-C(40)	1.40(2)
C(8)-C(9)	1.35(2)	C(39)-H(39)	0.9300
C(8)-S(2)	1.714(15)	C(40)-C(41)	1.33(2)
C(9)-C(10)	1.42(2)	C(40)-H(40)	0.9300
C(9)-H(9)	0.9300	C(41)-C(42)	1.49(2)
C(10)-C(11)	1.35(2)	C(41)-S(7)	1.711(16)
C(10)-H(10)	0.9300	C(42)-O(27)	1.23(2)
C(11)-C(12)	1.50(2)	C(42)-O(28)	1.278(18)
C(11)-S(2)	1.678(15)	C(43)-O(30)	1.25(2)
C(12)-O(8)	1.23(2)	C(43)-O(29)	1.265(19)
C(12)-O(7)	1.252(18)	C(43)-C(44)	1.47(2)
C(13)-O(9)	1.244(19)	C(43)-Ce(4)	3.078(17)
C(13)-O(10)	1.270(18)	C(44)-C(45)	1.34(2)
C(13)-C(14)	1.49(2)	C(44)-S(8)	1.701(15)
C(14)-C(15)	1.36(2)	C(45)-C(46)	1.42(2)
C(14)-S(3)	1.713(16)	C(45)-H(45)	0.9300

C(15)-C(16)	1.39(2)	C(46)-C(47)	1.36(2)
C(15)-H(15)	0.9300	C(46)-H(46)	0.9300
C(16)-C(17)	1.31(3)	C(47)-C(48)	1.49(2)
C(16)-H(16)	0.9300	C(48)-O(32)	1.28(2)
C(17)-C(18)	1.51(2)	C(49)-O(34)	1.230(18)
C(17)-S(3)	1.703(15)	C(49)-O(33)	1.244(19)
C(18)-O(11)	1.23(2)	C(49)-C(50)	1.52(2)
C(18)-O(12)	1.27(2)	C(50)-C(51)	1.35(2)
C(19)-O(13)	1.25(2)	C(50)-S(9)	1.702(15)
C(19)-O(14)	1.25(2)	C(51)-C(52)	1.42(2)
C(19)-C(20)	1.49(2)	C(51)-H(51)	0.9300
C(20)-C(21)	1.33(2)	C(52)-C(53)	1.38(2)
C(20)-S(4)	1.719(16)	C(52)-H(52)	0.9300
C(21)-C(22)	1.39(2)	C(53)-C(54)	1.46(2)
C(21)-H(21)	0.9300	C(53)-S(9)	1.698(16)
C(22)-C(23)	1.35(2)	C(54)-O(36)	1.26(2)
C(22)-H(22)	0.9300	C(54)-O(35)	1.25(2)
C(23)-C(24)	1.48(2)	C(54)-Ce(3)#3	3.076(18)
C(23)-S(4)	1.706(16)	O(1)-Ce(2)	2.456(10)
C(24)-O(16)	1.240(18)	O(2)-Ce(1)	2.419(11)
C(24)-O(15)	1.288(17)	O(3)-Ce(1)#4	2.477(11)
C(25)-O(18)	1.24(2)	O(4)-Ce(2)#4	2.373(10)
C(25)-O(17)	1.25(2)	O(5)-Ce(1)	2.521(10)
C(25)-C(26)	1.47(2)	O(5)-Ce(2)	2.791(11)
C(26)-C(27)	1.37(2)	O(6)-Ce(2)	2.487(11)
C(26)-S(5)	1.716(15)	O(7)-Ce(1)#5	2.399(11)
C(27)-C(28)	1.41(2)	O(8)-Ce(5)#2	2.443(10)
C(27)-H(27)	0.9300	O(9)-Ce(1)	2.527(11)
C(28)-C(29)	1.36(2)	O(10)-Ce(2)	2.407(10)
C(28)-H(28)	0.9300	O(11)-Ce(1)#6	2.488(11)
C(29)-C(30)	1.489(19)	O(12)-Ce(5)#7	2.325(10)
C(29)-S(5)	1.705(15)	O(13)-Ce(2)	2.359(10)
C(30)-O(20)	1.260(17)	O(14)-Ce(3)	2.492(11)
C(30)-O(43)	1.257(19)	O(15)-Ce(5)	2.441(11)
C(30)-Ce(5)#1	3.041(13)	O(16)-Ce(6)	2.539(10)
C(31)-O(21)	1.25(2)	O(17)-Ce(2)	2.482(11)

C(31)-O(22)	1.27(2)	O(18)-Ce(3)	2.377(11)
C(31)-C(32)	1.50(2)	O(19)-Ce(3)	2.683(9)
C(47)-S(8)	1.712(16)	O(19)-H(19B)	0.86(3)
C(48)-O(31)	1.20(2)	O(20)-Ce(6)#1	2.464(10)
O(19)-Ce(2)	2.773(9)	O(20)-Ce(5)#1	2.820(10)
O(19)-H(19A)	0.86(3)	O(21)-Ce(3)	2.441(11)
O(26)-Ce(4)	2.426(10)	O(22)-Ce(4)	2.474(10)
O(27)-Ce(6)#1	2.483(11)	O(23)-Ce(5)#2	2.413(10)
O(28)-Ce(4)#8	2.359(10)	O(23)-Ce(6)#2	2.893(11)
O(29)-Ce(3)	2.450(10)	O(24)-Ce(6)#2	2.516(11)
O(29)-Ce(4)	2.854(11)	O(25)-Ce(3)	2.524(10)
O(30)-Ce(4)	2.539(11)	O(32)-Ce(6)	2.377(12)
O(31)-Ce(4)#9	2.476(11)	O(33)-Ce(5)	2.440(10)
O(42)-H(42B)	0.86(3)	O(34)-Ce(6)	2.453(10)
O(43)-Ce(5)#1	2.546(10)	O(35)-Ce(3)#3	2.554(11)
O(44)-Ce(1)	2.604(10)	O(36)-Ce(4)#3	2.433(10)
O(44)-H(44A)	0.85(3)	O(36)-Ce(3)#3	2.840(10)
O(44)-H(44B)	0.85(3)	O(42)-Ce(6)	2.638(10)
Ce(1)-O(7)#6	2.399(11)	O(42)-H(42A)	0.86(3)
Ce(1)-O(37)	2.472(15)	Ce(5)-O(41)	2.548(13)
Ce(1)-O(3)#10	2.477(11)	Ce(5)-O(20)#14	2.820(11)
Ce(1)-O(11)#5	2.488(11)	Ce(5)-C(30)#14	3.042(14)
Ce(1)-H(44A)	2.20(17)	Ce(6)-O(40)	2.451(12)
Ce(2)-O(4)#10	2.373(10)	Ce(6)-O(20)#14	2.464(10)
Ce(2)-C(59')#11	3.09(6)	Ce(6)-O(27)#14	2.483(11)
Ce(2)-H(19B)	2.40(16)	Ce(6)-O(24)#11	2.516(11)
Ce(3)-O(38)	2.515(11)	Ce(6)-O(23)#11	2.893(11)
Ce(3)-O(35)#7	2.555(11)	Ce(6)-C(36)#11	3.065(15)
Ce(3)-O(36)#7	2.840(10)	N(1)-C(55)	1.47(3)
Ce(3)-C(54)#7	3.076(18)	N(1)-C(58)	1.52(3)
Ce(4)-O(28)#12	2.360(10)	N(1)-C(56)	1.54(3)
Ce(4)-O(39)	2.437(13)	C(55)-O(37)	1.12(4)
Ce(4)-O(36)#7	2.433(10)	C(55)-H(55)	0.9300
Ce(4)-O(31)#13	2.476(11)	C(56)-C(57)	1.59(3)
Ce(5)-O(12)#3	2.325(11)	C(56)-H(56A)	0.9700
Ce(5)-O(23)#11	2.413(10)	C(56)-H(56B)	0.9700

Ce(5)-O(8)#11	2.443(10)	C(57)-H(57A)	0.9600
Ce(5)-O(43)#14	2.546(10)	C(57)-H(57B)	0.9600
C(58)-H(58B)	0.9700	C(57)-H(57C)	0.9600
C(59)-H(59A)	0.9600	C(58)-C(59)	1.59(3)
C(59)-H(59B)	0.9600	C(58)-H(58A)	0.9700
C(59)-H(59C)	0.9600	N(1')-C(55')	1.46(3)
N(3)-C(68)	1.47(2)	N(1')-C(56')	1.46(3)
N(3)-C(66)	1.48(2)	N(1')-C(58')	1.48(3)
C(65)-O(39)	1.22(3)	C(55')-O(37)	1.48(8)
C(65)-H(65)	0.9300	C(55')-H(55')	0.9300
C(66)-C(67)	1.56(3)	C(56')-C(57')	1.48(3)
C(66)-H(66A)	0.9700	C(56')-H(56C)	0.9700
C(66)-H(66B)	0.9700	C(56')-H(56D)	0.9700
C(67)-H(67A)	0.9600	C(57')-H(57D)	0.9600
C(67)-H(67B)	0.9600	C(57')-H(57E)	0.9600
C(67)-H(67C)	0.9600	C(57')-H(57F)	0.9600
C(68)-C(69)	1.52(3)	C(58')-C(59')	1.56(3)
C(68)-H(68A)	0.9700	C(58')-H(58C)	0.9700
C(68)-H(68B)	0.9700	C(58')-H(58D)	0.9700
C(69)-H(69A)	0.9600	C(59')-Ce(2)#2	3.09(6)
C(69)-H(69B)	0.9600	C(59')-H(59D)	0.9600
C(69)-H(69C)	0.9600	C(59')-H(59E)	0.9600
N(3')-C(65')	1.42(2)	C(59')-H(59F)	0.9600
N(3')-C(66')	1.47(2)	O(38)-C(60)	1.23(2)
N(3')-C(68')	1.47(2)	N(2)-C(60)	1.43(2)
C(65')-O(39)	1.23(3)	N(2)-C(63)	1.48(2)
C(65')-H(65')	0.9300	N(2)-C(61)	1.51(2)
C(66')-C(67')	1.53(3)	C(60)-H(60)	0.9300
C(66')-H(66C)	0.9700	C(61)-C(62)	1.56(3)
C(66')-H(66D)	0.9700	C(61)-H(61A)	0.9700
C(67')-H(67D)	0.9600	C(61)-H(61B)	0.9700
C(67')-H(67E)	0.9600	C(62)-H(62A)	0.9600
C(67')-H(67F)	0.9600	C(62)-H(62B)	0.9600
C(68')-C(69')	1.54(3)	C(62)-H(624)	0.9600
C(68')-H(68C)	0.9700	C(63)-C(64)	1.51(3)
C(68')-H(68D)	0.9700	C(63)-H(63A)	0.9700

C(69')-H(69D)	0.9600	C(63)-H(63B)	0.9700
C(69')-H(69E)	0.9600	C(64)-H(64A)	0.9600
C(69')-H(69F)	0.9600	C(64)-H(64B)	0.9600
O(40)-C(70)	1.22(2)	C(64)-H(64C)	0.9600
N(4)-C(70)	1.366(19)	N(3)-C(65)	1.45(2)
N(4)-C(71)	1.46(2)	C(76')-H(76C)	0.9700
N(4)-C(73)	1.47(2)	C(76')-H(76D)	0.9700
C(70)-H(70)	0.9300	C(77')-H(77D)	0.9600
C(71)-C(72)	1.52(3)	C(77')-H(77E)	0.9600
C(71)-H(71A)	0.9700	C(77')-H(77F)	0.9600
C(71)-H(71B)	0.9700	C(78')-C(79')	1.53(3)
C(72)-H(72A)	0.9600	C(78')-H(78C)	0.9700
C(72)-H(72B)	0.9600	C(78')-H(78D)	0.9700
C(72)-H(72C)	0.9600	C(79')-H(79D)	0.9600
C(73)-C(74)	1.55(3)	C(79')-H(79E)	0.9600
C(73)-H(73A)	0.9700	C(79')-H(79F)	0.9600
C(73)-H(73B)	0.9700	C(77)-H(77C)	0.9600
C(74)-H(74A)	0.9600	C(78)-C(79)	1.54(3)
C(74)-H(74B)	0.9600	C(78)-H(78A)	0.9700
C(74)-H(74C)	0.9600	C(78)-H(78B)	0.9700
N(5)-C(76)	1.45(3)	C(79)-H(79A)	0.9600
N(5)-C(78)	1.48(3)	C(79)-H(79B)	0.9600
N(5)-C(75)	1.49(3)	C(79)-H(79C)	0.9600
C(75)-O(41)	1.24(3)	N(5')-C(75')	1.45(2)
C(75)-H(75)	0.9300	N(5')-C(76')	1.46(3)
C(76)-C(77)	1.55(3)	N(5')-C(78')	1.47(3)
C(76)-H(76A)	0.9700	C(75')-O(41)	1.19(2)
C(76)-H(76B)	0.9700	C(75')-H(75')	0.9300
C(77)-H(77A)	0.9600	C(76')-C(77')	1.52(3)
C(77)-H(77B)	0.9600	C(29)-C(28)-C(27)	112.0(15)
O(1)-C(1)-O(2)	126.1(15)	C(29)-C(28)-H(28)	124.0
O(1)-C(1)-C(2)	119.4(13)	C(27)-C(28)-H(28)	124.0
O(2)-C(1)-C(2)	114.4(14)	C(28)-C(29)-C(30)	126.4(14)
C(3)-C(2)-C(1)	128.6(15)	C(28)-C(29)-S(5)	112.1(11)
C(3)-C(2)-S(1)	110.4(12)	C(30)-C(29)-S(5)	121.5(12)
C(1)-C(2)-S(1)	120.9(12)	O(20)-C(30)-O(43)	122.3(13)

C(2)-C(3)-C(4)	113.7(16)	O(20)-C(30)-C(29)	120.0(13)
C(2)-C(3)-H(3)	123.1	O(43)-C(30)-C(29)	117.7(13)
C(4)-C(3)-H(3)	123.1	O(20)-C(30)-Ce(5)#1	67.9(7)
C(5)-C(4)-C(3)	112.3(15)	O(43)-C(30)-Ce(5)#1	55.3(7)
C(5)-C(4)-H(4)	123.8	C(29)-C(30)-Ce(5)#1	167.7(11)
C(3)-C(4)-H(4)	123.8	O(21)-C(31)-O(22)	126.8(16)
C(4)-C(5)-C(6)	128.3(14)	O(21)-C(31)-C(32)	117.8(16)
C(4)-C(5)-S(1)	111.6(12)	O(22)-C(31)-C(32)	114.9(16)
C(6)-C(5)-S(1)	120.1(12)	C(33)-C(32)-C(31)	124.6(16)
O(3)-C(6)-O(4)	121.6(14)	C(33)-C(32)-S(6)	112.9(12)
O(3)-C(6)-C(5)	119.3(14)	C(31)-C(32)-S(6)	122.3(13)
O(4)-C(6)-C(5)	119.0(14)	C(32)-C(33)-C(34)	110.0(15)
O(6)-C(7)-O(5)	123.5(13)	C(32)-C(33)-H(33)	125.0
O(6)-C(7)-C(8)	118.9(14)	C(34)-C(33)-H(33)	125.0
O(5)-C(7)-C(8)	117.6(14)	C(35)-C(34)-C(33)	113.5(15)
O(6)-C(7)-Ce(2)	54.8(7)	C(35)-C(34)-H(34)	123.3
O(5)-C(7)-Ce(2)	69.0(8)	C(33)-C(34)-H(34)	123.3
C(8)-C(7)-Ce(2)	172.5(11)	C(34)-C(35)-C(36)	128.2(14)
C(9)-C(8)-C(7)	130.5(14)	C(34)-C(35)-S(6)	112.2(11)
C(9)-C(8)-S(2)	110.1(12)	C(36)-C(35)-S(6)	119.6(12)
C(7)-C(8)-S(2)	119.4(12)	O(24)-C(36)-O(23)	122.2(14)
C(8)-C(9)-C(10)	113.9(15)	O(24)-C(36)-C(35)	119.0(14)
C(8)-C(9)-H(9)	123.0	O(23)-C(36)-C(35)	118.7(14)
C(10)-C(9)-H(9)	123.0	O(24)-C(36)-Ce(6)#2	52.9(7)
C(11)-C(10)-C(9)	110.4(15)	O(23)-C(36)-Ce(6)#2	70.2(8)
C(11)-C(10)-H(10)	124.8	C(35)-C(36)-Ce(6)#2	168.8(11)
C(9)-C(10)-H(10)	124.8	O(26)-C(37)-O(25)	127.4(15)
C(10)-C(11)-C(12)	124.2(14)	O(26)-C(37)-C(38)	116.9(15)
C(10)-C(11)-S(2)	113.2(11)	O(25)-C(37)-C(38)	115.7(15)
C(12)-C(11)-S(2)	122.5(12)	C(39)-C(38)-C(37)	128.5(16)
O(8)-C(12)-O(7)	123.8(15)	C(39)-C(38)-S(7)	111.4(12)
O(8)-C(12)-C(11)	118.6(13)	C(37)-C(38)-S(7)	120.0(12)
O(7)-C(12)-C(11)	117.6(15)	C(38)-C(39)-C(40)	112.2(16)
O(9)-C(13)-O(10)	127.7(15)	C(38)-C(39)-H(39)	123.9
O(9)-C(13)-C(14)	117.7(14)	C(40)-C(39)-H(39)	123.9
O(10)-C(13)-C(14)	114.5(13)	C(41)-C(40)-C(39)	113.3(15)

C(15)-C(14)-C(13)	129.3(15)	C(41)-C(40)-H(40)	123.4
C(15)-C(14)-S(3)	110.7(12)	C(39)-C(40)-H(40)	123.4
C(13)-C(14)-S(3)	119.9(12)	C(40)-C(41)-C(42)	128.5(15)
C(14)-C(15)-C(16)	111.2(15)	C(40)-C(41)-S(7)	111.9(13)
C(14)-C(15)-H(15)	124.4	C(42)-C(41)-S(7)	119.6(12)
C(16)-C(15)-H(15)	124.4	O(27)-C(42)-O(28)	126.0(14)
C(17)-C(16)-C(15)	115.9(16)	O(27)-C(42)-C(41)	120.3(14)
C(17)-C(16)-H(16)	122.1	O(28)-C(42)-C(41)	113.5(14)
C(15)-C(16)-H(16)	122.1	O(30)-C(43)-O(29)	120.9(15)
C(16)-C(17)-C(18)	129.6(15)	O(30)-C(43)-C(44)	119.3(15)
C(16)-C(17)-S(3)	110.4(13)	O(29)-C(43)-C(44)	119.7(16)
C(18)-C(17)-S(3)	120.0(13)	O(30)-C(43)-Ce(4)	53.4(8)
O(11)-C(18)-O(12)	127.9(15)	O(29)-C(43)-Ce(4)	67.9(9)
O(11)-C(18)-C(17)	119.5(15)	C(44)-C(43)-Ce(4)	169.2(12)
O(12)-C(18)-C(17)	112.0(15)	C(45)-C(44)-C(43)	126.4(15)
O(13)-C(19)-O(14)	125.0(16)	C(45)-C(44)-S(8)	113.2(11)
O(13)-C(19)-C(20)	116.8(16)	C(43)-C(44)-S(8)	120.4(12)
O(14)-C(19)-C(20)	118.1(15)	C(44)-C(45)-C(46)	111.1(14)
C(21)-C(20)-C(19)	127.8(15)	C(44)-C(45)-H(45)	124.4
C(21)-C(20)-S(4)	112.2(13)	C(46)-C(45)-H(45)	124.4
C(19)-C(20)-S(4)	120.0(13)	C(47)-C(46)-C(45)	113.2(16)
C(20)-C(21)-C(22)	112.7(15)	C(47)-C(46)-H(46)	123.4
C(20)-C(21)-H(21)	123.6	C(45)-C(46)-H(46)	123.4
C(22)-C(21)-H(21)	123.6	C(46)-C(47)-C(48)	126.9(15)
C(23)-C(22)-C(21)	112.9(15)	C(46)-C(47)-S(8)	111.0(12)
C(23)-C(22)-H(22)	123.5	C(48)-C(47)-S(8)	122.0(13)
C(21)-C(22)-H(22)	123.5	O(31)-C(48)-O(32)	126.4(16)
C(22)-C(23)-C(24)	129.5(15)	O(31)-C(48)-C(47)	120.8(15)
C(22)-C(23)-S(4)	111.4(12)	O(32)-C(48)-C(47)	112.8(16)
C(24)-C(23)-S(4)	119.0(12)	O(34)-C(49)-O(33)	126.7(15)
O(16)-C(24)-O(15)	123.4(13)	O(34)-C(49)-C(50)	115.8(14)
O(16)-C(24)-C(23)	119.8(13)	O(33)-C(49)-C(50)	117.3(13)
O(15)-C(24)-C(23)	116.3(14)	C(51)-C(50)-C(49)	124.8(14)
O(18)-C(25)-O(17)	123.4(16)	C(51)-C(50)-S(9)	114.6(12)
O(18)-C(25)-C(26)	116.2(16)	C(49)-C(50)-S(9)	120.5(11)
O(17)-C(25)-C(26)	120.3(15)	C(50)-C(51)-C(52)	109.9(15)

C(27)-C(26)-C(25)	124.9(15)	C(50)-C(51)-H(51)	125.0
C(27)-C(26)-S(5)	110.4(11)	C(52)-C(51)-H(51)	125.0
C(25)-C(26)-S(5)	124.7(13)	C(53)-C(52)-C(51)	113.2(15)
C(26)-C(27)-C(28)	113.4(15)	C(53)-C(52)-H(52)	123.4
C(26)-C(27)-H(27)	123.3	C(51)-C(52)-H(52)	123.4
C(28)-C(27)-H(27)	123.3	C(52)-C(53)-C(54)	128.8(15)
C(50)-S(9)-C(53)	91.1(8)	C(52)-C(53)-S(9)	111.2(12)
O(7)#6-Ce(1)-O(2)	137.6(4)	C(54)-C(53)-S(9)	120.0(13)
O(7)#6-Ce(1)-O(37)	77.8(5)	O(36)-C(54)-O(35)	121.1(15)
O(2)-Ce(1)-O(37)	138.1(5)	O(36)-C(54)-C(53)	120.3(16)
O(7)#6-Ce(1)-O(3)#10	73.9(4)	O(35)-C(54)-C(53)	118.4(15)
O(2)-Ce(1)-O(3)#10	83.0(4)	O(36)-C(54)-Ce(3)#3	67.3(9)
O(37)-Ce(1)-O(3)#10	136.8(5)	O(35)-C(54)-Ce(3)#3	54.2(9)
O(7)#6-Ce(1)-O(11)#5	98.3(5)	C(53)-C(54)-Ce(3)#3	166.7(13)
O(2)-Ce(1)-O(11)#5	80.5(4)	C(1)-O(1)-Ce(2)	130.0(10)
O(37)-Ce(1)-O(11)#5	70.9(5)	C(1)-O(2)-Ce(1)	145.9(11)
O(3)#10-Ce(1)-O(11)#5	144.8(4)	C(6)-O(3)-Ce(1)#4	114.0(10)
O(7)#6-Ce(1)-O(5)	153.6(4)	C(6)-O(4)-Ce(2)#4	173.6(11)
O(2)-Ce(1)-O(5)	68.8(4)	C(7)-O(5)-Ce(1)	166.6(10)
O(37)-Ce(1)-O(5)	79.4(4)	C(7)-O(5)-Ce(2)	86.0(8)
O(3)#10-Ce(1)-O(5)	115.7(4)	Ce(1)-O(5)-Ce(2)	106.6(3)
O(11)#5-Ce(1)-O(5)	86.8(4)	C(7)-O(6)-Ce(2)	101.5(9)
O(7)#6-Ce(1)-O(9)	86.3(4)	C(12)-O(7)-Ce(1)#5	172.5(12)
O(2)-Ce(1)-O(9)	121.8(4)	C(12)-O(8)-Ce(5)#2	132.8(10)
O(37)-Ce(1)-O(9)	71.0(5)	C(13)-O(9)-Ce(1)	141.1(10)
O(3)#10-Ce(1)-O(9)	75.1(4)	C(13)-O(10)-Ce(2)	132.2(10)
O(11)#5-Ce(1)-O(9)	139.7(4)	C(18)-O(11)-Ce(1)#6	123.7(11)
O(5)-Ce(1)-O(9)	73.6(3)	C(18)-O(12)-Ce(5)#7	143.6(12)
O(7)#6-Ce(1)-O(44)	70.6(4)	C(19)-O(13)-Ce(2)	144.2(14)
O(2)-Ce(1)-O(44)	68.1(4)	C(19)-O(14)-Ce(3)	130.2(11)
O(37)-Ce(1)-O(44)	128.9(4)	C(24)-O(15)-Ce(5)	134.4(10)
O(3)#10-Ce(1)-O(44)	69.9(4)	C(24)-O(16)-Ce(6)	141.6(9)
O(11)#5-Ce(1)-O(44)	75.1(4)	C(25)-O(17)-Ce(2)	128.5(11)
O(5)-Ce(1)-O(44)	135.4(4)	C(25)-O(18)-Ce(3)	170.3(13)
O(9)-Ce(1)-O(44)	142.1(4)	Ce(3)-O(19)-Ce(2)	122.0(4)
O(7)#6-Ce(1)-H(44A)	67(4)	Ce(3)-O(19)-H(19A)	100(9)

O(2)-Ce(1)-H(44A)	77(3)	Ce(2)-O(19)-H(19A)	123(10)
O(37)-Ce(1)-H(44A)	111.7(19)	Ce(3)-O(19)-H(19B)	148(10)
O(3)#10-Ce(1)-H(44A)	86(2)	Ce(2)-O(19)-H(19B)	56(10)
O(11)#5-Ce(1)-H(44A)	60(3)	H(19A)-O(19)-H(19B)	106(5)
O(5)-Ce(1)-H(44A)	136(4)	C(30)-O(20)-Ce(6)#1	168.2(10)
O(9)-Ce(1)-H(44A)	151(4)	C(30)-O(20)-Ce(5)#1	87.7(8)
O(44)-Ce(1)-H(44A)	18.0(17)	Ce(6)#1-O(20)-Ce(5)#1	104.1(3)
O(13)-Ce(2)-O(4)#10	144.2(4)	C(31)-O(21)-Ce(3)	136.3(12)
O(13)-Ce(2)-O(10)	135.1(4)	C(31)-O(22)-Ce(4)	133.7(11)
O(4)#10-Ce(2)-O(10)	76.2(4)	C(36)-O(23)-Ce(5)#2	167.4(11)
O(13)-Ce(2)-O(1)	81.5(4)	C(36)-O(23)-Ce(6)#2	85.5(9)
O(4)#10-Ce(2)-O(1)	80.7(4)	Ce(5)#2-O(23)-Ce(6)#2	103.4(3)
O(10)-Ce(2)-O(1)	137.2(4)	C(36)-O(24)-Ce(6)#2	103.6(9)
O(13)-Ce(2)-O(17)	83.8(4)	C(37)-O(25)-Ce(3)	135.3(10)
O(4)#10-Ce(2)-O(17)	81.2(4)	C(37)-O(26)-Ce(4)	134.4(12)
O(10)-Ce(2)-O(17)	86.6(5)	C(42)-O(27)-Ce(6)#1	133.4(10)
O(1)-Ce(2)-O(17)	124.8(5)	C(42)-O(28)-Ce(4)#8	144.4(10)
O(13)-Ce(2)-O(6)	77.8(4)	C(43)-O(29)-Ce(3)	167.8(11)
O(4)#10-Ce(2)-O(6)	129.9(4)	C(43)-O(29)-Ce(4)	87.8(10)
O(10)-Ce(2)-O(6)	85.3(4)	Ce(3)-O(29)-Ce(4)	104.3(3)
O(1)-Ce(2)-O(6)	82.6(4)	C(43)-O(30)-Ce(4)	103.3(10)
O(17)-Ce(2)-O(6)	144.3(4)	C(48)-O(31)-Ce(4)#9	133.1(11)
O(13)-Ce(2)-O(19)	71.3(4)	C(48)-O(32)-Ce(6)	163.3(15)
O(4)#10-Ce(2)-O(19)	137.8(4)	C(49)-O(33)-Ce(5)	135.3(10)
O(10)-Ce(2)-O(19)	64.1(4)	C(49)-O(34)-Ce(6)	138.2(10)
O(1)-Ce(2)-O(19)	138.9(4)	C(54)-O(35)-Ce(3)#3	102.5(10)
O(17)-Ce(2)-O(19)	83.0(4)	C(54)-O(36)-Ce(4)#3	166.3(11)
O(6)-Ce(2)-O(19)	62.3(4)	C(54)-O(36)-Ce(3)#3	88.5(10)
O(13)-Ce(2)-O(5)	121.1(3)	Ce(4)#3-O(36)-Ce(3)#3	105.2(3)
O(4)#10-Ce(2)-O(5)	81.3(4)	Ce(6)-O(42)-H(42A)	142(10)
O(10)-Ce(2)-O(5)	70.5(4)	Ce(6)-O(42)-H(42B)	105(10)
O(1)-Ce(2)-O(5)	70.8(4)	H(42A)-O(42)-H(42B)	107(5)
O(17)-Ce(2)-O(5)	153.9(4)	C(30)-O(43)-Ce(5)#1	100.7(8)
O(6)-Ce(2)-O(5)	48.5(3)	Ce(1)-O(44)-H(44A)	53(10)
O(19)-Ce(2)-O(5)	97.4(3)	Ce(1)-O(44)-H(44B)	126(10)
O(13)-Ce(2)-C(7)	98.4(4)	H(44A)-O(44)-H(44B)	109(5)

O(4)#10-Ce(2)-C(7)	106.2(4)	C(5)-S(1)-C(2)	91.9(8)
O(10)-Ce(2)-C(7)	78.4(4)	C(11)-S(2)-C(8)	92.1(8)
O(1)-Ce(2)-C(7)	74.2(5)	C(17)-S(3)-C(14)	91.6(8)
O(17)-Ce(2)-C(7)	161.0(5)	C(23)-S(4)-C(20)	90.6(8)
O(6)-Ce(2)-C(7)	23.7(4)	C(29)-S(5)-C(26)	92.1(8)
O(19)-Ce(2)-C(7)	79.9(4)	C(32)-S(6)-C(35)	91.4(8)
O(5)-Ce(2)-C(7)	24.9(4)	C(41)-S(7)-C(38)	91.1(8)
O(13)-Ce(2)-C(59')#11	67.9(14)	C(44)-S(8)-C(47)	91.5(7)
O(28)#12-Ce(4)-O(39)	77.3(4)	O(4)#10-Ce(2)-C(59')#11	76.3(14)
O(26)-Ce(4)-O(39)	139.2(4)	O(10)-Ce(2)-C(59')#11	140.9(15)
O(28)#12-Ce(4)-O(36)#7	156.4(4)	O(1)-Ce(2)-C(59')#11	63.1(13)
O(26)-Ce(4)-O(36)#7	74.2(4)	O(17)-Ce(2)-C(59')#11	62.0(14)
O(39)-Ce(4)-O(36)#7	79.5(4)	O(6)-Ce(2)-C(59')#11	133.8(15)
O(28)#12-Ce(4)-O(22)	88.1(4)	O(19)-Ce(2)-C(59')#11	127.9(12)
O(26)-Ce(4)-O(22)	131.5(4)	O(5)-Ce(2)-C(59')#11	131.1(12)
O(39)-Ce(4)-O(22)	72.4(4)	C(7)-Ce(2)-C(59')#11	136.3(14)
O(36)#7-Ce(4)-O(22)	81.1(4)	O(13)-Ce(2)-H(19B)	77(3)
O(28)#12-Ce(4)-O(31)#13	86.0(4)	O(4)#10-Ce(2)-H(19B)	138(3)
O(26)-Ce(4)-O(31)#13	79.2(4)	O(10)-Ce(2)-H(19B)	62(3)
O(39)-Ce(4)-O(31)#13	70.0(5)	O(1)-Ce(2)-H(19B)	127(3)
O(36)#7-Ce(4)-O(31)#13	89.8(4)	O(17)-Ce(2)-H(19B)	99.9(16)
O(22)-Ce(4)-O(31)#13	142.3(4)	O(6)-Ce(2)-H(19B)	46.3(19)
O(28)#12-Ce(4)-O(30)	75.3(4)	O(19)-Ce(2)-H(19B)	17.3(14)
O(26)-Ce(4)-O(30)	79.7(4)	O(5)-Ce(2)-H(19B)	80.7(15)
O(39)-Ce(4)-O(30)	141.0(4)	C(7)-Ce(2)-H(19B)	62.7(14)
O(36)#7-Ce(4)-O(30)	122.5(3)	C(59')#11-Ce(2)-H(19B)	141(3)
O(22)-Ce(4)-O(30)	79.5(4)	O(18)-Ce(3)-O(21)	134.6(4)
O(31)#13-Ce(4)-O(30)	134.0(4)	O(18)-Ce(3)-O(29)	152.8(4)
O(28)#12-Ce(4)-O(29)	119.3(3)	O(21)-Ce(3)-O(29)	72.3(4)
O(26)-Ce(4)-O(29)	67.4(3)	O(18)-Ce(3)-O(14)	93.0(4)
O(39)-Ce(4)-O(29)	134.0(4)	O(21)-Ce(3)-O(14)	77.1(4)
O(36)#7-Ce(4)-O(29)	75.2(3)	O(29)-Ce(3)-O(14)	89.9(4)
O(22)-Ce(4)-O(29)	66.2(3)	O(18)-Ce(3)-O(38)	73.5(5)
O(31)#13-Ce(4)-O(29)	146.0(4)	O(21)-Ce(3)-O(38)	138.2(4)
O(30)-Ce(4)-O(29)	47.5(3)	O(29)-Ce(3)-O(38)	82.2(4)
O(28)#12-Ce(4)-C(43)	96.4(4)	O(14)-Ce(3)-O(38)	70.2(4)

O(26)-Ce(4)-C(43)	73.8(4)	O(18)-Ce(3)-O(25)	84.8(4)
O(39)-Ce(4)-C(43)	142.1(4)	O(21)-Ce(3)-O(25)	129.5(4)
O(36)#7-Ce(4)-C(43)	99.5(4)	O(29)-Ce(3)-O(25)	76.2(3)
O(22)-Ce(4)-C(43)	70.0(4)	O(14)-Ce(3)-O(25)	141.3(4)
O(31)#13-Ce(4)-C(43)	147.7(5)	O(38)-Ce(3)-O(25)	72.2(4)
O(30)-Ce(4)-C(43)	23.3(4)	O(18)-Ce(3)-O(35)#7	71.7(5)
O(29)-Ce(4)-C(43)	24.3(4)	O(21)-Ce(3)-O(35)#7	84.7(5)
O(12)#3-Ce(5)-O(23)#11	165.0(4)	O(29)-Ce(3)-O(35)#7	122.7(4)
O(12)#3-Ce(5)-O(15)	113.7(4)	O(14)-Ce(3)-O(35)#7	135.6(4)
O(23)#11-Ce(5)-O(15)	76.1(4)	O(38)-Ce(3)-O(35)#7	137.0(5)
O(12)#3-Ce(5)-O(33)	98.0(4)	O(25)-Ce(3)-O(35)#7	80.2(4)
O(23)#11-Ce(5)-O(33)	81.3(4)	O(18)-Ce(3)-O(19)	67.7(4)
O(15)-Ce(5)-O(33)	133.6(4)	O(21)-Ce(3)-O(19)	67.3(4)
O(12)#3-Ce(5)-O(8)#11	83.6(4)	O(29)-Ce(3)-O(19)	138.0(4)
O(23)#11-Ce(5)-O(8)#11	88.3(4)	O(14)-Ce(3)-O(19)	70.6(4)
O(15)-Ce(5)-O(8)#11	75.2(4)	O(38)-Ce(3)-O(19)	121.9(4)
O(33)-Ce(5)-O(8)#11	144.2(4)	O(25)-Ce(3)-O(19)	140.5(4)
O(12)#3-Ce(5)-O(43)#14	69.4(4)	O(35)#7-Ce(3)-O(19)	65.0(4)
O(23)#11-Ce(5)-O(43)#14	125.1(4)	O(18)-Ce(3)-O(36)#7	114.2(4)
O(15)-Ce(5)-O(43)#14	78.1(4)	O(21)-Ce(3)-O(36)#7	69.3(4)
O(33)-Ce(5)-O(43)#14	82.9(4)	O(29)-Ce(3)-O(36)#7	75.2(3)
O(8)#11-Ce(5)-O(43)#14	129.7(4)	O(14)-Ce(3)-O(36)#7	146.0(4)
O(12)#3-Ce(5)-O(41)	78.6(5)	O(38)-Ce(3)-O(36)#7	135.2(4)
O(23)#11-Ce(5)-O(41)	86.9(5)	O(25)-Ce(3)-O(36)#7	65.1(3)
O(15)-Ce(5)-O(41)	143.7(6)	O(35)#7-Ce(3)-O(36)#7	47.5(3)
O(33)-Ce(5)-O(41)	72.9(5)	O(19)-Ce(3)-O(36)#7	100.2(3)
O(8)#11-Ce(5)-O(41)	72.4(5)	O(18)-Ce(3)-C(54)#7	92.0(5)
O(43)#14-Ce(5)-O(41)	136.4(6)	O(21)-Ce(3)-C(54)#7	77.5(5)
O(12)#3-Ce(5)-O(20)#14	116.4(4)	O(29)-Ce(3)-C(54)#7	99.4(4)
O(23)#11-Ce(5)-O(20)#14	77.3(3)	O(14)-Ce(3)-C(54)#7	148.8(5)
O(15)-Ce(5)-O(20)#14	68.8(3)	O(38)-Ce(3)-C(54)#7	140.4(5)
O(33)-Ce(5)-O(20)#14	66.9(4)	O(25)-Ce(3)-C(54)#7	69.8(5)
O(8)#11-Ce(5)-O(20)#14	143.4(4)	O(35)#7-Ce(3)-C(54)#7	23.4(4)
O(43)#14-Ce(5)-O(20)#14	48.2(3)	O(19)-Ce(3)-C(54)#7	83.0(4)
O(41)-Ce(5)-O(20)#14	138.5(4)	O(36)#7-Ce(3)-C(54)#7	24.2(4)
O(12)#3-Ce(5)-C(30)#14	92.1(4)	O(28)#12-Ce(4)-O(26)	127.3(4)

O(23)#11-Ce(5)-C(30)#14	101.7(4)	O(42)-Ce(6)-C(36)#11	85.8(5)
O(15)-Ce(5)-C(30)#14	74.3(4)	O(23)#11-Ce(6)-C(36)#11	24.3(4)
O(33)-Ce(5)-C(30)#14	71.4(4)	C(55)-N(1)-C(58)	110(3)
O(8)#11-Ce(5)-C(30)#14	144.4(4)	C(55)-N(1)-C(56)	109(3)
O(43)#14-Ce(5)-C(30)#14	24.0(4)	C(58)-N(1)-C(56)	112(4)
O(41)-Ce(5)-C(30)#14	141.4(5)	O(37)-C(55)-N(1)	121(4)
O(20)#14-Ce(5)-C(30)#14	24.4(3)	O(37)-C(55)-H(55)	119.6
O(32)-Ce(6)-O(40)	75.0(5)	N(1)-C(55)-H(55)	119.6
O(32)-Ce(6)-O(34)	138.7(4)	N(1)-C(56)-C(57)	121(3)
O(40)-Ce(6)-O(34)	134.1(4)	N(1)-C(56)-H(56A)	106.9
O(32)-Ce(6)-O(20)#14	149.5(4)	C(57)-C(56)-H(56A)	107.0
O(40)-Ce(6)-O(20)#14	76.8(4)	N(1)-C(56)-H(56B)	107.0
O(34)-Ce(6)-O(20)#14	71.1(4)	C(57)-C(56)-H(56B)	107.0
O(32)-Ce(6)-O(27)#14	90.8(4)	H(56A)-C(56)-H(56B)	106.7
O(40)-Ce(6)-O(27)#14	70.3(4)	C(56)-C(57)-H(57A)	109.5
O(34)-Ce(6)-O(27)#14	77.9(4)	C(56)-C(57)-H(57B)	109.5
O(20)#14-Ce(6)-O(27)#14	90.4(4)	H(57A)-C(57)-H(57B)	109.5
O(32)-Ce(6)-O(24)#11	72.8(4)	C(56)-C(57)-H(57C)	109.5
O(40)-Ce(6)-O(24)#11	135.2(4)	H(57A)-C(57)-H(57C)	109.5
O(34)-Ce(6)-O(24)#11	90.2(4)	H(57B)-C(57)-H(57C)	109.5
O(20)#14-Ce(6)-O(24)#11	122.5(4)	N(1)-C(58)-C(59)	122(3)
O(27)#14-Ce(6)-O(24)#11	139.4(4)	N(1)-C(58)-H(58A)	106.9
O(32)-Ce(6)-O(16)	84.8(4)	C(59)-C(58)-H(58A)	106.9
O(40)-Ce(6)-O(16)	71.8(4)	N(1)-C(58)-H(58B)	106.9
O(34)-Ce(6)-O(16)	127.7(4)	C(59)-C(58)-H(58B)	106.9
O(20)#14-Ce(6)-O(16)	75.6(3)	H(58A)-C(58)-H(58B)	106.7
O(27)#14-Ce(6)-O(16)	141.6(4)	C(58)-C(59)-H(59A)	109.5
O(24)#11-Ce(6)-O(16)	75.1(4)	C(58)-C(59)-H(59B)	109.5
O(32)-Ce(6)-O(42)	69.5(5)	H(59A)-C(59)-H(59B)	109.5
O(40)-Ce(6)-O(42)	126.1(4)	C(58)-C(59)-H(59C)	109.5
O(34)-Ce(6)-O(42)	69.2(4)	H(59A)-C(59)-H(59C)	109.5
O(20)#14-Ce(6)-O(42)	138.8(4)	H(59B)-C(59)-H(59C)	109.5
O(27)#14-Ce(6)-O(42)	71.1(4)	C(55')-N(1')-C(56')	115(3)
O(24)#11-Ce(6)-O(42)	68.4(4)	C(55')-N(1')-C(58')	114(3)
O(16)-Ce(6)-O(42)	140.0(4)	C(56')-N(1')-C(58')	108(6)
O(32)-Ce(6)-O(23)#11	116.5(4)	N(1')-C(55')-O(37)	105(5)

O(40)-Ce(6)-O(23)#11	131.5(4)	N(1')-C(55')-H(55')	127.5
O(34)-Ce(6)-O(23)#11	69.8(4)	N(2)-C(61)-H(61A)	110.2
O(20)#14-Ce(6)-O(23)#11	75.1(3)	C(62)-C(61)-H(61A)	110.2
O(27)#14-Ce(6)-O(23)#11	147.3(4)	N(2)-C(61)-H(61B)	110.2
O(24)#11-Ce(6)-O(23)#11	47.5(3)	C(62)-C(61)-H(61B)	110.2
O(16)-Ce(6)-O(23)#11	63.3(3)	H(61A)-C(61)-H(61B)	108.5
O(42)-Ce(6)-O(23)#11	100.7(4)	C(61)-C(62)-H(62A)	109.5
O(32)-Ce(6)-C(36)#11	93.4(4)	C(61)-C(62)-H(62B)	109.5
O(40)-Ce(6)-C(36)#11	136.2(4)	H(62A)-C(62)-H(62B)	109.5
O(34)-Ce(6)-C(36)#11	81.6(4)	C(61)-C(62)-H(624)	109.5
O(20)#14-Ce(6)-C(36)#11	99.0(4)	H(62A)-C(62)-H(624)	109.5
O(27)#14-Ce(6)-C(36)#11	153.3(4)	H(62B)-C(62)-H(624)	109.5
O(24)#11-Ce(6)-C(36)#11	23.5(4)	N(2)-C(63)-C(64)	108(3)
O(16)-Ce(6)-C(36)#11	65.1(4)	N(2)-C(63)-H(63A)	110.2
O(37)-C(55')-H(55')	127.5	C(64)-C(63)-H(63A)	110.2
N(1')-C(56')-C(57')	137(5)	N(2)-C(63)-H(63B)	110.2
N(1')-C(56')-H(56C)	102.9	C(64)-C(63)-H(63B)	110.2
C(57')-C(56')-H(56C)	102.9	H(63A)-C(63)-H(63B)	108.5
N(1')-C(56')-H(56D)	103.0	C(63)-C(64)-H(64A)	109.5
C(57')-C(56')-H(56D)	103.0	C(63)-C(64)-H(64B)	109.5
H(56C)-C(56')-H(56D)	105.1	H(64A)-C(64)-H(64B)	109.5
C(56')-C(57')-H(57D)	109.5	C(63)-C(64)-H(64C)	109.5
C(56')-C(57')-H(57E)	109.5	H(64A)-C(64)-H(64C)	109.5
H(57D)-C(57')-H(57E)	109.5	H(64B)-C(64)-H(64C)	109.5
C(56')-C(57')-H(57F)	109.4	C(65)-N(3)-C(68)	115(2)
H(57D)-C(57')-H(57F)	109.5	C(65)-N(3)-C(66)	114(2)
H(57E)-C(57')-H(57F)	109.5	C(68)-N(3)-C(66)	128(3)
N(1')-C(58')-C(59')	128(4)	O(39)-C(65)-N(3)	124(3)
N(1')-C(58')-H(58C)	105.4	O(39)-C(65)-H(65)	117.8
C(59')-C(58')-H(58C)	105.4	N(3)-C(65)-H(65)	117.8
N(1')-C(58')-H(58D)	105.4	N(3)-C(66)-C(67)	107(3)
C(59')-C(58')-H(58D)	105.4	N(3)-C(66)-H(66A)	110.3
H(58C)-C(58')-H(58D)	106.0	C(67)-C(66)-H(66A)	110.3
C(58')-C(59')-Ce(2)#2	134(5)	N(3)-C(66)-H(66B)	110.3
C(58')-C(59')-H(59D)	109.5	C(67)-C(66)-H(66B)	110.3
Ce(2)#2-C(59')-H(59D)	56.8	H(66A)-C(66)-H(66B)	108.5

C(58')-C(59')-H(59E)	109.4	C(66)-C(67)-H(67A)	109.5
Ce(2)#2-C(59')-H(59E)	53.7	C(66)-C(67)-H(67B)	109.5
H(59D)-C(59')-H(59E)	109.5	N(3')-C(68')-H(68D)	109.9
C(58')-C(59')-H(59F)	109.5	C(69')-C(68')-H(68D)	109.9
Ce(2)#2-C(59')-H(59F)	116.0	H(68C)-C(68')-H(68D)	108.3
H(59D)-C(59')-H(59F)	109.5	C(68')-C(69')-H(69D)	109.5
H(59E)-C(59')-H(59F)	109.5	C(68')-C(69')-H(69E)	109.5
C(60)-O(38)-Ce(3)	129.9(13)	H(69D)-C(69')-H(69E)	109.5
C(60)-N(2)-C(63)	117(2)	C(68')-C(69')-H(69F)	109.5
C(60)-N(2)-C(61)	113(2)	H(69D)-C(69')-H(69F)	109.5
C(63)-N(2)-C(61)	129(3)	H(69E)-C(69')-H(69F)	109.5
O(38)-C(60)-N(2)	121(2)	C(70)-O(40)-Ce(6)	127.6(12)
O(38)-C(60)-H(60)	119.3	C(70)-N(4)-C(71)	123(2)
N(2)-C(60)-H(60)	119.3	C(70)-N(4)-C(73)	121(2)
N(2)-C(61)-C(62)	108(3)	C(71)-N(4)-C(73)	116(2)
H(67A)-C(67)-H(67B)	109.5	O(40)-C(70)-N(4)	123.9(19)
C(66)-C(67)-H(67C)	109.5	O(40)-C(70)-H(70)	118.0
H(67A)-C(67)-H(67C)	109.5	N(4)-C(70)-H(70)	118.0
H(67B)-C(67)-H(67C)	109.5	N(4)-C(71)-C(72)	114(3)
N(3)-C(68)-C(69)	111(3)	N(4)-C(71)-H(71A)	108.9
N(3)-C(68)-H(68A)	109.5	C(72)-C(71)-H(71A)	108.9
C(69)-C(68)-H(68A)	109.4	N(4)-C(71)-H(71B)	108.9
N(3)-C(68)-H(68B)	109.5	C(72)-C(71)-H(71B)	108.9
C(69)-C(68)-H(68B)	109.5	H(71A)-C(71)-H(71B)	107.7
H(68A)-C(68)-H(68B)	108.1	C(71)-C(72)-H(72A)	109.5
C(68)-C(69)-H(69A)	109.5	C(71)-C(72)-H(72B)	109.5
C(68)-C(69)-H(69B)	109.5	H(72A)-C(72)-H(72B)	109.5
H(69A)-C(69)-H(69B)	109.5	C(71)-C(72)-H(72C)	109.5
C(68)-C(69)-H(69C)	109.4	H(72A)-C(72)-H(72C)	109.5
H(69A)-C(69)-H(69C)	109.5	H(72B)-C(72)-H(72C)	109.5
H(69B)-C(69)-H(69C)	109.5	N(4)-C(73)-C(74)	109(3)
C(65')-N(3')-C(66')	115(2)	N(4)-C(73)-H(73A)	109.9
C(65')-N(3')-C(68')	116(2)	C(74)-C(73)-H(73A)	109.9
C(66')-N(3')-C(68')	128(3)	N(4)-C(73)-H(73B)	109.9
O(39)-C(65')-N(3')	122(3)	C(74)-C(73)-H(73B)	109.9
O(39)-C(65')-H(65')	119.2	H(73A)-C(73)-H(73B)	108.3

N(3')-C(65')-H(65')	119.2	C(73)-C(74)-H(74A)	109.5
N(3')-C(66')-C(67')	109(3)	C(73)-C(74)-H(74B)	109.5
N(3')-C(66')-H(66C)	110.0	H(74A)-C(74)-H(74B)	109.5
C(67')-C(66')-H(66C)	110.0	O(41)-C(75')-H(75')	118.6
N(3')-C(66')-H(66D)	110.0	N(5')-C(75')-H(75')	118.7
C(67')-C(66')-H(66D)	110.0	N(5')-C(76')-C(77')	128(5)
H(66C)-C(66')-H(66D)	108.4	N(5')-C(76')-H(76C)	105.3
C(66')-C(67')-H(67D)	109.5	C(77')-C(76')-H(76C)	105.3
C(66')-C(67')-H(67E)	109.5	N(5')-C(76')-H(76D)	105.3
H(67D)-C(67')-H(67E)	109.5	C(77')-C(76')-H(76D)	105.3
C(66')-C(67')-H(67F)	109.5	H(76C)-C(76')-H(76D)	106.0
H(67D)-C(67')-H(67F)	109.5	C(76')-C(77')-H(77D)	109.5
H(67E)-C(67')-H(67F)	109.5	C(76')-C(77')-H(77E)	109.5
N(3')-C(68')-C(69')	109(3)	H(77D)-C(77')-H(77E)	109.5
N(3')-C(68')-H(68C)	109.9	C(76')-C(77')-H(77F)	109.5
C(69')-C(68')-H(68C)	109.9	H(77D)-C(77')-H(77F)	109.5
C(73)-C(74)-H(74C)	109.5	H(77E)-C(77')-H(77F)	109.5
H(74A)-C(74)-H(74C)	109.5	N(5')-C(78')-C(79')	112(4)
H(74B)-C(74)-H(74C)	109.5	N(5')-C(78')-H(78C)	109.2
C(76)-N(5)-C(78)	110(4)	C(79')-C(78')-H(78C)	109.2
C(76)-N(5)-C(75)	124(3)	N(5')-C(78')-H(78D)	109.2
C(78)-N(5)-C(75)	121(3)	C(79')-C(78')-H(78D)	109.2
O(41)-C(75)-N(5)	113(4)	H(78C)-C(78')-H(78D)	107.9
O(41)-C(75)-H(75)	123.7	C(78')-C(79')-H(79D)	109.5
N(5)-C(75)-H(75)	123.7	C(78')-C(79')-H(79E)	109.5
N(5)-C(76)-C(77)	127(5)	H(79D)-C(79')-H(79E)	109.5
N(5)-C(76)-H(76A)	105.7	C(78')-C(79')-H(79F)	109.5
C(77)-C(76)-H(76A)	105.7	H(79D)-C(79')-H(79F)	109.5
N(5)-C(76)-H(76B)	105.6	H(79E)-C(79')-H(79F)	109.5
C(77)-C(76)-H(76B)	105.6	C(55)-O(37)-Ce(1)	124(2)
H(76A)-C(76)-H(76B)	106.1	C(55')-O(37)-Ce(1)	130(2)
C(76)-C(77)-H(77A)	109.5	C(65)-O(39)-Ce(4)	134(2)
C(76)-C(77)-H(77B)	109.4	C(65')-O(39)-Ce(4)	131.0(18)
H(77A)-C(77)-H(77B)	109.5	C(75')-O(41)-Ce(5)	134(2)
C(76)-C(77)-H(77C)	109.5	C(75)-O(41)-Ce(5)	142(4)
H(77A)-C(77)-H(77C)	109.5	H(79A)-C(79)-H(79B)	109.5

H(77B)-C(77)-H(77C)	109.5	C(78)-C(79)-H(79C)	109.5
N(5)-C(78)-C(79)	112(4)	H(79A)-C(79)-H(79C)	109.5
N(5)-C(78)-H(78A)	109.2	H(79B)-C(79)-H(79C)	109.5
C(79)-C(78)-H(78A)	109.2	C(75')-N(5')-C(76')	126(3)
N(5)-C(78)-H(78B)	109.2	C(75')-N(5')-C(78')	124(3)
C(79)-C(78)-H(78B)	109.2	C(76')-N(5')-C(78')	109(4)
H(78A)-C(78)-H(78B)	107.9	O(41)-C(75')-N(5')	123(3)
C(78)-C(79)-H(79A)	109.5	C(78)-C(79)-H(79B)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z-1 #2 x,y-1,z #3 x,y+1,z+1 #4 -x+1,-y+1,z+1/2 #5 -x+1,-y,z+1/2 #6 -x+1,-y,z-1/2 #7 x,y-1,z-1 #8 -x+1/2,y+1/2,z-1/2 #9 -x+1/2,y+1/2,z+1/2 #10 -x+1,-y+1,z-1/2 #11 x,y+1,z #12 -x+1/2,y-1/2,z+1/2 #13 -x+1/2,y-1/2,z-1/2 #14 x,y,z+1

2

C(1)-O(2)	1.241(11)	O(1)-Pr(2)	2.432(6)
C(1)-C(2)	1.474(12)	O(2)-Pr(1)	2.380(6)
C(2)-S(1)	1.711(9)	O(3)-Pr(1)#4	2.451(6)
C(3)-H(3)	0.9300	O(4)-Pr(2)#4	2.352(6)
C(4)-H(4)	0.9300	O(5)-Pr(1)	2.505(6)
C(5)-S(1)	1.701(9)	O(5)-Pr(2)	2.783(6)
C(6)-O(4)	1.258(11)	O(6)-Pr(2)	2.475(6)
C(7)-O(5)	1.254(11)	O(7)-Pr(1)#5	2.398(7)
C(7)-Pr(2)	2.987(10)	O(8)-Pr(5)#2	2.429(6)
C(8)-S(2)	1.711(9)	O(9)-Pr(1)	2.508(6)
C(9)-H(9)	0.9300	O(10)-Pr(2)	2.378(6)
C(10)-H(10)	0.9300	O(11)-Pr(1)#6	2.469(6)
C(11)-S(2)	1.709(10)	O(12)-Pr(5)#7	2.327(6)
C(12)-O(8)	1.248(12)	O(13)-Pr(2)	2.343(6)
C(13)-O(10)	1.261(12)	O(14)-Pr(3)	2.462(6)
C(1)-O(1)	1.258(12)	O(15)-Pr(5)	2.425(6)
C(2)-C(3)	1.339(13)	O(16)-Pr(6)	2.533(6)
C(3)-C(4)	1.413(13)	O(17)-Pr(2)	2.475(6)
C(4)-C(5)	1.340(13)	O(18)-Pr(3)	2.358(6)

C(5)-C(6)	1.461(12)	O(19)-Pr(3)	2.675(5)
C(6)-O(3)	1.240(12)	O(19)-Pr(2)	2.720(5)
C(7)-O(6)	1.253(12)	O(19)-H(19A)	0.85(3)
C(7)-C(8)	1.469(13)	O(19)-H(19B)	0.84(3)
C(8)-C(9)	1.356(14)	O(20)-Pr(6)#1	2.446(6)
C(9)-C(10)	1.429(13)	O(20)-Pr(5)#1	2.814(6)
C(10)-C(11)	1.333(14)	O(21)-Pr(3)	2.429(6)
C(11)-C(12)	1.477(12)	O(22)-Pr(4)	2.463(6)
C(12)-O(7)	1.231(12)	O(23)-Pr(5)#2	2.379(6)
C(13)-O(9)	1.245(12)	O(23)-Pr(6)#2	2.884(7)
C(13)-C(14)	1.477(13)	O(24)-Pr(6)#2	2.497(7)
C(14)-C(15)	1.336(13)	O(25)-Pr(3)	2.495(6)
C(14)-S(3)	1.695(10)	O(26)-Pr(4)	2.401(6)
C(15)-C(16)	1.411(13)	O(27)-Pr(6)#1	2.458(6)
C(15)-H(15)	0.9300	O(28)-Pr(4)#8	2.332(6)
C(16)-C(17)	1.336(14)	O(29)-Pr(3)	2.420(6)
C(16)-H(16)	0.9300	O(29)-Pr(4)	2.854(6)
C(17)-C(18)	1.482(13)	O(30)-Pr(4)	2.519(6)
C(17)-S(3)	1.698(10)	O(31)-Pr(4)#9	2.453(6)
C(18)-O(12)	1.251(12)	O(32)-Pr(6)	2.351(6)
C(18)-O(11)	1.257(13)	O(33)-Pr(5)	2.418(6)
C(19)-O(14)	1.231(13)	O(34)-Pr(6)	2.415(6)
C(19)-O(13)	1.261(12)	O(35)-Pr(3)#3	2.530(6)
C(19)-C(20)	1.496(14)	O(36)-Pr(4)#3	2.394(6)
C(20)-C(21)	1.347(13)	O(36)-Pr(3)#3	2.845(6)
C(20)-S(4)	1.698(10)	O(42)-Pr(6)	2.632(6)
C(21)-C(22)	1.409(12)	O(42)-H(42B)	0.86(3)
C(21)-H(21)	0.9300	O(42)-H(42A)	0.86(3)
C(22)-C(23)	1.365(13)	O(43)-Pr(5)#1	2.521(6)
C(22)-H(22)	0.9300	O(44)-Pr(1)	2.574(6)
C(23)-C(24)	1.497(13)	O(44)-H(44A)	0.86(3)
C(23)-S(4)	1.705(10)	O(44)-H(44B)	0.86(3)
C(24)-O(16)	1.224(11)	Pr(1)-O(7)#6	2.398(7)
C(24)-O(15)	1.272(12)	Pr(1)-O(3)#10	2.451(6)
C(25)-O(17)	1.233(12)	Pr(1)-O(37)	2.463(6)
C(25)-O(18)	1.249(12)	Pr(1)-O(11)#5	2.469(6)

C(25)-C(26)	1.487(14)	Pr(2)-O(4)#10	2.352(6)
C(26)-C(27)	1.357(13)	Pr(3)-O(38)	2.503(7)
C(26)-S(5)	1.706(10)	Pr(3)-O(35)#7	2.530(6)
C(27)-C(28)	1.400(12)	Pr(3)-O(36)#7	2.845(6)
C(27)-H(27)	0.9300	Pr(3)-C(54)#7	3.040(10)
C(28)-C(29)	1.346(13)	Pr(4)-O(28)#11	2.331(6)
C(28)-H(28)	0.9300	Pr(4)-O(36)#7	2.394(6)
C(29)-C(30)	1.460(12)	Pr(4)-O(31)#12	2.453(6)
C(29)-S(5)	1.706(9)	Pr(4)-O(39)	2.467(7)
C(30)-O(43)	1.249(12)	Pr(5)-O(12)#3	2.327(6)
C(30)-O(20)	1.270(11)	Pr(5)-O(23)#13	2.379(6)
C(30)-Pr(5)#1	3.037(9)	Pr(5)-O(8)#13	2.429(6)
C(31)-O(22)	1.226(11)	Pr(5)-O(41)	2.464(7)
C(31)-O(21)	1.273(11)	Pr(5)-O(43)#14	2.521(6)
C(31)-C(32)	1.502(12)	Pr(5)-O(20)#14	2.814(6)
C(32)-C(33)	1.347(13)	Pr(5)-C(30)#14	3.037(9)
C(32)-S(6)	1.705(9)	Pr(6)-O(20)#14	2.446(6)
C(33)-C(34)	1.434(13)	Pr(6)-O(27)#14	2.458(6)
C(33)-H(33)	0.9300	Pr(6)-O(40)	2.472(6)
C(34)-C(35)	1.349(13)	Pr(6)-O(24)#13	2.497(7)
C(34)-H(34)	0.9300	Pr(6)-O(23)#13	2.884(7)
C(35)-C(36)	1.485(13)	Pr(6)-C(36)#13	3.048(10)
C(35)-S(6)	1.705(9)	N(1)-C(55)	1.41(2)
C(36)-O(24)	1.242(12)	N(1)-C(56)	1.48(2)
C(36)-O(23)	1.263(11)	N(1)-C(58)	1.54(2)
C(36)-Pr(6)#2	3.048(10)	C(55)-O(37)	1.11(4)
C(37)-O(25)	1.255(12)	C(55)-H(55)	0.9300
C(37)-O(26)	1.259(12)	C(56)-C(57)	1.50(3)
C(37)-C(38)	1.487(12)	C(56)-H(56A)	0.9700
C(38)-C(39)	1.348(13)	C(56)-H(56B)	0.9700
C(38)-S(7)	1.701(9)	C(57)-H(57A)	0.9600
C(39)-C(40)	1.403(13)	C(57)-H(57B)	0.9600
C(39)-H(39)	0.9300	C(57)-H(57C)	0.9600
C(40)-C(41)	1.341(13)	C(58)-C(59)	1.62(3)
C(40)-H(40)	0.9300	C(58)-H(58A)	0.9700
C(41)-C(42)	1.491(13)	C(58)-H(58B)	0.9700

C(41)-S(7)	1.702(10)	C(59)-H(59A)	0.9600
C(42)-O(27)	1.238(12)	C(59)-H(59B)	0.9600
C(42)-O(28)	1.244(11)	C(59)-H(59C)	0.9600
C(43)-O(30)	1.249(12)	N(1')-C(55')	1.40(2)
C(43)-O(29)	1.252(11)	N(1')-C(56')	1.44(2)
C(43)-C(44)	1.477(12)	N(1')-C(58')	1.49(2)
C(43)-Pr(4)	3.043(9)	C(55')-O(37)	1.24(4)
C(44)-C(45)	1.346(13)	C(55')-H(55')	0.9300
C(44)-S(8)	1.712(8)	C(56')-C(57')	1.47(3)
C(45)-C(46)	1.413(12)	C(56')-H(56C)	0.9700
C(45)-H(45)	0.9300	C(56')-H(56D)	0.9700
C(46)-C(47)	1.366(13)	C(57')-H(57D)	0.9600
C(46)-H(46)	0.9300	C(57')-H(57E)	0.9600
C(47)-C(48)	1.484(13)	C(57')-H(57F)	0.9600
C(47)-S(8)	1.703(9)	C(58')-C(59')	1.57(3)
C(48)-O(31)	1.222(12)	C(58')-H(58C)	0.9700
C(48)-O(32)	1.261(11)	C(58')-H(58D)	0.9700
C(49)-O(34)	1.253(11)	C(59')-H(59D)	0.9600
C(49)-O(33)	1.262(12)	C(59')-H(59E)	0.9600
C(49)-C(50)	1.494(13)	C(59')-H(59F)	0.9600
C(50)-C(51)	1.342(13)	O(38)-C(60)	1.219(13)
C(50)-S(9)	1.701(9)	N(2)-C(60)	1.349(13)
C(51)-C(52)	1.413(12)	N(2)-C(63)	1.478(18)
C(51)-H(51)	0.9300	N(2)-C(61)	1.526(17)
C(52)-C(53)	1.351(13)	C(60)-H(60)	0.9300
C(52)-H(52)	0.9300	C(61)-C(62)	1.45(2)
C(53)-C(54)	1.479(12)	C(61)-H(61A)	0.9700
C(53)-S(9)	1.705(9)	C(61)-H(61B)	0.9700
C(54)-O(35)	1.226(11)	C(62)-H(62A)	0.9600
C(54)-O(36)	1.264(11)	C(62)-H(62B)	0.9600
C(54)-Pr(3)#3	3.040(10)	C(62)-H(62C)	0.9600
C(75)-H(75)	0.9300	C(63)-C(64)	1.49(2)
C(76)-C(77)	1.51(3)	C(63)-H(63A)	0.9700
C(76)-H(76A)	0.9700	C(63)-H(63B)	0.9700
C(76)-H(76B)	0.9700	C(64)-H(64A)	0.9600
C(77)-H(77A)	0.9600	C(64)-H(64B)	0.9600

C(77)-H(77B)	0.9600	C(64)-H(64C)	0.9600
C(77)-H(77C)	0.9600	N(3)-C(65)	1.37(2)
C(78)-C(79)	1.56(3)	N(3)-C(68)	1.47(2)
C(78)-H(78A)	0.9700	N(3)-C(66)	1.47(2)
C(78)-H(78B)	0.9700	C(65)-O(39)	1.23(2)
C(79)-H(79A)	0.9600	C(65)-H(65)	0.9300
C(79)-H(79B)	0.9600	C(66)-C(67)	1.53(3)
C(79)-H(79C)	0.9600	C(66)-H(66A)	0.9700
N(5')-C(75')	1.43(2)	C(66)-H(66B)	0.9700
N(5')-C(76')	1.46(2)	C(67)-H(67A)	0.9600
N(5')-C(78')	1.51(2)	C(67)-H(67B)	0.9600
C(75')-O(41)	1.13(2)	C(67)-H(67C)	0.9600
C(75')-H(75')	0.9300	C(68)-C(69)	1.50(3)
C(76')-C(77')	1.51(3)	C(68)-H(68A)	0.9700
C(76')-H(76C)	0.9700	C(68)-H(68B)	0.9700
C(76')-H(76D)	0.9700	C(69)-H(69A)	0.9600
C(77')-H(77D)	0.9600	C(69)-H(69B)	0.9600
C(77')-H(77E)	0.9600	C(69)-H(69C)	0.9600
C(77')-H(77F)	0.9600	N(3')-C(65')	1.353(19)
C(78')-C(79')	1.52(3)	N(3')-C(68')	1.471(19)
C(78')-H(78C)	0.9700	N(3')-C(66')	1.48(2)
C(78')-H(78D)	0.9700	C(65')-O(39)	1.210(17)
C(79')-H(79D)	0.9600	C(65')-H(65')	0.9300
C(79')-H(79E)	0.9600	C(66')-C(67')	1.54(2)
C(79')-H(79F)	0.9600	C(66')-H(66C)	0.9700
N(4)-C(70)	1.333(12)	C(66')-H(66D)	0.9700
N(4)-C(71)	1.455(15)	C(67')-H(67D)	0.9600
N(4)-C(73)	1.487(17)	C(67')-H(67E)	0.9600
C(70)-H(70)	0.9300	C(67')-H(67F)	0.9600
C(71)-C(72)	1.491(19)	C(68')-C(69')	1.54(2)
C(71)-H(71A)	0.9700	C(68')-H(68C)	0.9700
C(71)-H(71B)	0.9700	C(68')-H(68D)	0.9700
C(72)-H(72A)	0.9600	C(69')-H(69D)	0.9600
C(72)-H(72B)	0.9600	C(69')-H(69E)	0.9600
C(72)-H(72C)	0.9600	C(69')-H(69F)	0.9600
C(73)-C(74)	1.491(19)	O(40)-C(70)	1.220(11)

C(73)-H(73A)	0.9700	N(5)-C(76)	1.45(2)
C(73)-H(73B)	0.9700	N(5)-C(75)	1.49(2)
C(74)-H(74A)	0.9600	N(5)-C(78)	1.50(2)
C(74)-H(74B)	0.9600	C(75)-O(41)	1.20(2)
C(74)-H(74C)	0.9600	O(2)-C(1)-O(1)	125.9(8)
O(12)-C(18)-C(17)	116.3(10)	O(2)-C(1)-C(2)	115.6(9)
O(11)-C(18)-C(17)	118.2(9)	O(1)-C(1)-C(2)	118.5(8)
O(14)-C(19)-O(13)	125.6(9)	C(3)-C(2)-C(1)	127.2(9)
O(14)-C(19)-C(20)	118.6(9)	C(3)-C(2)-S(1)	110.9(7)
O(13)-C(19)-C(20)	115.8(10)	C(1)-C(2)-S(1)	121.9(7)
C(21)-C(20)-C(19)	127.2(9)	C(2)-C(3)-C(4)	113.2(9)
C(21)-C(20)-S(4)	111.9(7)	C(2)-C(3)-H(3)	123.4
C(19)-C(20)-S(4)	120.7(8)	C(4)-C(3)-H(3)	123.4
C(20)-C(21)-C(22)	113.4(9)	C(5)-C(4)-C(3)	112.4(9)
C(20)-C(21)-H(21)	123.3	C(5)-C(4)-H(4)	123.8
C(22)-C(21)-H(21)	123.3	C(3)-C(4)-H(4)	123.8
C(23)-C(22)-C(21)	111.0(9)	C(4)-C(5)-C(6)	127.9(9)
C(23)-C(22)-H(22)	124.5	C(4)-C(5)-S(1)	111.7(7)
C(21)-C(22)-H(22)	124.5	C(6)-C(5)-S(1)	120.4(7)
C(22)-C(23)-C(24)	128.1(9)	O(3)-C(6)-O(4)	124.0(9)
C(22)-C(23)-S(4)	112.3(7)	O(3)-C(6)-C(5)	118.0(8)
C(24)-C(23)-S(4)	119.3(7)	O(4)-C(6)-C(5)	117.9(9)
O(16)-C(24)-O(15)	126.7(9)	O(6)-C(7)-O(5)	122.6(9)
O(16)-C(24)-C(23)	118.4(9)	O(6)-C(7)-C(8)	117.8(9)
O(15)-C(24)-C(23)	114.9(9)	O(5)-C(7)-C(8)	119.6(10)
O(17)-C(25)-O(18)	124.9(10)	O(6)-C(7)-Pr(2)	54.3(5)
O(17)-C(25)-C(26)	120.3(9)	O(5)-C(7)-Pr(2)	68.4(5)
O(18)-C(25)-C(26)	114.8(9)	C(8)-C(7)-Pr(2)	171.0(7)
C(27)-C(26)-C(25)	125.0(9)	C(9)-C(8)-C(7)	128.6(9)
C(27)-C(26)-S(5)	110.5(7)	C(9)-C(8)-S(2)	111.3(7)
C(25)-C(26)-S(5)	124.5(8)	C(7)-C(8)-S(2)	120.0(8)
C(26)-C(27)-C(28)	113.3(9)	C(8)-C(9)-C(10)	112.3(9)
C(26)-C(27)-H(27)	123.4	C(8)-C(9)-H(9)	123.8
C(28)-C(27)-H(27)	123.4	C(10)-C(9)-H(9)	123.8
C(29)-C(28)-C(27)	112.8(9)	C(11)-C(10)-C(9)	112.4(10)
C(29)-C(28)-H(28)	123.6	C(11)-C(10)-H(10)	123.8

C(27)-C(28)-H(28)	123.6	C(9)-C(10)-H(10)	123.8
C(28)-C(29)-C(30)	127.4(9)	C(10)-C(11)-C(12)	126.8(10)
C(28)-C(29)-S(5)	111.2(7)	C(10)-C(11)-S(2)	112.2(7)
C(30)-C(29)-S(5)	121.4(7)	C(12)-C(11)-S(2)	120.9(8)
O(43)-C(30)-O(20)	121.3(8)	O(7)-C(12)-O(8)	124.5(9)
O(43)-C(30)-C(29)	119.1(8)	O(7)-C(12)-C(11)	116.8(10)
O(20)-C(30)-C(29)	119.5(9)	O(8)-C(12)-C(11)	118.7(9)
O(43)-C(30)-Pr(5)#1	54.3(5)	O(9)-C(13)-O(10)	126.2(9)
O(20)-C(30)-Pr(5)#1	67.8(5)	O(9)-C(13)-C(14)	118.1(9)
C(29)-C(30)-Pr(5)#1	167.0(7)	O(10)-C(13)-C(14)	115.7(9)
O(22)-C(31)-O(21)	127.5(8)	C(15)-C(14)-C(13)	127.5(9)
O(22)-C(31)-C(32)	118.2(8)	C(15)-C(14)-S(3)	111.3(7)
O(21)-C(31)-C(32)	114.3(9)	C(13)-C(14)-S(3)	121.0(8)
C(33)-C(32)-C(31)	127.3(9)	C(14)-C(15)-C(16)	112.5(10)
C(33)-C(32)-S(6)	112.8(7)	C(14)-C(15)-H(15)	123.8
C(31)-C(32)-S(6)	119.8(7)	C(16)-C(15)-H(15)	123.8
C(32)-C(33)-C(34)	111.6(9)	C(17)-C(16)-C(15)	113.1(10)
C(32)-C(33)-H(33)	124.2	C(17)-C(16)-H(16)	123.5
C(34)-C(33)-H(33)	124.2	C(15)-C(16)-H(16)	123.5
C(35)-C(34)-C(33)	111.9(8)	C(16)-C(17)-C(18)	127.3(10)
C(35)-C(34)-H(34)	124.1	C(16)-C(17)-S(3)	110.9(8)
C(33)-C(34)-H(34)	124.1	C(18)-C(17)-S(3)	121.5(8)
C(34)-C(35)-C(36)	127.9(9)	O(12)-C(18)-O(11)	125.4(9)
C(34)-C(35)-S(6)	112.6(7)	(2)-Pr(1)-O(7)#6	137.7(3)
C(36)-C(35)-S(6)	119.4(8)	O(2)-Pr(1)-O(3)#10	82.2(2)
O(24)-C(36)-O(23)	122.3(9)	O(7)#6-Pr(1)-O(3)#10	73.9(2)
O(24)-C(36)-C(35)	118.9(9)	O(2)-Pr(1)-O(37)	139.0(3)
O(23)-C(36)-C(35)	118.7(10)	O(7)#6-Pr(1)-O(37)	78.0(3)
O(24)-C(36)-Pr(6)#2	52.6(5)	O(3)#10-Pr(1)-O(37)	136.1(3)
O(23)-C(36)-Pr(6)#2	70.5(5)	O(2)-Pr(1)-O(11)#5	81.6(2)
C(35)-C(36)-Pr(6)#2	166.9(7)	O(7)#6-Pr(1)-O(11)#5	99.1(3)
O(25)-C(37)-O(26)	126.7(9)	O(3)#10-Pr(1)-O(11)#5	145.9(2)
O(25)-C(37)-C(38)	116.9(9)	O(37)-Pr(1)-O(11)#5	71.1(3)
O(26)-C(37)-C(38)	116.3(9)	O(2)-Pr(1)-O(5)	68.7(2)
C(39)-C(38)-C(37)	128.0(9)	O(7)#6-Pr(1)-O(5)	153.5(2)
C(39)-C(38)-S(7)	112.0(7)	O(3)#10-Pr(1)-O(5)	115.1(2)

C(37)-C(38)-S(7)	120.0(7)	O(37)-Pr(1)-O(5)	79.4(2)
C(38)-C(39)-C(40)	112.3(9)	O(11)#5-Pr(1)-O(5)	86.4(2)
C(38)-C(39)-H(39)	123.8	O(2)-Pr(1)-O(9)	119.6(2)
C(40)-C(39)-H(39)	123.8	O(7)#6-Pr(1)-O(9)	86.9(2)
C(41)-C(40)-C(39)	112.5(9)	O(3)#10-Pr(1)-O(9)	74.1(2)
C(41)-C(40)-H(40)	123.7	O(37)-Pr(1)-O(9)	71.4(3)
C(39)-C(40)-H(40)	123.7	O(11)#5-Pr(1)-O(9)	139.8(2)
C(40)-C(41)-C(42)	127.1(9)	O(5)-Pr(1)-O(9)	72.89(19)
C(40)-C(41)-S(7)	112.1(7)	O(2)-Pr(1)-O(44)	68.2(2)
C(42)-C(41)-S(7)	120.6(7)	O(7)#6-Pr(1)-O(44)	71.1(3)
O(27)-C(42)-O(28)	125.9(9)	O(3)#10-Pr(1)-O(44)	70.9(2)
O(27)-C(42)-C(41)	118.4(9)	O(37)-Pr(1)-O(44)	129.2(2)
O(28)-C(42)-C(41)	115.6(9)	O(11)#5-Pr(1)-O(44)	75.2(3)
O(30)-C(43)-O(29)	122.9(8)	O(5)-Pr(1)-O(44)	135.0(2)
O(30)-C(43)-C(44)	118.5(8)	O(9)-Pr(1)-O(44)	142.6(3)
O(29)-C(43)-C(44)	118.6(9)	O(13)-Pr(2)-O(4)#10	140.6(2)
O(30)-C(43)-Pr(4)	53.9(4)	O(13)-Pr(2)-O(10)	136.9(2)
O(29)-C(43)-Pr(4)	69.4(5)	O(4)#10-Pr(2)-O(10)	77.1(2)
C(44)-C(43)-Pr(4)	169.8(7)	O(13)-Pr(2)-O(1)	80.0(2)
C(45)-C(44)-C(43)	127.6(8)	O(4)#10-Pr(2)-O(1)	80.3(2)
C(45)-C(44)-S(8)	111.8(7)	O(10)-Pr(2)-O(1)	138.2(2)
C(43)-C(44)-S(8)	120.6(7)	O(13)-Pr(2)-O(17)	82.9(2)
C(44)-C(45)-C(46)	112.9(8)	O(4)#10-Pr(2)-O(17)	79.2(2)
C(44)-C(45)-H(45)	123.5	O(10)-Pr(2)-O(17)	87.6(2)
C(46)-C(45)-H(45)	123.5	O(1)-Pr(2)-O(17)	122.0(2)
C(47)-C(46)-C(45)	111.9(9)	O(13)-Pr(2)-O(6)	78.5(2)
C(47)-C(46)-H(46)	124.1	O(4)#10-Pr(2)-O(6)	131.8(2)
C(45)-C(46)-H(46)	124.1	O(10)-Pr(2)-O(6)	86.8(3)
C(46)-C(47)-C(48)	125.4(9)	O(1)-Pr(2)-O(6)	82.6(2)
C(46)-C(47)-S(8)	111.8(7)	O(17)-Pr(2)-O(6)	145.9(2)
C(48)-C(47)-S(8)	122.7(7)	O(13)-Pr(2)-O(19)	72.5(2)
O(31)-C(48)-O(32)	125.6(9)	O(4)#10-Pr(2)-O(19)	138.5(2)
O(31)-C(48)-C(47)	120.4(9)	O(10)-Pr(2)-O(19)	64.7(2)
O(32)-C(48)-C(47)	113.9(9)	O(1)-Pr(2)-O(19)	139.8(2)
O(34)-C(49)-O(33)	126.3(9)	O(17)-Pr(2)-O(19)	83.4(2)
O(34)-C(49)-C(50)	116.5(9)	O(6)-Pr(2)-O(19)	63.9(2)

O(33)-C(49)-C(50)	117.1(9)	O(13)-Pr(2)-O(5)	121.8(2)
C(51)-C(50)-C(49)	126.7(9)	O(4)#10-Pr(2)-O(5)	82.8(2)
C(51)-C(50)-S(9)	112.4(7)	O(10)-Pr(2)-O(5)	71.3(2)
C(49)-C(50)-S(9)	120.9(7)	O(1)-Pr(2)-O(5)	71.3(2)
C(50)-C(51)-C(52)	112.5(9)	O(17)-Pr(2)-O(5)	154.9(2)
C(50)-C(51)-H(51)	123.7	O(6)-Pr(2)-O(5)	49.01(19)
C(52)-C(51)-H(51)	123.7	O(19)-Pr(2)-O(5)	99.03(18)
C(53)-C(52)-C(51)	111.7(9)	O(13)-Pr(2)-C(7)	99.7(3)
C(53)-C(52)-H(52)	124.1	O(4)#10-Pr(2)-C(7)	107.5(3)
C(51)-C(52)-H(52)	124.1	O(10)-Pr(2)-C(7)	79.1(3)
C(52)-C(53)-C(54)	128.8(8)	O(1)-Pr(2)-C(7)	74.7(3)
C(52)-C(53)-S(9)	112.4(7)	O(17)-Pr(2)-C(7)	163.1(3)
C(54)-C(53)-S(9)	118.8(7)	O(6)-Pr(2)-C(7)	24.3(2)
O(35)-C(54)-O(36)	122.7(9)	O(19)-Pr(2)-C(7)	81.5(3)
O(35)-C(54)-C(53)	119.1(8)	O(5)-Pr(2)-C(7)	24.8(2)
O(36)-C(54)-C(53)	118.1(8)	O(18)-Pr(3)-O(29)	152.6(2)
O(35)-C(54)-Pr(3)#3	54.4(5)	O(18)-Pr(3)-O(21)	134.2(2)
O(36)-C(54)-Pr(3)#3	69.1(5)	O(29)-Pr(3)-O(21)	72.9(2)
C(53)-C(54)-Pr(3)#3	167.9(7)	O(18)-Pr(3)-O(14)	92.8(2)
C(1)-O(1)-Pr(2)	128.3(6)	O(29)-Pr(3)-O(14)	90.0(2)
C(1)-O(2)-Pr(1)	146.2(7)	O(21)-Pr(3)-O(14)	76.7(2)
C(6)-O(3)-Pr(1)#4	114.7(6)	O(18)-Pr(3)-O(25)	85.0(2)
C(6)-O(4)-Pr(2)#4	169.5(7)	O(29)-Pr(3)-O(25)	76.30(19)
C(7)-O(5)-Pr(1)	165.6(6)	O(21)-Pr(3)-O(25)	129.6(2)
C(7)-O(5)-Pr(2)	86.8(6)	O(14)-Pr(3)-O(25)	142.1(2)
Pr(1)-O(5)-Pr(2)	107.0(2)	O(18)-Pr(3)-O(38)	73.7(3)
C(7)-O(6)-Pr(2)	101.4(6)	O(29)-Pr(3)-O(38)	81.8(2)
C(12)-O(7)-Pr(1)#5	169.6(8)	O(21)-Pr(3)-O(38)	137.8(2)
C(12)-O(8)-Pr(5)#2	132.4(6)	O(14)-Pr(3)-O(38)	70.0(2)
C(13)-O(9)-Pr(1)	144.0(6)	O(25)-Pr(3)-O(38)	73.1(2)
C(13)-O(10)-Pr(2)	133.5(6)	O(18)-Pr(3)-O(35)#7	72.2(2)
C(18)-O(11)-Pr(1)#6	122.9(6)	O(29)-Pr(3)-O(35)#7	122.7(2)
C(18)-O(12)-Pr(5)#7	143.7(7)	O(21)-Pr(3)-O(35)#7	84.3(2)
C(19)-O(13)-Pr(2)	142.7(7)	O(14)-Pr(3)-O(35)#7	135.1(2)
C(19)-O(14)-Pr(3)	131.3(6)	O(25)-Pr(3)-O(35)#7	80.0(2)
C(24)-O(15)-Pr(5)	132.0(6)	O(38)-Pr(3)-O(35)#7	137.9(2)

C(24)-O(16)-Pr(6)	139.5(6)	O(18)-Pr(3)-O(19)	67.5(2)
C(25)-O(17)-Pr(2)	127.8(7)	O(29)-Pr(3)-O(19)	138.4(2)
C(25)-O(18)-Pr(3)	170.7(8)	O(21)-Pr(3)-O(19)	67.0(2)
Pr(3)-O(19)-Pr(2)	122.69(18)	O(14)-Pr(3)-O(19)	70.8(2)
Pr(3)-O(19)-H(19A)	95(6)	O(25)-Pr(3)-O(19)	139.8(2)
Pr(2)-O(19)-H(19A)	106(7)	O(38)-Pr(3)-O(19)	122.1(2)
Pr(3)-O(19)-H(19B)	119(7)	O(35)#7-Pr(3)-O(19)	64.3(2)
Pr(2)-O(19)-H(19B)	103(7)	O(18)-Pr(3)-O(36)#7	114.6(2)
H(19A)-O(19)-H(19B)	110(4)	O(29)-Pr(3)-O(36)#7	75.20(18)
C(30)-O(20)-Pr(6)#1	168.7(6)	O(21)-Pr(3)-O(36)#7	69.44(19)
C(30)-O(20)-Pr(5)#1	87.6(5)	O(14)-Pr(3)-O(36)#7	145.7(2)
Pr(6)#1-O(20)-Pr(5)#1	103.75(19)	O(25)-Pr(3)-O(36)#7	64.7(2)
C(31)-O(21)-Pr(3)	136.2(6)	O(38)-Pr(3)-O(36)#7	135.4(2)
C(31)-O(22)-Pr(4)	135.5(6)	O(35)#7-Pr(3)-O(36)#7	47.53(18)
C(36)-O(23)-Pr(5)#2	167.4(6)	O(19)-Pr(3)-O(36)#7	99.91(17)
C(36)-O(23)-Pr(6)#2	85.1(6)	O(18)-Pr(3)-C(54)#7	91.9(3)
Pr(5)#2-O(23)-Pr(6)#2	103.5(2)	O(29)-Pr(3)-C(54)#7	99.7(2)
C(36)-O(24)-Pr(6)#2	104.1(6)	O(21)-Pr(3)-C(54)#7	78.0(2)
C(37)-O(25)-Pr(3)	137.1(6)	O(14)-Pr(3)-C(54)#7	148.8(2)
C(37)-O(26)-Pr(4)	134.1(6)	O(25)-Pr(3)-C(54)#7	69.0(2)
C(42)-O(27)-Pr(6)#1	133.5(6)	O(38)-Pr(3)-C(54)#7	140.5(2)
C(42)-O(28)-Pr(4)#8	146.4(7)	O(35)#7-Pr(3)-C(54)#7	23.2(2)
C(43)-O(29)-Pr(3)	169.2(6)	O(19)-Pr(3)-C(54)#7	82.7(2)
C(43)-O(29)-Pr(4)	86.4(5)	O(36)#7-Pr(3)-C(54)#7	24.5(2)
Pr(3)-O(29)-Pr(4)	104.19(19)	O(28)#11-Pr(4)-O(36)#7	156.3(2)
C(43)-O(30)-Pr(4)	102.4(5)	O(28)#11-Pr(4)-O(26)	126.7(2)
C(48)-O(31)-Pr(4)#9	134.0(6)	O(36)#7-Pr(4)-O(26)	75.0(2)
C(48)-O(32)-Pr(6)	163.1(7)	O(28)#11-Pr(4)-O(31)#12	85.7(2)
C(49)-O(33)-Pr(5)	134.9(6)	O(36)#7-Pr(4)-O(31)#12	90.1(2)
C(49)-O(34)-Pr(6)	138.3(6)	O(26)-Pr(4)-O(31)#12	79.3(2)
C(54)-O(35)-Pr(3)#3	102.4(6)	O(28)#11-Pr(4)-O(22)	88.4(2)
C(54)-O(36)-Pr(4)#3	168.3(6)	O(36)#7-Pr(4)-O(22)	80.80(19)
C(54)-O(36)-Pr(3)#3	86.4(5)	O(26)-Pr(4)-O(22)	131.6(2)
Pr(4)#3-O(36)-Pr(3)#3	105.2(2)	O(31)#12-Pr(4)-O(22)	142.5(2)
Pr(6)-O(42)-H(42B)	107(8)	O(28)#11-Pr(4)-O(39)	79.0(2)
Pr(6)-O(42)-H(42A)	113(8)	O(36)#7-Pr(4)-O(39)	77.6(2)

H(42B)-O(42)-H(42A)	108(5)	O(26)-Pr(4)-O(39)	138.9(2)
C(30)-O(43)-Pr(5)#1	102.0(5)	O(31)#12-Pr(4)-O(39)	70.6(2)
Pr(1)-O(44)-H(44A)	128(7)	O(22)-Pr(4)-O(39)	71.9(2)
Pr(1)-O(44)-H(44B)	112(6)	O(28)#11-Pr(4)-O(30)	74.6(2)
H(44A)-O(44)-H(44B)	106(4)	O(36)#7-Pr(4)-O(30)	123.1(2)
C(5)-S(1)-C(2)	91.8(4)	O(26)-Pr(4)-O(30)	80.2(2)
C(11)-S(2)-C(8)	91.6(5)	O(31)#12-Pr(4)-O(30)	134.1(2)
C(14)-S(3)-C(17)	92.2(5)	O(22)-Pr(4)-O(30)	79.0(2)
C(20)-S(4)-C(23)	91.3(5)	O(39)-Pr(4)-O(30)	141.0(2)
C(29)-S(5)-C(26)	92.2(5)	O(28)#11-Pr(4)-O(29)	119.17(19)
C(35)-S(6)-C(32)	91.0(5)	O(36)#7-Pr(4)-O(29)	75.41(18)
C(38)-S(7)-C(41)	91.1(4)	O(26)-Pr(4)-O(29)	67.63(19)
C(47)-S(8)-C(44)	91.5(5)	O(31)#12-Pr(4)-O(29)	146.2(2)
C(50)-S(9)-C(53)	90.9(5)	O(22)-Pr(4)-O(29)	65.95(19)
O(12)#3-Pr(5)-O(8)#13	81.7(2)	O(39)-Pr(4)-O(29)	132.7(2)
O(23)#13-Pr(5)-O(8)#13	89.1(2)	O(30)-Pr(4)-O(29)	47.78(18)
O(33)-Pr(5)-O(8)#13	144.1(2)	O(28)#11-Pr(4)-C(43)	96.1(2)
O(15)-Pr(5)-O(8)#13	75.2(2)	O(36)#7-Pr(4)-C(43)	99.7(2)
O(12)#3-Pr(5)-O(41)	79.0(3)	O(26)-Pr(4)-C(43)	74.1(2)
O(23)#13-Pr(5)-O(41)	87.1(3)	O(31)#12-Pr(4)-C(43)	148.1(2)
O(33)-Pr(5)-O(41)	72.6(3)	O(22)-Pr(4)-C(43)	69.4(2)
O(15)-Pr(5)-O(41)	143.9(4)	O(39)-Pr(4)-C(43)	141.2(2)
O(8)#13-Pr(5)-O(41)	72.4(3)	O(30)-Pr(4)-C(43)	23.6(2)
O(12)#3-Pr(5)-O(43)#14	69.2(2)	O(29)-Pr(4)-C(43)	24.2(2)
O(23)#13-Pr(5)-O(43)#14	125.5(2)	O(12)#3-Pr(5)-O(23)#13	165.1(2)
O(33)-Pr(5)-O(43)#14	82.4(2)	O(12)#3-Pr(5)-O(33)	99.3(2)
O(15)-Pr(5)-O(43)#14	78.7(2)	O(23)#13-Pr(5)-O(33)	81.3(2)
O(8)#13-Pr(5)-O(43)#14	129.7(2)	O(12)#3-Pr(5)-O(15)	111.7(2)
O(41)-Pr(5)-O(43)#14	135.4(4)	O(23)#13-Pr(5)-O(15)	76.8(2)
O(12)#3-Pr(5)-O(20)#14	116.56(19)	O(33)-Pr(5)-O(15)	134.5(2)
O(23)#13-Pr(5)-O(20)#14	77.57(19)	H(56A)-C(56)-H(56B)	107.9
O(33)-Pr(5)-O(20)#14	66.9(2)	C(56)-C(57)-H(57A)	109.5
O(15)-Pr(5)-O(20)#14	69.56(19)	C(56)-C(57)-H(57B)	109.5
O(8)#13-Pr(5)-O(20)#14	144.3(2)	H(57A)-C(57)-H(57B)	109.5
O(41)-Pr(5)-O(20)#14	138.3(2)	C(56)-C(57)-H(57C)	109.5
O(43)#14-Pr(5)-O(20)#14	48.23(18)	H(57A)-C(57)-H(57C)	109.5

O(12)#3-Pr(5)-C(30)#14	92.0(2)	H(57B)-C(57)-H(57C)	109.5
O(23)#13-Pr(5)-C(30)#14	102.3(2)	N(1)-C(58)-C(59)	102(2)
O(33)-Pr(5)-C(30)#14	71.4(2)	N(1)-C(58)-H(58A)	111.4
O(15)-Pr(5)-C(30)#14	74.8(2)	C(59)-C(58)-H(58A)	111.4
O(8)#13-Pr(5)-C(30)#14	144.5(2)	N(1)-C(58)-H(58B)	111.4
O(41)-Pr(5)-C(30)#14	140.8(4)	C(59)-C(58)-H(58B)	111.4
O(43)#14-Pr(5)-C(30)#14	23.7(2)	H(58A)-C(58)-H(58B)	109.2
O(20)#14-Pr(5)-C(30)#14	24.7(2)	C(58)-C(59)-H(59A)	109.5
O(32)-Pr(6)-O(34)	138.3(2)	C(58)-C(59)-H(59B)	109.5
O(32)-Pr(6)-O(20)#14	149.4(2)	H(59A)-C(59)-H(59B)	109.5
O(34)-Pr(6)-O(20)#14	71.4(2)	C(58)-C(59)-H(59C)	109.5
O(32)-Pr(6)-O(27)#14	90.5(2)	H(59A)-C(59)-H(59C)	109.5
O(34)-Pr(6)-O(27)#14	77.6(2)	H(59B)-C(59)-H(59C)	109.5
O(20)#14-Pr(6)-O(27)#14	90.5(2)	C(55')-N(1')-C(56')	122(2)
O(32)-Pr(6)-O(40)	75.4(2)	C(55')-N(1')-C(58')	117(2)
O(34)-Pr(6)-O(40)	133.9(2)	C(56')-N(1')-C(58')	117(3)
O(20)#14-Pr(6)-O(40)	76.1(2)	O(37)-C(55')-N(1')	115(3)
O(27)#14-Pr(6)-O(40)	70.9(2)	O(37)-C(55')-H(55')	122.5
O(32)-Pr(6)-O(24)#13	73.3(2)	N(1')-C(55')-H(55')	122.5
O(34)-Pr(6)-O(24)#13	89.7(2)	N(1')-C(56')-C(57')	116(3)
O(20)#14-Pr(6)-O(24)#13	122.5(2)	N(1')-C(56')-H(56C)	108.3
O(27)#14-Pr(6)-O(24)#13	138.9(2)	C(57')-C(56')-H(56C)	108.3
O(40)-Pr(6)-O(24)#13	135.8(2)	N(1')-C(56')-H(56D)	108.3
O(32)-Pr(6)-O(16)	84.5(2)	C(57')-C(56')-H(56D)	108.3
O(34)-Pr(6)-O(16)	128.2(2)	H(56C)-C(56')-H(56D)	107.4
O(20)#14-Pr(6)-O(16)	76.20(19)	C(56')-C(57')-H(57D)	109.5
O(27)#14-Pr(6)-O(16)	142.2(2)	C(56')-C(57')-H(57E)	109.5
O(40)-Pr(6)-O(16)	71.6(2)	H(57D)-C(57')-H(57E)	109.5
O(24)#13-Pr(6)-O(16)	74.9(2)	C(56')-C(57')-H(57F)	109.5
O(32)-Pr(6)-O(42)	69.1(3)	H(57D)-C(57')-H(57F)	109.5
O(34)-Pr(6)-O(42)	69.3(2)	H(57E)-C(57')-H(57F)	109.5
O(20)#14-Pr(6)-O(42)	139.1(2)	N(1')-C(58')-C(59')	107(2)
O(27)#14-Pr(6)-O(42)	70.6(2)	N(1')-C(58')-H(58C)	110.3
O(40)-Pr(6)-O(42)	126.4(2)	C(59')-C(58')-H(58C)	110.3
O(24)#13-Pr(6)-O(42)	68.3(3)	N(1')-C(58')-H(58D)	110.3
O(16)-Pr(6)-O(42)	139.4(2)	C(59')-C(58')-H(58D)	110.3

O(32)-Pr(6)-O(23)#13	117.0(2)	H(58C)-C(58')-H(58D)	108.6
O(34)-Pr(6)-O(23)#13	69.5(2)	C(58')-C(59')-H(59D)	109.5
O(20)#14-Pr(6)-O(23)#13	75.19(18)	C(58')-C(59')-H(59E)	109.5
O(27)#14-Pr(6)-O(23)#13	146.8(2)	H(59D)-C(59')-H(59E)	109.5
O(40)-Pr(6)-O(23)#13	131.2(2)	C(58')-C(59')-H(59F)	109.5
O(24)#13-Pr(6)-O(23)#13	47.5(2)	H(59D)-C(59')-H(59F)	109.5
O(16)-Pr(6)-O(23)#13	63.78(19)	H(59E)-C(59')-H(59F)	109.5
O(42)-Pr(6)-O(23)#13	100.8(2)	C(60)-O(38)-Pr(3)	128.3(7)
O(32)-Pr(6)-C(36)#13	93.9(3)	C(60)-N(2)-C(63)	120.4(13)
O(34)-Pr(6)-C(36)#13	81.1(2)	C(60)-N(2)-C(61)	116.5(15)
O(20)#14-Pr(6)-C(36)#13	99.2(2)	C(63)-N(2)-C(61)	121.3(13)
O(27)#14-Pr(6)-C(36)#13	152.3(3)	O(38)-C(60)-N(2)	123.3(12)
O(40)-Pr(6)-C(36)#13	136.5(2)	O(38)-C(60)-H(60)	118.3
O(24)#13-Pr(6)-C(36)#13	23.3(2)	N(2)-C(60)-H(60)	118.3
O(16)-Pr(6)-C(36)#13	65.4(2)	C(62)-C(61)-N(2)	111.9(18)
O(42)-Pr(6)-C(36)#13	85.5(3)	C(62)-C(61)-H(61A)	109.2
O(23)#13-Pr(6)-C(36)#13	24.4(2)	N(2)-C(61)-H(61A)	109.2
C(55)-N(1)-C(56)	118(2)	C(62)-C(61)-H(61B)	109.2
C(55)-N(1)-C(58)	114(2)	N(2)-C(61)-H(61B)	109.2
C(56)-N(1)-C(58)	127(3)	H(61A)-C(61)-H(61B)	107.9
O(37)-C(55)-N(1)	129(4)	C(61)-C(62)-H(62A)	109.5
O(37)-C(55)-H(55)	115.5	C(61)-C(62)-H(62B)	109.5
N(1)-C(55)-H(55)	115.5	H(62A)-C(62)-H(62B)	109.5
N(1)-C(56)-C(57)	112(2)	C(61)-C(62)-H(62C)	109.5
N(1)-C(56)-H(56A)	109.3	H(62A)-C(62)-H(62C)	109.5
C(57)-C(56)-H(56A)	109.3	H(62B)-C(62)-H(62C)	109.5
N(1)-C(56)-H(56B)	109.3	N(2)-C(63)-C(64)	108.7(17)
C(57)-C(56)-H(56B)	109.3	N(2)-C(63)-H(63A)	110.0
N(3)-C(66)-H(66A)	109.6	C(64)-C(63)-H(63A)	110.0
C(67)-C(66)-H(66A)	109.6	N(2)-C(63)-H(63B)	110.0
N(3)-C(66)-H(66B)	109.6	C(64)-C(63)-H(63B)	110.0
C(67)-C(66)-H(66B)	109.6	H(63A)-C(63)-H(63B)	108.3
H(66A)-C(66)-H(66B)	108.1	C(63)-C(64)-H(64A)	109.5
C(66)-C(67)-H(67A)	109.5	C(63)-C(64)-H(64B)	109.5
C(66)-C(67)-H(67B)	109.5	H(64A)-C(64)-H(64B)	109.5
H(67A)-C(67)-H(67B)	109.5	C(63)-C(64)-H(64C)	109.5

C(66)-C(67)-H(67C)	109.5	H(64A)-C(64)-H(64C)	109.5
H(67A)-C(67)-H(67C)	109.5	H(64B)-C(64)-H(64C)	109.5
H(67B)-C(67)-H(67C)	109.5	C(65)-N(3)-C(68)	120.6(18)
N(3)-C(68)-C(69)	114(2)	C(65)-N(3)-C(66)	118(2)
N(3)-C(68)-H(68A)	108.9	C(68)-N(3)-C(66)	121(2)
C(69)-C(68)-H(68A)	108.9	O(39)-C(65)-N(3)	125(3)
N(3)-C(68)-H(68B)	108.8	O(39)-C(65)-H(65)	117.3
C(69)-C(68)-H(68B)	108.8	N(3)-C(65)-H(65)	117.3
H(68A)-C(68)-H(68B)	107.7	N(3)-C(66)-C(67)	110(2)
C(68)-C(69)-H(69A)	109.5	N(3')-C(65')-H(65')	119.6
C(68)-C(69)-H(69B)	109.5	N(3')-C(66')-C(67')	108.7(17)
H(69A)-C(69)-H(69B)	109.5	N(3')-C(66')-H(66C)	109.9
C(68)-C(69)-H(69C)	109.5	C(67')-C(66')-H(66C)	109.9
H(69A)-C(69)-H(69C)	109.5	N(3')-C(66')-H(66D)	109.9
H(69B)-C(69)-H(69C)	109.5	C(67')-C(66')-H(66D)	109.9
C(65')-N(3')-C(68')	120.0(16)	H(66C)-C(66')-H(66D)	108.3
C(65')-N(3')-C(66')	118.6(15)	C(66')-C(67')-H(67D)	109.5
C(68')-N(3')-C(66')	121.1(17)	C(66')-C(67')-H(67E)	109.5
O(39)-C(65')-N(3')	120.7(19)	H(67D)-C(67')-H(67E)	109.5
O(39)-C(65')-H(65')	119.7	C(66')-C(67')-H(67F)	109.5
C(76)-N(5)-C(78)	120(3)	H(67D)-C(67')-H(67F)	109.5
C(75)-N(5)-C(78)	115(2)	H(67E)-C(67')-H(67F)	109.5
O(41)-C(75)-N(5)	117(3)	N(3')-C(68')-C(69')	110.3(18)
O(41)-C(75)-H(75)	121.7	N(3')-C(68')-H(68C)	109.6
N(5)-C(75)-H(75)	121.7	C(69')-C(68')-H(68C)	109.6
N(5)-C(76)-C(77)	122(4)	N(3')-C(68')-H(68D)	109.6
N(5)-C(76)-H(76A)	106.8	C(69')-C(68')-H(68D)	109.6
C(77)-C(76)-H(76A)	106.8	H(68C)-C(68')-H(68D)	108.1
N(5)-C(76)-H(76B)	106.8	C(68')-C(69')-H(69D)	109.5
C(77)-C(76)-H(76B)	106.8	C(68')-C(69')-H(69E)	109.5
H(76A)-C(76)-H(76B)	106.6	H(69D)-C(69')-H(69E)	109.5
C(76)-C(77)-H(77A)	109.5	C(68')-C(69')-H(69F)	109.5
C(76)-C(77)-H(77B)	109.4	H(69D)-C(69')-H(69F)	109.5
H(77A)-C(77)-H(77B)	109.5	H(69E)-C(69')-H(69F)	109.5
C(76)-C(77)-H(77C)	109.5	C(70)-O(40)-Pr(6)	126.8(7)
H(77A)-C(77)-H(77C)	109.5	C(70)-N(4)-C(71)	123.8(13)

H(77B)-C(77)-H(77C)	109.5	C(70)-N(4)-C(73)	119.5(11)
N(5)-C(78)-C(79)	96(3)	C(71)-N(4)-C(73)	116.7(12)
N(5)-C(78)-H(78A)	112.6	O(40)-C(70)-N(4)	123.7(11)
C(79)-C(78)-H(78A)	112.6	O(40)-C(70)-H(70)	118.1
N(5)-C(78)-H(78B)	112.6	N(4)-C(70)-H(70)	118.1
C(79)-C(78)-H(78B)	112.6	N(4)-C(71)-C(72)	113.7(14)
H(78A)-C(78)-H(78B)	110.1	N(4)-C(71)-H(71A)	108.8
C(78)-C(79)-H(79A)	109.5	C(72)-C(71)-H(71A)	108.8
C(78)-C(79)-H(79B)	109.5	N(4)-C(71)-H(71B)	108.8
H(79A)-C(79)-H(79B)	109.5	C(72)-C(71)-H(71B)	108.8
C(78)-C(79)-H(79C)	109.5	H(71A)-C(71)-H(71B)	107.7
H(79A)-C(79)-H(79C)	109.5	C(71)-C(72)-H(72A)	109.5
H(79B)-C(79)-H(79C)	109.5	C(71)-C(72)-H(72B)	109.5
C(75')-N(5')-C(76')	121(2)	H(72A)-C(72)-H(72B)	109.5
C(75')-N(5')-C(78')	116(2)	C(71)-C(72)-H(72C)	109.5
C(76')-N(5')-C(78')	120(3)	H(72A)-C(72)-H(72C)	109.5
O(41)-C(75')-N(5')	127(3)	H(72B)-C(72)-H(72C)	109.5
O(41)-C(75')-H(75')	116.7	N(4)-C(73)-C(74)	107.9(15)
N(5')-C(75')-H(75')	116.8	N(4)-C(73)-H(73A)	110.1
N(5')-C(76')-C(77')	121(3)	C(74)-C(73)-H(73A)	110.1
N(5')-C(76')-H(76C)	107.1	N(4)-C(73)-H(73B)	110.1
C(77')-C(76')-H(76C)	107.2	C(74)-C(73)-H(73B)	110.1
N(5')-C(76')-H(76D)	107.2	H(73A)-C(73)-H(73B)	108.4
C(77')-C(76')-H(76D)	107.2	C(73)-C(74)-H(74A)	109.5
H(76C)-C(76')-H(76D)	106.8	C(73)-C(74)-H(74B)	109.5
C(76')-C(77')-H(77D)	109.5	H(74A)-C(74)-H(74B)	109.5
C(76')-C(77')-H(77E)	109.5	C(73)-C(74)-H(74C)	109.5
H(77D)-C(77')-H(77E)	109.5	H(74A)-C(74)-H(74C)	109.5
C(76')-C(77')-H(77F)	109.5	H(74B)-C(74)-H(74C)	109.5
H(77D)-C(77')-H(77F)	109.5	C(76)-N(5)-C(75)	117(2)
H(77E)-C(77')-H(77F)	109.5	H(79D)-C(79')-H(79F)	109.5
N(5')-C(78')-C(79')	98(3)	H(79E)-C(79')-H(79F)	109.5
N(5')-C(78')-H(78C)	112.2	C(55)-O(37)-Pr(1)	130(2)
C(79')-C(78')-H(78C)	112.2	C(55')-O(37)-Pr(1)	129.9(19)
N(5')-C(78')-H(78D)	112.2	C(65')-O(39)-Pr(4)	128.5(12)
C(79')-C(78')-H(78D)	112.2	C(65)-O(39)-Pr(4)	123.5(19)

H(78C)-C(78')-H(78D)	109.8	C(75')-O(41)-Pr(5)	126.8(18)
C(78')-C(79')-H(79D)	109.5	C(75)-O(41)-Pr(5)	146(2)
C(78')-C(79')-H(79E)	109.5	C(78')-C(79')-H(79F)	109.5
H(79D)-C(79')-H(79E)	109.5		

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z-1 #2 x,y-1,z #3 x,y+1,z+1 #4 -x-2,-y-1,z+1/2 #5 -x-2,-y-2,z+1/2 #6 -x-2,-y-2,z-1/2 #7 x,y-1,z-1 #8 -x-5/2,y+1/2,z-1/2 #9 -x-5/2,y+1/2,z+1/2 #10 -x-2,-y-1,z-1/2 #11 -x-5/2,y-1/2,z+1/2 #12 -x-5/2,y-1/2,z-1/2 #13 x,y+1,z #14 x,y,z+1

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C(1)-O(2)	1.236(12)	C(30)-O(43)	1.268(13)
C(1)-O(1)	1.266(13)	C(30)-Nd(5)#1	3.032(10)
C(1)-C(2)	1.480(13)	C(31)-O(21)	1.242(12)
C(2)-C(3)	1.346(14)	C(31)-O(22)	1.259(13)
C(2)-S(1)	1.702(10)	C(31)-C(32)	1.494(13)
C(3)-C(4)	1.412(14)	C(32)-C(33)	1.363(14)
C(3)-H(3)	0.9300	C(32)-S(6)	1.704(10)
C(4)-C(5)	1.341(15)	C(33)-C(34)	1.423(13)
C(4)-H(4)	0.9300	C(33)-H(33)	0.9300
C(5)-C(6)	1.473(14)	C(34)-C(35)	1.344(14)
C(5)-S(1)	1.692(10)	C(34)-H(34)	0.9300
C(6)-O(3)	1.243(13)	C(35)-C(36)	1.473(14)
C(6)-O(4)	1.256(12)	C(35)-S(6)	1.707(10)
C(7)-O(5)	1.244(12)	C(36)-O(24)	1.240(13)
C(7)-O(6)	1.250(13)	C(36)-O(23)	1.272(12)
C(7)-C(8)	1.491(14)	C(36)-Nd(6)#2	3.041(11)
C(7)-Nd(2)	2.964(10)	C(37)-O(26)	1.248(13)
C(8)-C(9)	1.344(15)	C(37)-O(25)	1.265(13)
C(8)-S(2)	1.712(10)	C(37)-C(38)	1.480(13)
C(9)-C(10)	1.407(14)	C(38)-C(39)	1.359(14)
C(9)-H(9)	0.9300	C(38)-S(7)	1.706(10)
C(10)-C(11)	1.353(16)	C(39)-C(40)	1.411(14)

C(10)-H(10)	0.9300	C(39)-H(39)	0.9300
C(11)-C(12)	1.485(13)	C(40)-C(41)	1.341(15)
C(11)-S(2)	1.694(11)	C(40)-H(40)	0.9300
C(12)-O(7)	1.234(12)	C(41)-C(42)	1.498(14)
C(12)-O(8)	1.248(13)	C(41)-S(7)	1.701(11)
C(13)-O(9)	1.247(13)	C(42)-O(27)	1.230(13)
C(13)-O(10)	1.264(13)	C(42)-O(28)	1.259(12)
C(13)-C(14)	1.465(14)	C(43)-O(30)	1.250(13)
C(14)-C(15)	1.342(15)	C(43)-O(29)	1.267(12)
C(14)-S(3)	1.698(10)	C(43)-C(44)	1.468(13)
C(15)-C(16)	1.394(14)	C(43)-Nd(4)	3.040(10)
C(15)-H(15)	0.9300	C(44)-C(45)	1.347(14)
C(16)-C(17)	1.355(16)	C(44)-S(8)	1.709(10)
C(16)-H(16)	0.9300	C(45)-C(46)	1.403(13)
C(17)-C(18)	1.490(14)	C(45)-H(45)	0.9300
C(17)-S(3)	1.688(11)	C(46)-C(47)	1.349(14)
C(18)-O(11)	1.255(14)	C(46)-H(46)	0.9300
C(18)-O(12)	1.255(14)	C(47)-C(48)	1.495(14)
C(19)-O(14)	1.241(14)	C(47)-S(8)	1.703(10)
C(19)-O(13)	1.245(14)	C(48)-O(31)	1.216(13)
C(19)-C(20)	1.499(15)	C(48)-O(32)	1.267(13)
C(20)-C(21)	1.338(15)	C(49)-O(33)	1.247(13)
C(20)-S(4)	1.711(11)	C(49)-O(34)	1.262(13)
C(21)-C(22)	1.409(13)	C(49)-C(50)	1.510(13)
C(21)-H(21)	0.9300	C(50)-C(51)	1.356(14)
C(22)-C(23)	1.346(14)	C(50)-S(9)	1.697(10)
C(22)-H(22)	0.9300	C(51)-C(52)	1.395(13)
C(23)-C(24)	1.500(14)	C(51)-H(51)	0.9300
C(23)-S(4)	1.712(10)	C(52)-C(53)	1.368(14)
C(24)-O(16)	1.231(14)	C(52)-H(52)	0.9300
C(24)-O(15)	1.289(13)	C(53)-C(54)	1.472(14)
C(25)-O(18)	1.241(13)	C(53)-S(9)	1.700(10)
C(25)-O(17)	1.261(13)	C(54)-O(36)	1.243(12)
C(25)-C(26)	1.478(15)	C(54)-O(35)	1.252(13)
C(26)-C(27)	1.346(15)	C(54)-Nd(3)#3	3.027(11)
C(26)-S(5)	1.715(11)	O(1)-Nd(2)	2.416(6)

C(27)-C(28)	1.401(13)	O(2)-Nd(1)	2.367(6)
C(27)-H(27)	0.9300	O(3)-Nd(1)#4	2.431(6)
C(28)-C(29)	1.351(14)	O(4)-Nd(2)#4	2.324(7)
C(28)-H(28)	0.9300	O(5)-Nd(1)	2.495(6)
C(29)-C(30)	1.452(13)	O(5)-Nd(2)	2.767(7)
C(29)-S(5)	1.720(9)	O(6)-Nd(2)	2.452(7)
C(30)-O(20)	1.258(12)	O(7)-Nd(1)#5	2.375(7)
O(22)-Nd(4)	2.457(6)	O(8)-Nd(5)#2	2.415(6)
O(23)-Nd(5)#2	2.364(6)	O(9)-Nd(1)	2.490(7)
O(23)-Nd(6)#2	2.876(7)	O(10)-Nd(2)	2.360(6)
O(24)-Nd(6)#2	2.480(7)	O(11)-Nd(1)#6	2.451(7)
O(25)-Nd(3)	2.470(6)	O(12)-Nd(5)#7	2.322(7)
O(26)-Nd(4)	2.392(6)	O(13)-Nd(2)	2.340(6)
O(27)-Nd(6)#1	2.435(7)	O(14)-Nd(3)	2.451(7)
O(28)-Nd(4)#8	2.318(7)	O(15)-Nd(5)	2.406(6)
O(29)-Nd(3)	2.400(6)	O(16)-Nd(6)	2.512(7)
O(29)-Nd(4)	2.845(7)	O(17)-Nd(2)	2.457(7)
O(30)-Nd(4)	2.494(6)	O(18)-Nd(3)	2.341(7)
O(31)-Nd(4)#9	2.429(7)	O(19)-Nd(3)	2.668(6)
O(32)-Nd(6)	2.341(7)	O(19)-Nd(2)	2.695(6)
O(33)-Nd(5)	2.408(6)	O(19)-H(19A)	0.85(3)
O(34)-Nd(6)	2.403(6)	O(19)-H(19B)	0.85(3)
O(35)-Nd(3)#3	2.505(7)	O(20)-Nd(6)#1	2.426(6)
O(36)-Nd(4)#3	2.378(6)	O(20)-Nd(5)#1	2.807(6)
O(36)-Nd(3)#3	2.843(7)	O(21)-Nd(3)	2.413(6)
O(42)-Nd(6)	2.610(6)	O(43)-Nd(5)#1	2.502(6)
O(42)-H(42B)	0.85(3)	O(44)-Nd(1)	2.561(6)
O(42)-H(42A)	0.85(3)	O(44)-H(44A)	0.86(3)
O(44)-H(44B)	0.85(3)	C(68')-C(69')	1.55(2)
Nd(1)-O(7)#6	2.375(7)	C(68')-H(68C)	0.9700
Nd(1)-O(3)#10	2.431(6)	C(68')-H(68D)	0.9700
Nd(1)-O(37)	2.444(7)	C(69')-H(69D)	0.9600
Nd(1)-O(11)#5	2.451(7)	C(69')-H(69E)	0.9600
Nd(2)-O(4)#10	2.324(7)	C(69')-H(69F)	0.9600
Nd(3)-O(38)	2.484(7)	O(40)-C(70)	1.226(12)
Nd(3)-O(35)#7	2.505(7)	N(4)-C(70)	1.336(12)

Nd(3)-O(36)#7	2.843(7)	N(4)-C(71)	1.456(15)
Nd(3)-C(54)#7	3.027(11)	N(4)-C(73)	1.483(17)
Nd(4)-O(28)#11	2.318(7)	C(70)-H(70)	0.9300
Nd(4)-O(36)#7	2.378(6)	C(71)-C(72)	1.491(19)
Nd(4)-O(31)#12	2.429(7)	C(71)-H(71A)	0.9700
Nd(4)-O(39)	2.445(7)	C(71)-H(71B)	0.9700
Nd(5)-O(12)#3	2.322(7)	C(72)-H(72A)	0.9600
Nd(5)-O(23)#13	2.364(6)	C(72)-H(72B)	0.9600
Nd(5)-O(8)#13	2.416(6)	C(72)-H(72C)	0.9600
Nd(5)-O(41)	2.454(6)	C(73)-C(74)	1.50(2)
Nd(5)-O(43)#14	2.503(6)	C(73)-H(73A)	0.9700
Nd(5)-O(20)#14	2.807(6)	C(73)-H(73B)	0.9700
Nd(5)-C(30)#14	3.032(10)	C(74)-H(74A)	0.9600
Nd(6)-O(20)#14	2.426(6)	C(74)-H(74B)	0.9600
Nd(6)-O(27)#14	2.435(7)	C(74)-H(74C)	0.9600
Nd(6)-O(40)	2.463(6)	N(5)-C(76)	1.43(2)
Nd(6)-O(24)#13	2.480(7)	N(5)-C(78)	1.46(3)
Nd(6)-O(23)#13	2.877(7)	N(5)-C(75)	1.46(2)
Nd(6)-C(36)#13	3.041(11)	C(75)-O(41)	1.19(2)
N(1)-C(55)	1.40(2)	C(75)-H(75)	0.9300
N(1)-C(56)	1.47(2)	C(76)-C(77)	1.53(3)
N(1)-C(58)	1.52(2)	C(76)-H(76A)	0.9700
C(55)-O(37)	1.18(3)	C(76)-H(76B)	0.9700
C(55)-H(55)	0.9300	C(77)-H(77A)	0.9600
C(56)-C(57)	1.52(3)	C(77)-H(77B)	0.9600
C(56)-H(56A)	0.9700	C(77)-H(77C)	0.9600
C(56)-H(56B)	0.9700	C(78)-C(79)	1.55(3)
C(57)-H(57A)	0.9600	C(78)-H(78A)	0.9700
C(57)-H(57B)	0.9600	C(78)-H(78B)	0.9700
C(57)-H(57C)	0.9600	C(79)-H(79A)	0.9600
C(58)-C(59)	1.60(3)	C(79)-H(79B)	0.9600
C(58)-H(58A)	0.9700	C(79)-H(79C)	0.9600
C(58)-H(58B)	0.9700	N(5')-C(75')	1.42(2)
C(59)-H(59A)	0.9600	N(5')-C(78')	1.46(2)
C(59)-H(59B)	0.9600	N(5')-C(76')	1.46(2)
C(59)-H(59C)	0.9600	C(75')-O(41)	1.17(2)

N(1')-C(55')	1.41(2)	C(75')-H(75')	0.9300
N(1')-C(56')	1.44(3)	C(76')-C(77')	1.47(3)
N(1')-C(58')	1.47(2)	C(76')-H(76C)	0.9700
C(55')-O(37)	1.23(3)	C(76')-H(76D)	0.9700
C(55')-H(55')	0.9300	C(77')-H(77D)	0.9600
C(56')-C(57')	1.46(3)	C(77')-H(77E)	0.9600
C(56')-H(56C)	0.9700	C(77')-H(77F)	0.9600
C(56')-H(56D)	0.9700	C(78')-C(79')	1.53(3)
C(57')-H(57D)	0.9600	C(78')-H(78C)	0.9700
C(57')-H(57E)	0.9600	C(78')-H(78D)	0.9700
C(57')-H(57F)	0.9600	C(79')-H(79D)	0.9600
C(58')-C(59')	1.55(3)	C(79')-H(79E)	0.9600
C(58')-H(58C)	0.9700	C(79')-H(79F)	0.9600
C(58')-H(58D)	0.9700	C(68)-H(68B)	0.9700
C(59')-H(59D)	0.9600	C(69)-H(69A)	0.9600
C(59')-H(59E)	0.9600	C(69)-H(69B)	0.9600
C(59')-H(59F)	0.9600	C(69)-H(69C)	0.9600
O(38)-C(60)	1.217(12)	N(3')-C(65')	1.370(19)
N(2)-C(60)	1.358(13)	N(3')-C(68')	1.45(2)
N(2)-C(63)	1.472(18)	N(3')-C(66')	1.47(2)
N(2)-C(61)	1.502(17)	C(65')-O(39)	1.213(18)
C(60)-H(60)	0.9300	C(65')-H(65')	0.9300
C(61)-C(62)	1.48(2)	C(66')-C(67')	1.53(2)
C(61)-H(61A)	0.9700	C(66')-H(66C)	0.9700
C(61)-H(61B)	0.9700	C(66')-H(66D)	0.9700
C(62)-H(62A)	0.9600	C(67')-H(67D)	0.9600
C(62)-H(62B)	0.9600	C(65)-O(39)	1.22(2)
C(62)-H(624)	0.9600	C(65)-H(65)	0.9300
C(63)-C(64)	1.47(2)	C(66)-C(67)	1.52(3)
C(63)-H(63A)	0.9700	C(66)-H(66A)	0.9700
C(63)-H(63B)	0.9700	C(66)-H(66B)	0.9700
C(64)-H(64A)	0.9600	C(67)-H(67A)	0.9600
C(64)-H(64B)	0.9600	C(67)-H(67B)	0.9600
C(64)-H(64C)	0.9600	C(67)-H(67C)	0.9600
N(3)-C(65)	1.38(2)	C(68)-C(69)	1.50(3)
N(3)-C(66)	1.45(2)	C(68)-H(68A)	0.9700

N(3)-C(68)	1.46(2)	C(67')-H(67E)	0.9600
C(67')-H(67F)	0.9600		

O(2)-C(1)-O(1)	126.6(9)	C(33)-C(32)-C(31)	126.2(10)
O(2)-C(1)-C(2)	115.7(10)	C(33)-C(32)-S(6)	112.5(7)
O(1)-C(1)-C(2)	117.7(9)	C(31)-C(32)-S(6)	121.2(8)
C(3)-C(2)-C(1)	126.6(10)	C(32)-C(33)-C(34)	111.3(9)
C(3)-C(2)-S(1)	110.8(7)	C(32)-C(33)-H(33)	124.4
C(1)-C(2)-S(1)	122.6(8)	C(34)-C(33)-H(33)	124.4
C(2)-C(3)-C(4)	113.6(10)	C(35)-C(34)-C(33)	112.7(9)
C(2)-C(3)-H(3)	123.2	C(35)-C(34)-H(34)	123.6
C(4)-C(3)-H(3)	123.2	C(33)-C(34)-H(34)	123.6
C(5)-C(4)-C(3)	111.2(10)	C(34)-C(35)-C(36)	128.5(9)
C(5)-C(4)-H(4)	124.4	C(34)-C(35)-S(6)	112.3(7)
C(3)-C(4)-H(4)	124.4	C(36)-C(35)-S(6)	119.1(8)
C(4)-C(5)-C(6)	126.2(10)	O(24)-C(36)-O(23)	121.7(10)
C(4)-C(5)-S(1)	112.8(8)	O(24)-C(36)-C(35)	120.0(9)
C(6)-C(5)-S(1)	121.1(8)	O(23)-C(36)-C(35)	118.2(10)
O(3)-C(6)-O(4)	124.1(9)	O(24)-C(36)-Nd(6)#2	52.1(5)
O(3)-C(6)-C(5)	117.2(10)	O(23)-C(36)-Nd(6)#2	70.4(6)
O(4)-C(6)-C(5)	118.6(10)	C(35)-C(36)-Nd(6)#2	168.0(8)
O(5)-C(7)-O(6)	122.9(9)	O(26)-C(37)-O(25)	126.0(9)
O(5)-C(7)-C(8)	119.2(10)	O(26)-C(37)-C(38)	116.6(10)
O(6)-C(7)-C(8)	117.9(9)	O(25)-C(37)-C(38)	117.3(10)
O(5)-C(7)-Nd(2)	68.8(5)	C(39)-C(38)-C(37)	127.7(10)
O(6)-C(7)-Nd(2)	54.2(5)	C(39)-C(38)-S(7)	112.1(7)
C(8)-C(7)-Nd(2)	170.8(8)	C(37)-C(38)-S(7)	120.1(8)
C(9)-C(8)-C(7)	129.1(10)	C(38)-C(39)-C(40)	111.7(10)
C(9)-C(8)-S(2)	111.5(8)	C(38)-C(39)-H(39)	124.2
C(7)-C(8)-S(2)	119.3(9)	C(40)-C(39)-H(39)	124.2
C(8)-C(9)-C(10)	112.8(10)	C(41)-C(40)-C(39)	112.7(10)
C(8)-C(9)-H(9)	123.6	C(41)-C(40)-H(40)	123.6
C(10)-C(9)-H(9)	123.6	C(39)-C(40)-H(40)	123.6
C(11)-C(10)-C(9)	112.2(11)	C(40)-C(41)-C(42)	127.3(10)
C(11)-C(10)-H(10)	123.9	C(40)-C(41)-S(7)	112.4(8)
C(9)-C(10)-H(10)	123.9	C(42)-C(41)-S(7)	120.2(8)

C(10)-C(11)-C(12)	125.8(10)	O(27)-C(42)-O(28)	126.2(10)
C(10)-C(11)-S(2)	112.0(8)	O(27)-C(42)-C(41)	119.3(10)
C(12)-C(11)-S(2)	122.2(9)	O(28)-C(42)-C(41)	114.5(10)
O(7)-C(12)-O(8)	125.1(9)	O(30)-C(43)-O(29)	121.5(9)
O(7)-C(12)-C(11)	117.2(10)	O(30)-C(43)-C(44)	119.6(9)
O(8)-C(12)-C(11)	117.6(9)	O(29)-C(43)-C(44)	118.9(10)
O(9)-C(13)-O(10)	126.3(10)	O(30)-C(43)-Nd(4)	52.9(5)
O(9)-C(13)-C(14)	118.0(10)	O(29)-C(43)-Nd(4)	69.1(5)
O(10)-C(13)-C(14)	115.8(10)	C(44)-C(43)-Nd(4)	170.0(7)
C(15)-C(14)-C(13)	127.7(10)	C(45)-C(44)-C(43)	127.5(9)
C(15)-C(14)-S(3)	110.7(8)	C(45)-C(44)-S(8)	111.9(7)
C(13)-C(14)-S(3)	121.6(8)	C(43)-C(44)-S(8)	120.6(8)
C(14)-C(15)-C(16)	112.9(10)	C(44)-C(45)-C(46)	112.2(9)
C(14)-C(15)-H(15)	123.6	C(44)-C(45)-H(45)	123.9
C(16)-C(15)-H(15)	123.6	C(46)-C(45)-H(45)	123.9
C(17)-C(16)-C(15)	113.2(10)	C(47)-C(46)-C(45)	113.1(10)
C(17)-C(16)-H(16)	123.4	C(47)-C(46)-H(46)	123.5
C(15)-C(16)-H(16)	123.4	C(45)-C(46)-H(46)	123.5
C(16)-C(17)-C(18)	127.3(11)	C(46)-C(47)-C(48)	126.1(10)
C(16)-C(17)-S(3)	110.3(8)	C(46)-C(47)-S(8)	111.5(8)
C(18)-C(17)-S(3)	122.0(9)	C(48)-C(47)-S(8)	122.3(8)
O(11)-C(18)-O(12)	125.8(10)	O(31)-C(48)-O(32)	125.9(11)
O(11)-C(18)-C(17)	117.7(11)	O(31)-C(48)-C(47)	120.8(10)
O(12)-C(18)-C(17)	116.4(11)	O(32)-C(48)-C(47)	113.2(11)
O(14)-C(19)-O(13)	127.0(10)	O(33)-C(49)-O(34)	127.6(10)
O(14)-C(19)-C(20)	117.6(10)	O(33)-C(49)-C(50)	117.3(9)
O(13)-C(19)-C(20)	115.4(11)	O(34)-C(49)-C(50)	115.1(10)
C(21)-C(20)-C(19)	127.5(10)	C(51)-C(50)-C(49)	126.9(10)
C(21)-C(20)-S(4)	111.4(8)	C(51)-C(50)-S(9)	112.9(7)
C(19)-C(20)-S(4)	120.9(9)	C(49)-C(50)-S(9)	120.2(8)
C(20)-C(21)-C(22)	114.1(10)	C(50)-C(51)-C(52)	111.3(10)
C(20)-C(21)-H(21)	122.9	C(50)-C(51)-H(51)	124.3
C(22)-C(21)-H(21)	122.9	C(52)-C(51)-H(51)	124.3
C(23)-C(22)-C(21)	110.9(10)	C(53)-C(52)-C(51)	113.3(10)
C(23)-C(22)-H(22)	124.6	C(53)-C(52)-H(52)	123.3
C(21)-C(22)-H(22)	124.6	C(51)-C(52)-H(52)	123.3

C(22)-C(23)-C(24)	129.0(10)	C(52)-C(53)-C(54)	128.2(9)
C(22)-C(23)-S(4)	112.9(8)	C(52)-C(53)-S(9)	111.1(7)
C(24)-C(23)-S(4)	117.9(8)	C(54)-C(53)-S(9)	120.7(8)
O(16)-C(24)-O(15)	126.3(10)	O(36)-C(54)-O(35)	122.9(10)
O(16)-C(24)-C(23)	119.6(10)	O(36)-C(54)-C(53)	119.4(10)
O(15)-C(24)-C(23)	114.1(11)	O(35)-C(54)-C(53)	117.7(9)
O(18)-C(25)-O(17)	124.0(10)	O(36)-C(54)-Nd(3)#3	69.6(6)
O(18)-C(25)-C(26)	115.9(10)	O(35)-C(54)-Nd(3)#3	54.0(5)
O(17)-C(25)-C(26)	120.1(10)	C(53)-C(54)-Nd(3)#3	166.9(8)
C(27)-C(26)-C(25)	124.6(10)	C(1)-O(1)-Nd(2)	127.8(6)
C(27)-C(26)-S(5)	110.6(8)	C(1)-O(2)-Nd(1)	146.5(7)
C(25)-C(26)-S(5)	124.8(8)	C(6)-O(3)-Nd(1)#4	115.7(6)
C(26)-C(27)-C(28)	114.1(10)	C(6)-O(4)-Nd(2)#4	168.7(8)
C(26)-C(27)-H(27)	122.9	C(7)-O(5)-Nd(1)	165.7(7)
C(28)-C(27)-H(27)	122.9	C(7)-O(5)-Nd(2)	86.5(6)
C(29)-C(28)-C(27)	112.3(10)	Nd(1)-O(5)-Nd(2)	107.3(2)
C(29)-C(28)-H(28)	123.8	C(7)-O(6)-Nd(2)	101.3(6)
C(27)-C(28)-H(28)	123.8	C(12)-O(7)-Nd(1)#5	170.8(8)
C(28)-C(29)-C(30)	127.1(9)	C(12)-O(8)-Nd(5)#2	132.4(6)
C(28)-C(29)-S(5)	111.2(7)	C(13)-O(9)-Nd(1)	144.0(7)
C(30)-C(29)-S(5)	121.7(8)	C(13)-O(10)-Nd(2)	133.1(7)
O(20)-C(30)-O(43)	120.8(9)	C(18)-O(11)-Nd(1)#6	122.8(7)
O(20)-C(30)-C(29)	120.6(10)	C(18)-O(12)-Nd(5)#7	143.3(7)
O(43)-C(30)-C(29)	118.5(9)	C(19)-O(13)-Nd(2)	141.9(8)
O(20)-C(30)-Nd(5)#1	67.7(5)	C(19)-O(14)-Nd(3)	130.6(7)
O(43)-C(30)-Nd(5)#1	53.8(5)	C(24)-O(15)-Nd(5)	131.8(7)
C(29)-C(30)-Nd(5)#1	167.2(7)	C(24)-O(16)-Nd(6)	139.7(7)
O(21)-C(31)-O(22)	126.7(9)	C(25)-O(17)-Nd(2)	128.3(7)
O(21)-C(31)-C(32)	117.0(10)	C(25)-O(18)-Nd(3)	169.6(8)
O(22)-C(31)-C(32)	116.3(9)	Nd(3)-O(19)-Nd(2)	123.55(18)
C(37)-O(25)-Nd(3)	137.8(6)	Nd(3)-O(19)-H(19A)	88(6)
C(37)-O(26)-Nd(4)	134.0(7)	Nd(2)-O(19)-H(19A)	114(7)
C(42)-O(27)-Nd(6)#1	134.0(7)	Nd(3)-O(19)-H(19B)	120(6)
C(42)-O(28)-Nd(4)#8	146.3(7)	Nd(2)-O(19)-H(19B)	101(7)
C(43)-O(29)-Nd(3)	169.1(7)	H(19A)-O(19)-H(19B)	110(4)
C(43)-O(29)-Nd(4)	86.3(6)	C(30)-O(20)-Nd(6)#1	168.4(7)

Nd(3)-O(29)-Nd(4)	104.4(2)	C(30)-O(20)-Nd(5)#1	87.8(6)
C(43)-O(30)-Nd(4)	103.5(6)	Nd(6)#1-O(20)-Nd(5)#1	103.8(2)
C(48)-O(31)-Nd(4)#9	134.5(7)	C(31)-O(21)-Nd(3)	137.1(7)
C(48)-O(32)-Nd(6)	161.8(8)	C(31)-O(22)-Nd(4)	134.7(6)
C(49)-O(33)-Nd(5)	134.3(6)	C(36)-O(23)-Nd(5)#2	167.7(7)
C(49)-O(34)-Nd(6)	137.3(7)	C(36)-O(23)-Nd(6)#2	84.9(6)
C(54)-O(35)-Nd(3)#3	102.2(6)	Nd(5)#2-O(23)-Nd(6)#2	103.4(2)
C(54)-O(36)-Nd(4)#3	168.6(7)	C(36)-O(24)-Nd(6)#2	104.7(6)
C(54)-O(36)-Nd(3)#3	86.2(6)	O(18)-Nd(3)-O(14)	92.7(3)
Nd(4)#3-O(36)-Nd(3)#3	105.0(2)	O(29)-Nd(3)-O(14)	90.0(2)
Nd(6)-O(42)-H(42B)	115(5)	O(21)-Nd(3)-O(14)	76.8(3)
Nd(6)-O(42)-H(42A)	131(8)	O(18)-Nd(3)-O(25)	85.0(2)
H(42B)-O(42)-H(42A)	110(5)	O(29)-Nd(3)-O(25)	76.3(2)
C(30)-O(43)-Nd(5)#1	102.0(6)	O(21)-Nd(3)-O(25)	129.3(2)
Nd(1)-O(44)-H(44A)	123(10)	O(14)-Nd(3)-O(25)	142.2(2)
Nd(1)-O(44)-H(44B)	114(9)	O(18)-Nd(3)-O(38)	73.8(3)
H(44A)-O(44)-H(44B)	107(4)	O(29)-Nd(3)-O(38)	81.3(2)
C(5)-S(1)-C(2)	91.7(5)	O(21)-Nd(3)-O(38)	137.8(2)
C(11)-S(2)-C(8)	91.5(5)	O(14)-Nd(3)-O(38)	70.3(2)
C(17)-S(3)-C(14)	92.8(5)	O(25)-Nd(3)-O(38)	72.9(2)
C(20)-S(4)-C(23)	90.7(5)	O(18)-Nd(3)-O(35)#7	72.1(3)
C(26)-S(5)-C(29)	91.7(5)	O(29)-Nd(3)-O(35)#7	123.0(2)
C(32)-S(6)-C(35)	91.2(5)	O(21)-Nd(3)-O(35)#7	84.5(3)
C(41)-S(7)-C(38)	91.0(5)	O(14)-Nd(3)-O(35)#7	135.0(2)
C(47)-S(8)-C(44)	91.3(5)	O(25)-Nd(3)-O(35)#7	79.9(2)
C(50)-S(9)-C(53)	91.4(5)	O(38)-Nd(3)-O(35)#7	137.6(2)
O(2)-Nd(1)-O(7)#6	137.9(3)	O(18)-Nd(3)-O(19)	67.5(2)
O(2)-Nd(1)-O(3)#10	82.1(3)	O(29)-Nd(3)-O(19)	138.5(2)
O(7)#6-Nd(1)-O(3)#10	74.5(3)	O(21)-Nd(3)-O(19)	67.3(2)
O(2)-Nd(1)-O(37)	138.8(3)	O(14)-Nd(3)-O(19)	70.6(2)
O(7)#6-Nd(1)-O(37)	77.9(3)	O(25)-Nd(3)-O(19)	139.8(2)
O(3)#10-Nd(1)-O(37)	136.2(3)	O(38)-Nd(3)-O(19)	122.3(2)
O(2)-Nd(1)-O(11)#5	81.4(3)	O(35)#7-Nd(3)-O(19)	64.4(2)
O(7)#6-Nd(1)-O(11)#5	99.1(3)	O(18)-Nd(3)-O(36)#7	114.8(2)
O(3)#10-Nd(1)-O(11)#5	146.1(3)	O(29)-Nd(3)-O(36)#7	75.1(2)
O(37)-Nd(1)-O(11)#5	71.2(3)	O(21)-Nd(3)-O(36)#7	69.3(2)

O(2)-Nd(1)-O(9)	119.6(2)	O(14)-Nd(3)-O(36)#7	145.6(2)
O(7)#6-Nd(1)-O(9)	86.9(2)	O(25)-Nd(3)-O(36)#7	64.6(2)
O(3)#10-Nd(1)-O(9)	73.8(2)	O(38)-Nd(3)-O(36)#7	134.9(2)
O(37)-Nd(1)-O(9)	71.4(3)	O(35)#7-Nd(3)-O(36)#7	47.9(2)
O(11)#5-Nd(1)-O(9)	139.9(3)	O(19)-Nd(3)-O(36)#7	100.24(19)
O(2)-Nd(1)-O(5)	68.7(2)	O(18)-Nd(3)-C(54)#7	92.5(3)
O(7)#6-Nd(1)-O(5)	153.3(3)	O(29)-Nd(3)-C(54)#7	99.3(3)
O(3)#10-Nd(1)-O(5)	114.3(2)	O(21)-Nd(3)-C(54)#7	77.7(2)
O(37)-Nd(1)-O(5)	79.3(2)	O(14)-Nd(3)-C(54)#7	148.9(3)
O(11)#5-Nd(1)-O(5)	86.6(2)	O(25)-Nd(3)-C(54)#7	68.8(3)
O(9)-Nd(1)-O(5)	72.7(2)	O(38)-Nd(3)-C(54)#7	140.3(3)
O(2)-Nd(1)-O(44)	68.0(2)	O(35)#7-Nd(3)-C(54)#7	23.8(3)
O(7)#6-Nd(1)-O(44)	71.5(3)	O(19)-Nd(3)-C(54)#7	83.2(3)
O(3)#10-Nd(1)-O(44)	71.3(3)	O(36)#7-Nd(3)-C(54)#7	24.2(2)
O(37)-Nd(1)-O(44)	129.6(2)	O(28)#11-Nd(4)-O(36)#7	156.2(2)
O(11)#5-Nd(1)-O(44)	75.1(3)	O(28)#11-Nd(4)-O(26)	126.7(2)
O(9)-Nd(1)-O(44)	142.6(3)	O(36)#7-Nd(4)-O(26)	75.1(2)
O(5)-Nd(1)-O(44)	134.9(2)	O(28)#11-Nd(4)-O(31)#12	85.8(3)
O(4)#10-Nd(2)-O(13)	139.3(3)	O(36)#7-Nd(4)-O(31)#12	90.0(2)
O(4)#10-Nd(2)-O(10)	77.6(3)	O(26)-Nd(4)-O(31)#12	79.2(3)
O(13)-Nd(2)-O(10)	137.4(2)	O(28)#11-Nd(4)-O(39)	78.9(2)
O(4)#10-Nd(2)-O(1)	80.4(2)	O(36)#7-Nd(4)-O(39)	77.6(2)
O(13)-Nd(2)-O(1)	79.4(2)	O(26)-Nd(4)-O(39)	138.9(2)
O(10)-Nd(2)-O(1)	138.5(2)	O(31)#12-Nd(4)-O(39)	70.5(3)
O(4)#10-Nd(2)-O(6)	132.4(2)	O(28)#11-Nd(4)-O(22)	88.3(2)
O(13)-Nd(2)-O(6)	79.0(3)	O(36)#7-Nd(4)-O(22)	80.9(2)
O(10)-Nd(2)-O(6)	86.8(3)	O(26)-Nd(4)-O(22)	131.7(2)
O(1)-Nd(2)-O(6)	82.7(3)	O(31)#12-Nd(4)-O(22)	142.5(3)
O(4)#10-Nd(2)-O(17)	78.6(2)	O(39)-Nd(4)-O(22)	72.0(2)
O(13)-Nd(2)-O(17)	82.7(2)	O(28)#11-Nd(4)-O(30)	74.6(2)
O(10)-Nd(2)-O(17)	87.4(3)	O(36)#7-Nd(4)-O(30)	123.4(2)
O(1)-Nd(2)-O(17)	121.9(3)	O(26)-Nd(4)-O(30)	80.0(2)
O(6)-Nd(2)-O(17)	145.9(2)	O(31)#12-Nd(4)-O(30)	133.8(2)
O(4)#10-Nd(2)-O(19)	139.0(2)	O(39)-Nd(4)-O(30)	141.1(2)
O(13)-Nd(2)-O(19)	72.5(2)	O(22)-Nd(4)-O(30)	79.3(2)
O(10)-Nd(2)-O(19)	65.2(2)	O(28)#11-Nd(4)-O(29)	119.3(2)

O(1)-Nd(2)-O(19)	139.6(3)	O(36)#7-Nd(4)-O(29)	75.4(2)
O(6)-Nd(2)-O(19)	64.2(3)	O(26)-Nd(4)-O(29)	67.7(2)
O(17)-Nd(2)-O(19)	83.0(2)	O(31)#12-Nd(4)-O(29)	146.2(2)
O(4)#10-Nd(2)-O(5)	83.3(2)	O(39)-Nd(4)-O(29)	132.7(2)
O(13)-Nd(2)-O(5)	122.3(2)	O(22)-Nd(4)-O(29)	66.0(2)
O(10)-Nd(2)-O(5)	71.2(2)	O(30)-Nd(4)-O(29)	48.0(2)
O(1)-Nd(2)-O(5)	71.6(2)	O(28)#11-Nd(4)-C(43)	95.9(3)
O(6)-Nd(2)-O(5)	49.2(2)	O(36)#7-Nd(4)-C(43)	100.0(3)
O(17)-Nd(2)-O(5)	154.6(2)	O(26)-Nd(4)-C(43)	74.2(2)
O(19)-Nd(2)-O(5)	99.65(19)	O(31)#12-Nd(4)-C(43)	147.9(3)
O(4)#10-Nd(2)-C(7)	108.0(3)	O(39)-Nd(4)-C(43)	141.3(3)
O(13)-Nd(2)-C(7)	100.4(3)	O(22)-Nd(4)-C(43)	69.5(2)
O(10)-Nd(2)-C(7)	78.8(3)	O(30)-Nd(4)-C(43)	23.6(3)
O(1)-Nd(2)-C(7)	75.2(3)	O(29)-Nd(4)-C(43)	24.6(2)
O(6)-Nd(2)-C(7)	24.4(3)	O(12)#3-Nd(5)-O(23)#13	164.6(2)
O(17)-Nd(2)-C(7)	162.9(3)	O(12)#3-Nd(5)-O(15)	111.3(2)
O(19)-Nd(2)-C(7)	82.0(3)	(23)#13-Nd(5)-O(15)	77.1(2)
O(5)-Nd(2)-C(7)	24.8(2)	O(12)#3-Nd(5)-O(33)	99.3(2)
O(18)-Nd(3)-O(29)	152.4(3)	O(23)#13-Nd(5)-O(33)	81.9(2)
O(18)-Nd(3)-O(21)	134.5(3)	O(15)-Nd(5)-O(33)	134.8(2)
O(29)-Nd(3)-O(21)	72.8(2)	O(12)#3-Nd(5)-O(8)#13	81.1(2)
O(23)#13-Nd(5)-O(43)#14	125.7(2)	O(23)#13-Nd(5)-O(8)#13	89.1(2)
O(15)-Nd(5)-O(43)#14	78.6(2)	O(15)-Nd(5)-O(8)#13	75.0(2)
O(33)-Nd(5)-O(43)#14	82.1(2)	O(33)-Nd(5)-O(8)#13	144.4(2)
O(8)#13-Nd(5)-O(43)#14	129.5(2)	O(12)#3-Nd(5)-O(41)	78.7(3)
O(41)-Nd(5)-O(43)#14	135.2(4)	O(23)#13-Nd(5)-O(41)	87.1(3)
O(12)#3-Nd(5)-O(20)#14	117.2(2)	O(15)-Nd(5)-O(41)	144.0(4)
O(23)#13-Nd(5)-O(20)#14	77.5(2)	O(33)-Nd(5)-O(41)	72.6(3)
O(15)-Nd(5)-O(20)#14	69.5(2)	O(8)#13-Nd(5)-O(41)	72.6(4)
O(33)-Nd(5)-O(20)#14	67.1(2)	O(12)#3-Nd(5)-O(43)#14	69.5(2)
O(8)#13-Nd(5)-O(20)#14	144.0(2)	C(58)-C(59)-H(59B)	109.5
O(41)-Nd(5)-O(20)#14	138.4(3)	H(59A)-C(59)-H(59B)	109.5
O(43)#14-Nd(5)-O(20)#14	48.4(2)	C(58)-C(59)-H(59C)	109.5
O(12)#3-Nd(5)-C(30)#14	92.8(3)	H(59A)-C(59)-H(59C)	109.5
O(23)#13-Nd(5)-C(30)#14	102.0(3)	H(59B)-C(59)-H(59C)	109.5
O(15)-Nd(5)-C(30)#14	74.7(3)	C(55')-N(1')-C(56')	119(2)

O(33)-Nd(5)-C(30)#14	71.2(3)	C(55')-N(1')-C(58')	116(2)
O(8)#13-Nd(5)-C(30)#14	144.4(3)	C(56')-N(1')-C(58')	114(3)
O(41)-Nd(5)-C(30)#14	140.9(4)	O(37)-C(55')-N(1')	119(3)
O(43)#14-Nd(5)-C(30)#14	24.1(3)	O(37)-C(55')-H(55')	120.7
O(20)#14-Nd(5)-C(30)#14	24.5(2)	N(1')-C(55')-H(55')	120.7
O(32)-Nd(6)-O(34)	138.3(3)	N(1')-C(56')-C(57')	118(3)
O(32)-Nd(6)-O(20)#14	148.9(3)	N(1')-C(56')-H(56C)	107.8
O(34)-Nd(6)-O(20)#14	71.8(2)	C(57')-C(56')-H(56C)	107.8
O(32)-Nd(6)-O(27)#14	90.3(3)	N(1')-C(56')-H(56D)	107.8
O(34)-Nd(6)-O(27)#14	77.5(3)	C(57')-C(56')-H(56D)	107.8
O(20)#14-Nd(6)-O(27)#14	90.4(2)	H(56C)-C(56')-H(56D)	107.2
O(32)-Nd(6)-O(40)	75.3(3)	C(56')-C(57')-H(57D)	109.5
O(34)-Nd(6)-O(40)	133.9(2)	C(56')-C(57')-H(57E)	109.5
O(20)#14-Nd(6)-O(40)	75.7(2)	H(57D)-C(57')-H(57E)	109.5
O(27)#14-Nd(6)-O(40)	70.9(3)	C(56')-C(57')-H(57F)	109.5
O(32)-Nd(6)-O(24)#13	73.5(3)	H(57D)-C(57')-H(57F)	109.5
O(34)-Nd(6)-O(24)#13	89.9(3)	H(57E)-C(57')-H(57F)	109.5
O(20)#14-Nd(6)-O(24)#13	122.7(2)	N(1')-C(58')-C(59')	110(2)
O(27)#14-Nd(6)-O(24)#13	139.0(2)	N(1')-C(58')-H(58C)	109.7
O(40)-Nd(6)-O(24)#13	135.7(3)	C(59')-C(58')-H(58C)	109.7
O(32)-Nd(6)-O(16)	84.4(2)	N(1')-C(58')-H(58D)	109.7
O(34)-Nd(6)-O(16)	128.6(2)	C(59')-C(58')-H(58D)	109.7
O(20)#14-Nd(6)-O(16)	76.1(2)	H(58C)-C(58')-H(58D)	108.2
O(27)#14-Nd(6)-O(16)	141.9(2)	C(58')-C(59')-H(59D)	109.5
O(40)-Nd(6)-O(16)	71.3(2)	C(58')-C(59')-H(59E)	109.5
O(24)#13-Nd(6)-O(16)	75.0(2)	H(59D)-C(59')-H(59E)	109.5
O(32)-Nd(6)-O(42)	69.7(3)	C(58')-C(59')-H(59F)	109.5
O(34)-Nd(6)-O(42)	68.6(3)	H(59D)-C(59')-H(59F)	109.5
O(20)#14-Nd(6)-O(42)	138.9(3)	H(59E)-C(59')-H(59F)	109.5
O(27)#14-Nd(6)-O(42)	70.7(3)	C(60)-O(38)-Nd(3)	127.8(7)
O(40)-Nd(6)-O(42)	126.9(2)	C(60)-N(2)-C(63)	120.4(13)
O(24)#13-Nd(6)-O(42)	68.3(3)	C(60)-N(2)-C(61)	118.3(14)
O(16)-Nd(6)-O(42)	139.6(3)	C(63)-N(2)-C(61)	119.9(13)
O(32)-Nd(6)-O(23)#13	117.3(2)	O(38)-C(60)-N(2)	123.5(12)
O(34)-Nd(6)-O(23)#13	69.8(2)	O(38)-C(60)-H(60)	118.2
O(20)#14-Nd(6)-O(23)#13	75.2(2)	N(2)-C(60)-H(60)	118.2

O(27)#14-Nd(6)-O(23)#13	147.0(2)	C(62)-C(61)-N(2)	111.5(18)
O(40)-Nd(6)-O(23)#13	130.9(2)	C(62)-C(61)-H(61A)	109.3
O(24)#13-Nd(6)-O(23)#13	47.7(2)	N(2)-C(61)-H(61A)	109.3
O(16)-Nd(6)-O(23)#13	63.8(2)	C(62)-C(61)-H(61B)	109.3
O(42)-Nd(6)-O(23)#13	100.7(2)	N(2)-C(61)-H(61B)	109.3
O(32)-Nd(6)-C(36)#13	94.0(3)	H(61A)-C(61)-H(61B)	108.0
O(34)-Nd(6)-C(36)#13	81.4(2)	C(61)-C(62)-H(62A)	109.5
O(20)#14-Nd(6)-C(36)#13	99.5(3)	C(61)-C(62)-H(62B)	109.5
O(27)#14-Nd(6)-C(36)#13	152.6(3)	H(62A)-C(62)-H(62B)	109.5
O(40)-Nd(6)-C(36)#13	136.3(3)	C(61)-C(62)-H(624)	109.5
O(24)#13-Nd(6)-C(36)#13	23.2(3)	H(62A)-C(62)-H(624)	109.5
O(16)-Nd(6)-C(36)#13	65.5(3)	H(62B)-C(62)-H(624)	109.5
O(42)-Nd(6)-C(36)#13	85.4(3)	N(2)-C(63)-C(64)	110.2(18)
O(23)#13-Nd(6)-C(36)#13	24.6(2)	N(2)-C(63)-H(63A)	109.6
C(55)-N(1)-C(56)	117(2)	C(64)-C(63)-H(63A)	109.6
C(55)-N(1)-C(58)	113(2)	N(2)-C(63)-H(63B)	109.6
C(56)-N(1)-C(58)	131(3)	C(64)-C(63)-H(63B)	109.6
O(37)-C(55)-N(1)	123(3)	H(63A)-C(63)-H(63B)	108.1
O(37)-C(55)-H(55)	118.5	C(63)-C(64)-H(64A)	109.5
N(1)-C(55)-H(55)	118.5	C(63)-C(64)-H(64B)	109.5
N(1)-C(56)-C(57)	112(3)	H(64A)-C(64)-H(64B)	109.5
N(1)-C(56)-H(56A)	109.1	C(63)-C(64)-H(64C)	109.5
C(57)-C(56)-H(56A)	109.1	H(64A)-C(64)-H(64C)	109.5
N(1)-C(56)-H(56B)	109.1	H(64B)-C(64)-H(64C)	109.5
C(57)-C(56)-H(56B)	109.1	C(65)-N(3)-C(66)	118(2)
H(56A)-C(56)-H(56B)	107.9	C(65)-N(3)-C(68)	120.0(18)
C(56)-C(57)-H(57A)	109.5	C(66)-N(3)-C(68)	120(2)
C(56)-C(57)-H(57B)	109.5	O(39)-C(65)-N(3)	124(3)
H(57A)-C(57)-H(57B)	109.5	O(39)-C(65)-H(65)	118.0
C(56)-C(57)-H(57C)	109.5	N(3)-C(65)-H(65)	118.0
H(57A)-C(57)-H(57C)	109.5	N(3)-C(66)-C(67)	111(2)
H(57B)-C(57)-H(57C)	109.5	N(3)-C(66)-H(66A)	109.4
N(1)-C(58)-C(59)	104(2)	C(67)-C(66)-H(66A)	109.4
N(1)-C(58)-H(58A)	110.9	N(3)-C(66)-H(66B)	109.4
C(59)-C(58)-H(58A)	110.9	C(67)-C(66)-H(66B)	109.4
N(1)-C(58)-H(58B)	110.9	H(66A)-C(66)-H(66B)	108.0

C(59)-C(58)-H(58B)	110.9	C(66)-C(67)-H(67A)	109.5
H(58A)-C(58)-H(58B)	108.9	C(66)-C(67)-H(67B)	109.5
C(58)-C(59)-H(59A)	109.5	H(67A)-C(67)-H(67B)	109.5
N(4)-C(73)-C(74)	109.2(16)	C(66)-C(67)-H(67C)	109.5
N(4)-C(73)-H(73A)	109.8	H(67A)-C(67)-H(67C)	109.5
C(74)-C(73)-H(73A)	109.8	H(67B)-C(67)-H(67C)	109.5
N(4)-C(73)-H(73B)	109.8	N(3)-C(68)-C(69)	112(2)
C(74)-C(73)-H(73B)	109.8	N(3)-C(68)-H(68A)	109.2
H(73A)-C(73)-H(73B)	108.3	C(69)-C(68)-H(68A)	109.2
C(73)-C(74)-H(74A)	109.5	N(3)-C(68)-H(68B)	109.2
C(73)-C(74)-H(74B)	109.5	C(69)-C(68)-H(68B)	109.2
H(74A)-C(74)-H(74B)	109.5	H(68A)-C(68)-H(68B)	107.9
C(73)-C(74)-H(74C)	109.5	C(68)-C(69)-H(69A)	109.5
H(74A)-C(74)-H(74C)	109.5	C(68)-C(69)-H(69B)	109.5
H(74B)-C(74)-H(74C)	109.5	H(69A)-C(69)-H(69B)	109.5
C(76)-N(5)-C(78)	110(3)	C(68)-C(69)-H(69C)	109.5
C(76)-N(5)-C(75)	125(2)	H(69A)-C(69)-H(69C)	109.5
C(78)-N(5)-C(75)	124(2)	H(69B)-C(69)-H(69C)	109.5
O(41)-C(75)-N(5)	117(3)	C(65')-N(3')-C(68')	120.1(17)
O(41)-C(75)-H(75)	121.3	C(65')-N(3')-C(66')	117.3(16)
N(5)-C(75)-H(75)	121.3	C(68')-N(3')-C(66')	120.9(18)
N(5)-C(76)-C(77)	120(4)	O(39)-C(65')-N(3')	120(2)
N(5)-C(76)-H(76A)	107.2	O(39)-C(65')-H(65')	120.2
C(77)-C(76)-H(76A)	107.2	N(3')-C(65')-H(65')	120.2
N(5)-C(76)-H(76B)	107.3	N(3')-C(66')-C(67')	108.9(19)
C(77)-C(76)-H(76B)	107.3	N(3')-C(66')-H(66C)	109.9
H(76A)-C(76)-H(76B)	106.9	C(67')-C(66')-H(66C)	109.9
C(76)-C(77)-H(77A)	109.5	N(3')-C(66')-H(66D)	109.9
C(76)-C(77)-H(77B)	109.5	C(67')-C(66')-H(66D)	109.9
H(77A)-C(77)-H(77B)	109.5	H(66C)-C(66')-H(66D)	108.3
C(76)-C(77)-H(77C)	109.5	C(66')-C(67')-H(67D)	109.5
H(77A)-C(77)-H(77C)	109.5	C(66')-C(67')-H(67E)	109.5
H(77B)-C(77)-H(77C)	109.5	H(67D)-C(67')-H(67E)	109.5
N(5)-C(78)-C(79)	101(3)	C(66')-C(67')-H(67F)	109.5
N(5)-C(78)-H(78A)	111.6	H(67D)-C(67')-H(67F)	109.5
C(79)-C(78)-H(78A)	111.6	H(67E)-C(67')-H(67F)	109.5

N(5)-C(78)-H(78B)	111.5	N(3')-C(68')-C(69')	110(2)
C(79)-C(78)-H(78B)	111.5	N(3')-C(68')-H(68C)	109.7
H(78A)-C(78)-H(78B)	109.3	C(69')-C(68')-H(68C)	109.7
C(78)-C(79)-H(79A)	109.5	N(3')-C(68')-H(68D)	109.7
C(78)-C(79)-H(79B)	109.5	C(69')-C(68')-H(68D)	109.7
H(79A)-C(79)-H(79B)	109.5	H(68C)-C(68')-H(68D)	108.2
C(78)-C(79)-H(79C)	109.4	C(68')-C(69')-H(69D)	109.5
H(79A)-C(79)-H(79C)	109.5	C(68')-C(69')-H(69E)	109.5
H(79B)-C(79)-H(79C)	109.5	H(69D)-C(69')-H(69E)	109.5
C(75')-N(5')-C(78')	125(2)	C(68')-C(69')-H(69F)	109.5
C(75')-N(5')-C(76')	125(2)	H(69D)-C(69')-H(69F)	109.5
C(78')-N(5')-C(76')	107(2)	H(69E)-C(69')-H(69F)	109.5
O(41)-C(75')-N(5')	123(2)	C(70)-O(40)-Nd(6)	126.2(7)
O(41)-C(75')-H(75')	118.3	C(70)-N(4)-C(71)	123.2(13)
N(5')-C(75')-H(75')	118.3	C(70)-N(4)-C(73)	118.8(11)
N(5')-C(76')-C(77')	122(3)	C(71)-N(4)-C(73)	117.9(12)
N(5')-C(76')-H(76C)	106.8	O(40)-C(70)-N(4)	123.3(11)
C(77')-C(76')-H(76C)	106.8	O(40)-C(70)-H(70)	118.4
N(5')-C(76')-H(76D)	106.8	N(4)-C(70)-H(70)	118.4
C(77')-C(76')-H(76D)	106.8	N(4)-C(71)-C(72)	115.1(15)
H(76C)-C(76')-H(76D)	106.6	N(4)-C(71)-H(71A)	108.5
C(76')-C(77')-H(77D)	109.5	C(72)-C(71)-H(71A)	108.5
C(76')-C(77')-H(77E)	109.5	N(4)-C(71)-H(71B)	108.5
H(77D)-C(77')-H(77E)	109.5	C(72)-C(71)-H(71B)	108.5
C(76')-C(77')-H(77F)	109.5	H(71A)-C(71)-H(71B)	107.5
H(77D)-C(77')-H(77F)	109.5	C(71)-C(72)-H(72A)	109.5
H(77E)-C(77')-H(77F)	109.5	C(71)-C(72)-H(72B)	109.5
N(5')-C(78')-C(79')	104(3)	H(72A)-C(72)-H(72B)	109.5
N(5')-C(78')-H(78C)	111.0	C(71)-C(72)-H(72C)	109.5
C(79')-C(78')-H(78C)	111.0	H(72A)-C(72)-H(72C)	109.5
N(5')-C(78')-H(78D)	111.0	H(72B)-C(72)-H(72C)	109.5
C(79')-C(78')-H(78D)	111.0	H(79D)-C(79')-H(79F)	109.5
H(78C)-C(78')-H(78D)	109.0	H(79E)-C(79')-H(79F)	109.5
C(78')-C(79')-H(79D)	109.5	C(55)-O(37)-Nd(1)	128.3(17)
C(78')-C(79')-H(79E)	109.5	C(55')-O(37)-Nd(1)	130.8(18)
H(79D)-C(79')-H(79E)	109.5	C(65')-O(39)-Nd(4)	128.8(12)

C(78')-C(79')-H(79F)	109.5	C(65)-O(39)-Nd(4)	122.9(18)
C(75)-O(41)-Nd(5)	150(2)	C(75')-O(41)-Nd(5)	129.3(16)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z+1 #2 x,y+1,z #3 x,y-1,z-1 #4 -x+1,-y+1,z-1/2
#5 -x+1,-y+2,z-1/2 #6 -x+1,-y+2,z+1/2 #7 x,y+1,z+1
#8 -x+3/2,y-1/2,z+1/2 #9 -x+3/2,y-1/2,z-1/2
#10 -x+1,-y+1,z+1/2 #11 -x+3/2,y+1/2,z-1/2 #12 -x+3/2,y+1/2,z+1/2
#13 x,y-1,z #14 x,y,z-1

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C(1)-O(2)	1.241(8)	C(44)-C(45)	1.366(9)
C(1)-O(1)	1.263(8)	C(44)-S(8)	1.712(6)
C(1)-C(2)	1.475(8)	C(45)-C(46)	1.406(9)
C(2)-C(3)	1.352(10)	C(45)-H(45)	0.9300
C(2)-S(1)	1.701(7)	C(46)-C(47)	1.357(9)
C(3)-C(4)	1.417(10)	C(46)-H(46)	0.9300
C(3)-H(3)	0.9300	C(47)-C(48)	1.496(9)
C(4)-C(5)	1.342(10)	C(47)-S(8)	1.712(6)
C(4)-H(4)	0.9300	C(48)-O(31)	1.222(8)
C(5)-C(6)	1.484(9)	C(48)-O(32)	1.253(8)
C(5)-S(1)	1.699(6)	C(49)-O(33)	1.250(8)
C(6)-O(3)	1.229(8)	C(49)-O(34)	1.250(8)
C(6)-O(4)	1.262(8)	C(49)-C(50)	1.496(8)
C(7)-O(6)	1.241(9)	C(50)-C(51)	1.359(9)
C(7)-O(5)	1.246(8)	C(50)-S(9)	1.700(6)
C(7)-C(8)	1.489(9)	C(51)-C(52)	1.412(9)

C(7)-Sm(2)	2.944(7)	C(51)-H(51)	0.9300
C(8)-C(9)	1.353(10)	C(52)-C(53)	1.365(9)
C(8)-S(2)	1.708(7)	C(52)-H(52)	0.9300
C(9)-C(10)	1.419(10)	C(53)-C(54)	1.473(9)
C(9)-H(9)	0.9300	C(53)-S(9)	1.709(6)
C(10)-C(11)	1.336(10)	C(54)-O(36)	1.249(8)
C(10)-H(10)	0.9300	C(54)-O(35)	1.249(9)
C(11)-C(12)	1.476(9)	C(54)-Sm(3)#3	3.022(7)
C(11)-S(2)	1.713(7)	O(1)-Sm(2)	2.385(4)
C(12)-O(7)	1.231(8)	O(2)-Sm(1)	2.338(4)
C(12)-O(8)	1.254(8)	O(3)-Sm(1)#4	2.399(4)
C(13)-O(9)	1.243(9)	O(4)-Sm(2)#4	2.297(4)
C(13)-O(10)	1.261(8)	O(5)-Sm(1)	2.473(4)
C(13)-C(14)	1.481(9)	O(5)-Sm(2)	2.759(5)
C(14)-C(15)	1.342(10)	O(6)-Sm(2)	2.421(5)
C(14)-S(3)	1.707(7)	O(7)-Sm(1)#5	2.344(5)
C(15)-C(16)	1.406(10)	O(8)-Sm(5)#2	2.394(4)
C(15)-H(15)	0.9300	O(9)-Sm(1)	2.462(4)
C(16)-C(17)	1.340(10)	O(10)-Sm(2)	2.328(4)
C(16)-H(16)	0.9300	O(11)-Sm(1)#6	2.425(5)
C(17)-C(18)	1.497(9)	O(12)-Sm(5)#7	2.294(4)
C(17)-S(3)	1.689(7)	O(13)-Sm(2)	2.310(4)
C(18)-O(12)	1.248(9)	O(14)-Sm(3)	2.414(4)
C(18)-O(11)	1.253(9)	O(15)-Sm(5)	2.382(4)
C(19)-O(14)	1.246(9)	O(16)-Sm(6)	2.483(4)
C(19)-O(13)	1.257(8)	O(17)-Sm(2)	2.434(4)
C(19)-C(20)	1.488(10)	O(18)-Sm(3)	2.312(4)
C(20)-C(21)	1.352(9)	O(19)-Sm(3)	2.655(4)
C(20)-S(4)	1.707(7)	O(19)-Sm(2)	2.664(4)
C(21)-C(22)	1.407(9)	O(19)-H(19A)	0.84(3)
C(21)-H(21)	0.9300	O(19)-H(19B)	0.83(3)
C(22)-C(23)	1.367(9)	O(20)-Sm(6)#1	2.389(4)
C(22)-H(22)	0.9300	O(20)-Sm(5)#1	2.812(4)
C(23)-C(24)	1.480(8)	O(21)-Sm(3)	2.384(4)
C(23)-S(4)	1.706(6)	O(22)-Sm(4)	2.422(4)
C(24)-O(16)	1.241(8)	O(23)-Sm(5)#2	2.328(4)

C(24)-O(15)	1.277(8)	O(23)-Sm(6)#2	2.896(5)
C(25)-O(17)	1.246(8)	O(24)-Sm(6)#2	2.450(5)
C(25)-O(18)	1.244(8)	O(25)-Sm(3)	2.448(4)
C(25)-C(26)	1.481(9)	O(26)-Sm(4)	2.366(4)
C(26)-C(27)	1.354(10)	O(27)-Sm(6)#1	2.408(4)
C(26)-S(5)	1.722(7)	O(28)-Sm(4)#8	2.286(4)
C(27)-C(28)	1.413(9)	O(29)-Sm(3)	2.356(4)
C(27)-H(27)	0.9300	O(29)-Sm(4)	2.857(4)
C(28)-C(29)	1.352(9)	O(30)-Sm(4)	2.470(4)
C(28)-H(28)	0.9300	O(31)-Sm(4)#9	2.412(4)
C(29)-C(30)	1.471(8)	O(32)-Sm(6)	2.309(5)
C(29)-S(5)	1.715(6)	O(33)-Sm(5)	2.378(4)
C(30)-O(20)	1.255(7)	O(34)-Sm(6)	2.379(4)
C(30)-O(43)	1.259(8)	O(35)-Sm(3)#3	2.473(5)
C(30)-Sm(5)#1	3.004(6)	O(36)-Sm(4)#3	2.339(4)
C(31)-O(22)	1.251(8)	O(36)-Sm(3)#3	2.854(5)
C(31)-O(21)	1.249(8)	O(42)-Sm(6)	2.585(4)
C(31)-C(32)	1.490(8)	O(42)-H(42B)	0.84(3)
C(32)-C(33)	1.374(9)	O(42)-H(42A)	0.86(3)
C(32)-S(6)	1.704(6)	O(43)-Sm(5)#1	2.468(4)
C(33)-C(34)	1.425(9)	O(44)-Sm(1)	2.540(4)
C(33)-H(33)	0.9300	O(44)-H(44A)	0.85(3)
C(34)-C(35)	1.349(10)	O(44)-H(44B)	0.85(3)
C(34)-H(34)	0.9300	Sm(1)-O(7)#6	2.344(5)
C(35)-C(36)	1.474(9)	Sm(1)-O(3)#10	2.399(4)
C(35)-S(6)	1.710(6)	Sm(1)-O(11)#5	2.425(5)
C(36)-O(24)	1.250(9)	Sm(1)-O(37)	2.432(4)
C(36)-O(23)	1.265(8)	Sm(2)-O(4)#10	2.297(4)
C(36)-Sm(6)#2	3.039(7)	Sm(3)-O(38)	2.463(5)
C(37)-O(25)	1.260(8)	Sm(3)-O(35)#7	2.473(5)
C(37)-O(26)	1.262(8)	Sm(3)-O(36)#7	2.854(5)
C(37)-C(38)	1.470(8)	Sm(3)-C(54)#7	3.022(7)
C(38)-C(39)	1.357(10)	Sm(4)-O(28)#11	2.286(4)
C(38)-S(7)	1.711(6)	Sm(4)-O(36)#7	2.340(4)
C(39)-C(40)	1.410(9)	Sm(4)-O(31)#12	2.412(4)
C(39)-H(39)	0.9300	Sm(4)-O(39)	2.432(5)

C(40)-C(41)	1.351(10)	Sm(5)-O(12)#3	2.294(4)
C(40)-H(40)	0.9300	Sm(5)-O(23)#13	2.328(4)
C(41)-C(42)	1.475(9)	Sm(5)-O(8)#13	2.394(4)
C(41)-S(7)	1.704(7)	Sm(5)-O(41)	2.421(4)
C(42)-O(27)	1.239(8)	Sm(5)-O(43)#14	2.468(4)
C(42)-O(28)	1.258(8)	Sm(5)-O(20)#14	2.812(4)
C(43)-O(30)	1.255(8)	Sm(5)-C(30)#14	3.004(6)
C(43)-O(29)	1.258(8)	Sm(6)-O(20)#14	2.389(4)
C(43)-C(44)	1.474(8)	Sm(6)-O(27)#14	2.408(4)
C(43)-Sm(4)	3.018(6)	Sm(6)-O(40)	2.447(5)
C(57)-H(57C)	0.9600	Sm(6)-O(24)#13	2.450(5)
C(58)-C(59)	1.60(3)	Sm(6)-O(23)#13	2.896(5)
C(58)-H(58A)	0.9700	Sm(6)-C(36)#13	3.039(7)
C(58)-H(58B)	0.9700	N(1)-C(55)	1.39(2)
C(59)-H(59A)	0.9600	N(1)-C(56)	1.42(2)
C(59)-H(59B)	0.9600	N(1)-C(58)	1.53(2)
C(59)-H(59C)	0.9600	C(55)-O(37)	1.22(2)
N(1')-C(55')	1.382(19)	C(55)-H(55)	0.9300
N(1')-C(56')	1.45(2)	C(56)-C(57)	1.50(3)
N(1')-C(58')	1.47(2)	C(56)-H(56A)	0.9700
C(55')-O(37)	1.17(2)	C(56)-H(56B)	0.9700
C(55')-H(55')	0.9300	C(57)-H(57A)	0.9600
C(56')-C(57')	1.47(2)	C(57)-H(57B)	0.9600
C(56')-H(56C)	0.9700	C(76)-H(76A)	0.9700
C(56')-H(56D)	0.9700	C(76)-H(76B)	0.9700
C(57')-H(57D)	0.9600	C(77)-H(77A)	0.9600
C(57')-H(57E)	0.9600	C(77)-H(77B)	0.9600
C(57')-H(57F)	0.9600	C(77)-H(77C)	0.9600
C(58')-C(59')	1.53(2)	C(78)-C(79)	1.52(3)
C(58')-H(58C)	0.9700	C(78)-H(78A)	0.9700
C(58')-H(58D)	0.9700	C(78)-H(78B)	0.9700
C(59')-H(59D)	0.9600	C(79)-H(79A)	0.9600
C(59')-H(59E)	0.9600	C(79)-H(79B)	0.9600
C(59')-H(59F)	0.9600	C(79)-H(79C)	0.9600
O(38)-C(60)	1.215(9)	N(5')-C(75')	1.353(19)
N(2)-C(60)	1.341(10)	N(5')-C(76')	1.48(2)

N(2)-C(63)	1.467(14)	N(5')-C(78')	1.50(2)
N(2)-C(61)	1.515(13)	C(75')-O(41)	1.154(15)
C(60)-H(60)	0.9300	C(75')-H(75')	0.9300
C(61)-C(62)	1.475(18)	C(76')-C(77')	1.47(2)
C(61)-H(61A)	0.9700	C(76')-H(76C)	0.9700
C(61)-H(61B)	0.9700	C(76')-H(76D)	0.9700
C(62)-H(62A)	0.9600	C(77')-H(77D)	0.9600
C(62)-H(62B)	0.9600	C(77')-H(77E)	0.9600
C(62)-H(624)	0.9600	C(77')-H(77F)	0.9600
C(63)-C(64)	1.462(16)	C(78')-C(79')	1.52(2)
C(63)-H(63A)	0.9700	C(78')-H(78C)	0.9700
C(63)-H(63B)	0.9700	C(78')-H(78D)	0.9700
C(64)-H(64A)	0.9600	C(79')-H(79D)	0.9600
C(64)-H(64B)	0.9600	C(79')-H(79E)	0.9600
C(64)-H(64C)	0.9600	C(79')-H(79F)	0.9600
N(3)-C(65)	1.39(2)	C(69')-H(69E)	0.9600
N(3)-C(66)	1.44(2)	C(69')-H(69F)	0.9600
N(3)-C(68)	1.489(19)	O(40)-C(70)	1.224(8)
C(65)-O(39)	1.219(17)	N(4)-C(70)	1.313(9)
C(65)-H(65)	0.9300	N(4)-C(71)	1.463(12)
C(66)-C(67)	1.54(2)	N(4)-C(73)	1.478(13)
C(66)-H(66A)	0.9700	C(70)-H(70)	0.9300
C(66)-H(66B)	0.9700	C(71)-C(72)	1.439(16)
C(67)-H(67A)	0.9600	C(71)-H(71A)	0.9700
C(67)-H(67B)	0.9600	C(71)-H(71B)	0.9700
C(67)-H(67C)	0.9600	C(72)-H(72A)	0.9600
C(68)-C(69)	1.50(2)	C(72)-H(72B)	0.9600
C(68)-H(68A)	0.9700	C(72)-H(72C)	0.9600
C(68)-H(68B)	0.9700	C(73)-C(74)	1.482(16)
C(69)-H(69A)	0.9600	C(73)-H(73A)	0.9700
C(69)-H(69B)	0.9600	C(73)-H(73B)	0.9700
C(69)-H(69C)	0.9600	C(74)-H(74A)	0.9600
N(3')-C(65')	1.381(18)	C(74)-H(74B)	0.9600
N(3')-C(68')	1.457(17)	C(74)-H(74C)	0.9600
N(3')-C(66')	1.471(18)	N(5)-C(75)	1.45(2)
C(65')-O(39)	1.221(14)	N(5)-C(76)	1.45(3)

C(65')-H(65')	0.9300	N(5)-C(78)	1.52(3)
C(66')-C(67')	1.53(2)	C(75)-O(41)	1.15(2)
C(66')-H(66C)	0.9700	C(75)-H(75)	0.9300
C(66')-H(66D)	0.9700	C(76)-C(77)	1.52(3)
C(67')-H(67D)	0.9600	C(68')-H(68C)	0.9700
C(67')-H(67E)	0.9600	C(68')-H(68D)	0.9700
C(67')-H(67F)	0.9600	C(69')-H(69D)	0.9600
C(68')-C(69')	1.54(2)	C(29)-C(30)-Sm(5)#1	167.1(4)
O(2)-C(1)-O(1)	125.5(6)	O(22)-C(31)-O(21)	126.9(6)
O(2)-C(1)-C(2)	115.9(6)	O(22)-C(31)-C(32)	116.4(6)
O(1)-C(1)-C(2)	118.5(6)	O(21)-C(31)-C(32)	116.7(6)
C(3)-C(2)-C(1)	125.8(6)	C(33)-C(32)-C(31)	126.1(6)
C(3)-C(2)-S(1)	111.6(5)	C(33)-C(32)-S(6)	112.1(5)
C(1)-C(2)-S(1)	122.6(5)	C(31)-C(32)-S(6)	121.6(5)
C(2)-C(3)-C(4)	112.6(7)	C(32)-C(33)-C(34)	111.5(6)
C(2)-C(3)-H(3)	123.7	C(32)-C(33)-H(33)	124.2
C(4)-C(3)-H(3)	123.7	C(34)-C(33)-H(33)	124.2
C(5)-C(4)-C(3)	111.8(7)	C(35)-C(34)-C(33)	112.4(6)
C(5)-C(4)-H(4)	124.1	C(35)-C(34)-H(34)	123.8
C(3)-C(4)-H(4)	124.1	C(33)-C(34)-H(34)	123.8
C(4)-C(5)-C(6)	127.1(6)	C(34)-C(35)-C(36)	127.8(6)
C(4)-C(5)-S(1)	112.5(5)	C(34)-C(35)-S(6)	112.5(5)
C(6)-C(5)-S(1)	120.3(5)	C(36)-C(35)-S(6)	119.7(5)
O(3)-C(6)-O(4)	125.5(6)	O(24)-C(36)-O(23)	121.6(6)
O(3)-C(6)-C(5)	118.0(6)	O(24)-C(36)-C(35)	119.6(6)
O(4)-C(6)-C(5)	116.4(6)	O(23)-C(36)-C(35)	118.8(7)
O(6)-C(7)-O(5)	122.5(6)	O(24)-C(36)-Sm(6)#2	50.9(3)
O(6)-C(7)-C(8)	118.2(6)	O(23)-C(36)-Sm(6)#2	71.4(4)
O(5)-C(7)-C(8)	119.3(7)	C(35)-C(36)-Sm(6)#2	166.9(5)
O(6)-C(7)-Sm(2)	53.5(3)	O(25)-C(37)-O(26)	125.7(6)
O(5)-C(7)-Sm(2)	69.2(4)	O(25)-C(37)-C(38)	117.7(6)
C(8)-C(7)-Sm(2)	170.4(5)	O(26)-C(37)-C(38)	116.5(6)
C(9)-C(8)-C(7)	129.0(6)	C(39)-C(38)-C(37)	128.5(6)
C(9)-C(8)-S(2)	111.4(5)	C(39)-C(38)-S(7)	111.4(5)
C(7)-C(8)-S(2)	119.6(5)	C(37)-C(38)-S(7)	120.1(5)
C(8)-C(9)-C(10)	112.3(7)	C(38)-C(39)-C(40)	112.2(6)

C(8)-C(9)-H(9)	123.8	C(38)-C(39)-H(39)	123.9
C(10)-C(9)-H(9)	123.8	C(40)-C(39)-H(39)	123.9
C(11)-C(10)-C(9)	112.9(7)	C(41)-C(40)-C(39)	113.1(6)
C(11)-C(10)-H(10)	123.5	C(41)-C(40)-H(40)	123.5
C(9)-C(10)-H(10)	123.5	C(39)-C(40)-H(40)	123.5
C(10)-C(11)-C(12)	126.4(6)	C(40)-C(41)-C(42)	127.3(6)
C(10)-C(11)-S(2)	111.6(5)	C(40)-C(41)-S(7)	111.4(5)
C(12)-C(11)-S(2)	122.0(5)	C(42)-C(41)-S(7)	121.2(5)
O(7)-C(12)-O(8)	125.4(6)	O(27)-C(42)-O(28)	125.3(6)
O(7)-C(12)-C(11)	117.0(7)	O(27)-C(42)-C(41)	119.3(6)
O(8)-C(12)-C(11)	117.6(6)	O(28)-C(42)-C(41)	115.4(6)
O(9)-C(13)-O(10)	127.5(6)	O(30)-C(43)-O(29)	122.9(6)
O(9)-C(13)-C(14)	117.6(6)	O(30)-C(43)-C(44)	118.3(6)
O(10)-C(13)-C(14)	115.0(6)	O(29)-C(43)-C(44)	118.8(6)
C(15)-C(14)-C(13)	128.3(7)	O(30)-C(43)-Sm(4)	52.7(3)
C(15)-C(14)-S(3)	110.3(5)	O(29)-C(43)-Sm(4)	70.5(3)
C(13)-C(14)-S(3)	121.2(5)	C(44)-C(43)-Sm(4)	168.6(5)
C(14)-C(15)-C(16)	113.3(7)	C(45)-C(44)-C(43)	127.0(6)
C(14)-C(15)-H(15)	123.4	C(45)-C(44)-S(8)	111.5(5)
C(16)-C(15)-H(15)	123.4	C(43)-C(44)-S(8)	121.5(5)
C(17)-C(16)-C(15)	112.7(7)	C(44)-C(45)-C(46)	112.2(6)
C(17)-C(16)-H(16)	123.7	C(44)-C(45)-H(45)	123.9
C(15)-C(16)-H(16)	123.7	C(46)-C(45)-H(45)	123.9
C(16)-C(17)-C(18)	127.0(7)	C(47)-C(46)-C(45)	113.1(6)
C(16)-C(17)-S(3)	111.3(5)	C(47)-C(46)-H(46)	123.4
C(18)-C(17)-S(3)	121.4(5)	C(45)-C(46)-H(46)	123.4
O(12)-C(18)-O(11)	126.3(6)	C(46)-C(47)-C(48)	125.4(6)
O(12)-C(18)-C(17)	115.4(7)	C(46)-C(47)-S(8)	111.4(5)
O(11)-C(18)-C(17)	118.3(6)	C(48)-C(47)-S(8)	123.0(5)
O(14)-C(19)-O(13)	126.2(6)	O(31)-C(48)-O(32)	126.6(6)
O(14)-C(19)-C(20)	118.1(6)	O(31)-C(48)-C(47)	119.6(6)
O(13)-C(19)-C(20)	115.6(6)	O(32)-C(48)-C(47)	113.7(6)
C(21)-C(20)-C(19)	127.2(6)	O(33)-C(49)-O(34)	127.0(6)
C(21)-C(20)-S(4)	111.4(5)	O(33)-C(49)-C(50)	117.2(6)
C(19)-C(20)-S(4)	121.3(5)	O(34)-C(49)-C(50)	115.8(6)
C(20)-C(21)-C(22)	113.6(6)	C(51)-C(50)-C(49)	126.7(6)

C(20)-C(21)-H(21)	123.2	C(51)-C(50)-S(9)	112.1(5)
C(22)-C(21)-H(21)	123.2	C(49)-C(50)-S(9)	121.2(5)
C(23)-C(22)-C(21)	111.3(6)	C(50)-C(51)-C(52)	112.4(6)
C(23)-C(22)-H(22)	124.3	C(50)-C(51)-H(51)	123.8
C(21)-C(22)-H(22)	124.3	C(52)-C(51)-H(51)	123.8
C(22)-C(23)-C(24)	128.5(6)	C(53)-C(52)-C(51)	112.2(6)
C(22)-C(23)-S(4)	112.1(5)	C(53)-C(52)-H(52)	123.9
C(24)-C(23)-S(4)	119.3(5)	C(51)-C(52)-H(52)	123.9
O(16)-C(24)-O(15)	124.8(6)	C(52)-C(53)-C(54)	128.0(6)
O(16)-C(24)-C(23)	119.3(6)	C(52)-C(53)-S(9)	111.7(5)
O(15)-C(24)-C(23)	115.7(6)	C(54)-C(53)-S(9)	120.3(5)
O(17)-C(25)-O(18)	125.0(6)	O(36)-C(54)-O(35)	122.2(6)
O(17)-C(25)-C(26)	120.8(6)	O(36)-C(54)-C(53)	119.3(6)
O(18)-C(25)-C(26)	114.3(6)	O(35)-C(54)-C(53)	118.5(6)
C(27)-C(26)-C(25)	124.8(6)	O(36)-C(54)-Sm(3)#3	70.3(4)
C(27)-C(26)-S(5)	110.4(5)	O(35)-C(54)-Sm(3)#3	52.7(3)
C(25)-C(26)-S(5)	124.7(5)	C(53)-C(54)-Sm(3)#3	167.4(5)
C(26)-C(27)-C(28)	113.7(6)	C(1)-O(1)-Sm(2)	128.3(4)
C(26)-C(27)-H(27)	123.2	C(1)-O(2)-Sm(1)	147.3(5)
C(28)-C(27)-H(27)	123.2	C(6)-O(3)-Sm(1)#4	117.3(4)
C(29)-C(28)-C(27)	112.5(6)	C(6)-O(4)-Sm(2)#4	165.6(5)
C(29)-C(28)-H(28)	123.8	C(7)-O(5)-Sm(1)	165.4(5)
C(27)-C(28)-H(28)	123.8	C(7)-O(5)-Sm(2)	85.8(4)
C(28)-C(29)-C(30)	126.8(6)	Sm(1)-O(5)-Sm(2)	107.66(15)
C(28)-C(29)-S(5)	111.4(5)	C(7)-O(6)-Sm(2)	102.2(4)
C(30)-C(29)-S(5)	121.8(5)	C(12)-O(7)-Sm(1)#5	169.2(5)
O(20)-C(30)-O(43)	121.7(5)	C(12)-O(8)-Sm(5)#2	132.8(4)
O(20)-C(30)-C(29)	120.2(6)	C(13)-O(9)-Sm(1)	143.3(4)
O(43)-C(30)-C(29)	118.1(5)	C(13)-O(10)-Sm(2)	133.3(5)
O(20)-C(30)-Sm(5)#1	69.1(3)	C(18)-O(11)-Sm(1)#6	123.3(4)
O(43)-C(30)-Sm(5)#1	53.3(3)	C(18)-O(12)-Sm(5)#7	144.0(5)
C(36)-O(23)-Sm(6)#2	84.1(4)	C(19)-O(13)-Sm(2)	141.7(5)
Sm(5)#2-O(23)-Sm(6)#2	103.16(15)	C(19)-O(14)-Sm(3)	131.8(4)
C(36)-O(24)-Sm(6)#2	105.8(4)	C(24)-O(15)-Sm(5)	133.2(4)
C(37)-O(25)-Sm(3)	138.0(4)	C(24)-O(16)-Sm(6)	140.5(4)
C(37)-O(26)-Sm(4)	134.2(4)	C(25)-O(17)-Sm(2)	129.5(4)

C(42)-O(27)-Sm(6)#1	134.4(4)	C(25)-O(18)-Sm(3)	167.6(5)
C(42)-O(28)-Sm(4)#8	147.9(4)	Sm(3)-O(19)-Sm(2)	124.35(13)
C(43)-O(29)-Sm(3)	170.5(4)	Sm(3)-O(19)-H(19A)	94(5)
C(43)-O(29)-Sm(4)	84.9(4)	Sm(2)-O(19)-H(19A)	110(6)
Sm(3)-O(29)-Sm(4)	104.47(14)	Sm(3)-O(19)-H(19B)	110(5)
C(43)-O(30)-Sm(4)	103.4(4)	Sm(2)-O(19)-H(19B)	106(5)
C(48)-O(31)-Sm(4)#9	134.1(4)	H(19A)-O(19)-H(19B)	112(4)
C(48)-O(32)-Sm(6)	162.0(5)	C(30)-O(20)-Sm(6)#1	169.7(4)
C(49)-O(33)-Sm(5)	134.5(4)	C(30)-O(20)-Sm(5)#1	86.3(3)
C(49)-O(34)-Sm(6)	138.1(4)	Sm(6)#1-O(20)-Sm(5)#1	104.03(14)
C(54)-O(35)-Sm(3)#3	103.6(4)	C(31)-O(21)-Sm(3)	136.7(4)
C(54)-O(36)-Sm(4)#3	169.1(4)	C(31)-O(22)-Sm(4)	134.9(4)
C(54)-O(36)-Sm(3)#3	85.4(4)	C(36)-O(23)-Sm(5)#2	167.9(5)
Sm(4)#3-O(36)-Sm(3)#3	105.01(14)	O(2)-Sm(1)-O(11)#5	81.57(17)
Sm(6)-O(42)-H(42B)	118(4)	O(7)#6-Sm(1)-O(11)#5	99.36(19)
Sm(6)-O(42)-H(42A)	128(6)	O(3)#10-Sm(1)-O(11)#5	145.84(18)
H(42B)-O(42)-H(42A)	110(4)	O(2)-Sm(1)-O(37)	138.7(2)
C(30)-O(43)-Sm(5)#1	102.5(4)	O(7)#6-Sm(1)-O(37)	78.2(2)
Sm(1)-O(44)-H(44A)	126(6)	O(3)#10-Sm(1)-O(37)	136.9(2)
Sm(1)-O(44)-H(44B)	109(5)	O(11)#5-Sm(1)-O(37)	71.5(2)
H(44A)-O(44)-H(44B)	109(4)	O(2)-Sm(1)-O(9)	118.98(15)
C(5)-S(1)-C(2)	91.5(3)	O(7)#6-Sm(1)-O(9)	86.51(17)
C(8)-S(2)-C(11)	91.7(3)	O(3)#10-Sm(1)-O(9)	73.16(17)
C(17)-S(3)-C(14)	92.5(3)	O(11)#5-Sm(1)-O(9)	140.85(18)
C(23)-S(4)-C(20)	91.5(3)	O(37)-Sm(1)-O(9)	71.96(19)
C(29)-S(5)-C(26)	92.0(3)	O(2)-Sm(1)-O(5)	68.72(16)
C(32)-S(6)-C(35)	91.4(3)	O(7)#6-Sm(1)-O(5)	152.91(19)
C(41)-S(7)-C(38)	91.8(3)	O(3)#10-Sm(1)-O(5)	113.42(15)
C(47)-S(8)-C(44)	91.7(3)	O(11)#5-Sm(1)-O(5)	87.09(16)
C(50)-S(9)-C(53)	91.6(3)	O(37)-Sm(1)-O(5)	78.99(18)
O(2)-Sm(1)-O(7)#6	138.09(19)	O(9)-Sm(1)-O(5)	72.58(15)
O(2)-Sm(1)-O(3)#10	81.21(18)	O(2)-Sm(1)-O(44)	68.11(16)
O(7)#6-Sm(1)-O(3)#10	75.06(19)	O(7)#6-Sm(1)-O(44)	71.71(19)
O(1)-Sm(2)-C(7)	75.06(19)	O(3)#10-Sm(1)-O(44)	71.22(18)
O(6)-Sm(2)-C(7)	24.34(18)	O(11)#5-Sm(1)-O(44)	75.03(18)
O(17)-Sm(2)-C(7)	162.56(19)	O(37)-Sm(1)-O(44)	129.97(16)

O(19)-Sm(2)-C(7)	82.95(18)	O(9)-Sm(1)-O(44)	141.89(18)
O(5)-Sm(2)-C(7)	24.96(17)	O(5)-Sm(1)-O(44)	135.10(17)
O(18)-Sm(3)-O(29)	151.43(17)	O(4)#10-Sm(2)-O(13)	136.91(18)
O(18)-Sm(3)-O(21)	134.86(17)	O(4)#10-Sm(2)-O(10)	78.35(18)
O(29)-Sm(3)-O(21)	73.31(15)	O(13)-Sm(2)-O(10)	138.41(17)
O(18)-Sm(3)-O(14)	92.52(18)	O(4)#10-Sm(2)-O(1)	80.02(16)
O(29)-Sm(3)-O(14)	89.84(15)	O(13)-Sm(2)-O(1)	79.16(16)
O(21)-Sm(3)-O(14)	77.07(17)	O(10)-Sm(2)-O(1)	138.24(16)
O(18)-Sm(3)-O(25)	84.49(16)	O(4)#10-Sm(2)-O(6)	133.45(17)
O(29)-Sm(3)-O(25)	76.64(14)	O(13)-Sm(2)-O(6)	80.06(17)
O(21)-Sm(3)-O(25)	129.15(15)	O(10)-Sm(2)-O(6)	87.08(19)
O(14)-Sm(3)-O(25)	142.76(16)	O(1)-Sm(2)-O(6)	82.49(18)
O(18)-Sm(3)-O(38)	73.31(18)	O(4)#10-Sm(2)-O(17)	77.81(16)
O(29)-Sm(3)-O(38)	80.76(16)	O(13)-Sm(2)-O(17)	82.22(17)
O(21)-Sm(3)-O(38)	138.02(16)	O(10)-Sm(2)-O(17)	87.11(17)
O(14)-Sm(3)-O(38)	70.32(17)	O(1)-Sm(2)-O(17)	122.32(18)
O(25)-Sm(3)-O(38)	73.30(16)	O(6)-Sm(2)-O(17)	145.84(16)
O(18)-Sm(3)-O(35)#7	72.78(18)	O(4)#10-Sm(2)-O(19)	139.52(17)
O(29)-Sm(3)-O(35)#7	123.00(15)	O(13)-Sm(2)-O(19)	72.76(15)
O(21)-Sm(3)-O(35)#7	84.32(17)	O(10)-Sm(2)-O(19)	65.96(15)
O(14)-Sm(3)-O(35)#7	135.47(16)	O(1)-Sm(2)-O(19)	139.93(17)
O(25)-Sm(3)-O(35)#7	78.88(16)	O(6)-Sm(2)-O(19)	65.14(17)
O(38)-Sm(3)-O(35)#7	137.65(17)	O(17)-Sm(2)-O(19)	81.81(16)
O(18)-Sm(3)-O(19)	67.72(16)	O(4)#10-Sm(2)-O(5)	84.27(16)
O(29)-Sm(3)-O(19)	138.99(15)	O(13)-Sm(2)-O(5)	123.46(15)
O(21)-Sm(3)-O(19)	67.37(15)	O(10)-Sm(2)-O(5)	70.71(16)
O(14)-Sm(3)-O(19)	70.76(16)	O(1)-Sm(2)-O(5)	71.94(15)
O(25)-Sm(3)-O(19)	139.01(16)	O(6)-Sm(2)-O(5)	49.26(15)
O(38)-Sm(3)-O(19)	122.35(14)	O(17)-Sm(2)-O(5)	153.94(15)
O(35)#7-Sm(3)-O(19)	64.75(16)	O(19)-Sm(2)-O(5)	100.52(13)
O(18)-Sm(3)-O(36)#7	115.62(15)	O(4)#10-Sm(2)-C(7)	109.12(19)
O(29)-Sm(3)-O(36)#7	75.16(13)	O(13)-Sm(2)-C(7)	101.28(18)
O(21)-Sm(3)-O(36)#7	68.76(14)	O(10)-Sm(2)-C(7)	78.95(19)
O(14)-Sm(3)-O(36)#7	145.32(15)	O(28)#11-Sm(4)-O(22)	88.52(15)
O(25)-Sm(3)-O(36)#7	64.41(14)	O(36)#7-Sm(4)-O(22)	81.05(15)
O(38)-Sm(3)-O(36)#7	134.91(15)	O(26)-Sm(4)-O(22)	131.44(15)

O(35)#7-Sm(3)-O(36)#7	47.84(14)	O(31)#12-Sm(4)-O(22)	143.07(17)
O(19)-Sm(3)-O(36)#7	100.33(12)	O(28)#11-Sm(4)-O(39)	78.75(17)
O(18)-Sm(3)-C(54)#7	93.06(19)	O(36)#7-Sm(4)-O(39)	77.88(17)
O(29)-Sm(3)-C(54)#7	99.41(17)	O(26)-Sm(4)-O(39)	139.11(17)
O(21)-Sm(3)-C(54)#7	77.51(17)	O(31)#12-Sm(4)-O(39)	70.36(19)
O(14)-Sm(3)-C(54)#7	149.10(18)	O(22)-Sm(4)-O(39)	72.75(17)
O(25)-Sm(3)-C(54)#7	68.09(17)	O(28)#11-Sm(4)-O(30)	74.54(16)
O(38)-Sm(3)-C(54)#7	140.11(18)	O(36)#7-Sm(4)-O(30)	123.49(15)
O(35)#7-Sm(3)-C(54)#7	23.69(17)	O(26)-Sm(4)-O(30)	79.47(17)
O(19)-Sm(3)-C(54)#7	83.39(17)	O(31)#12-Sm(4)-O(30)	133.50(17)
O(36)#7-Sm(3)-C(54)#7	24.33(16)	O(22)-Sm(4)-O(30)	79.18(16)
O(28)#11-Sm(4)-O(36)#7	156.33(16)	O(39)-Sm(4)-O(30)	141.42(17)
O(28)#11-Sm(4)-O(26)	126.18(16)	O(28)#11-Sm(4)-O(29)	119.49(14)
O(36)#7-Sm(4)-O(26)	75.44(16)	O(36)#7-Sm(4)-O(29)	75.33(14)
O(28)#11-Sm(4)-O(31)#12	85.95(17)	O(26)-Sm(4)-O(29)	67.38(14)
O(36)#7-Sm(4)-O(31)#12	89.71(15)	O(31)#12-Sm(4)-O(29)	145.63(16)
O(26)-Sm(4)-O(31)#12	79.05(17)	O(22)-Sm(4)-O(29)	65.80(14)
O(32)-Sm(6)-O(23)#13	117.71(15)	O(39)-Sm(4)-O(29)	133.25(16)
O(34)-Sm(6)-O(23)#13	69.05(15)	O(30)-Sm(4)-O(29)	48.28(13)
O(20)#14-Sm(6)-O(23)#13	75.10(14)	O(28)#11-Sm(4)-C(43)	96.24(17)
O(27)#14-Sm(6)-O(23)#13	146.47(15)	O(36)#7-Sm(4)-C(43)	99.85(17)
O(40)-Sm(6)-O(23)#13	130.97(15)	O(26)-Sm(4)-C(43)	73.46(16)
O(24)#13-Sm(6)-O(23)#13	47.59(14)	O(31)#12-Sm(4)-C(43)	147.40(18)
O(16)-Sm(6)-O(23)#13	63.77(14)	O(22)-Sm(4)-C(43)	69.51(16)
O(42)-Sm(6)-O(23)#13	100.65(16)	O(39)-Sm(4)-C(43)	142.05(18)
O(32)-Sm(6)-C(36)#13	94.45(19)	O(30)-Sm(4)-C(43)	23.85(17)
O(34)-Sm(6)-C(36)#13	80.77(17)	O(29)-Sm(4)-C(43)	24.52(15)
O(20)#14-Sm(6)-C(36)#13	99.11(17)	O(12)#3-Sm(5)-O(23)#13	163.91(17)
O(27)#14-Sm(6)-C(36)#13	152.58(19)	O(12)#3-Sm(5)-O(33)	99.19(16)
O(40)-Sm(6)-C(36)#13	136.40(18)	O(23)#13-Sm(5)-O(33)	81.96(16)
O(24)#13-Sm(6)-C(36)#13	23.32(18)	O(12)#3-Sm(5)-O(15)	111.63(16)
O(16)-Sm(6)-C(36)#13	65.19(17)	O(23)#13-Sm(5)-O(15)	77.34(16)
O(42)-Sm(6)-C(36)#13	85.5(2)	O(33)-Sm(5)-O(15)	134.27(16)
O(23)#13-Sm(6)-C(36)#13	24.46(16)	O(12)#3-Sm(5)-O(8)#13	80.98(16)
C(55)-N(1)-C(56)	119.7(19)	O(23)#13-Sm(5)-O(8)#13	88.88(16)
C(55)-N(1)-C(58)	112.1(18)	O(33)-Sm(5)-O(8)#13	144.91(16)

C(56)-N(1)-C(58)	128(2)	O(15)-Sm(5)-O(8)#13	75.14(17)
O(37)-C(55)-N(1)	122(2)	O(12)#3-Sm(5)-O(41)	78.9(2)
O(37)-C(55)-H(55)	119.2	O(23)#13-Sm(5)-O(41)	86.2(2)
N(1)-C(55)-H(55)	119.2	O(33)-Sm(5)-O(41)	73.0(2)
N(1)-C(56)-C(57)	116(2)	O(15)-Sm(5)-O(41)	144.0(3)
N(1)-C(56)-H(56A)	108.4	O(8)#13-Sm(5)-O(41)	72.7(2)
C(57)-C(56)-H(56A)	108.4	O(12)#3-Sm(5)-O(43)#14	69.82(16)
N(1)-C(56)-H(56B)	108.4	O(23)#13-Sm(5)-O(43)#14	126.02(16)
C(57)-C(56)-H(56B)	108.4	O(33)-Sm(5)-O(43)#14	81.85(16)
H(56A)-C(56)-H(56B)	107.4	O(15)-Sm(5)-O(43)#14	78.34(17)
C(56)-C(57)-H(57A)	109.5	O(8)#13-Sm(5)-O(43)#14	129.27(16)
C(56)-C(57)-H(57B)	109.5	O(41)-Sm(5)-O(43)#14	135.7(3)
H(57A)-C(57)-H(57B)	109.5	O(12)#3-Sm(5)-O(20)#14	117.67(14)
C(56)-C(57)-H(57C)	109.5	O(23)#13-Sm(5)-O(20)#14	77.69(15)
H(57A)-C(57)-H(57C)	109.5	O(33)-Sm(5)-O(20)#14	67.06(14)
H(57B)-C(57)-H(57C)	109.5	O(15)-Sm(5)-O(20)#14	68.89(14)
N(1)-C(58)-C(59)	104(2)	O(8)#13-Sm(5)-O(20)#14	143.51(16)
N(1)-C(58)-H(58A)	111.1	O(41)-Sm(5)-O(20)#14	138.49(18)
C(59)-C(58)-H(58A)	111.1	O(43)#14-Sm(5)-O(20)#14	48.61(13)
N(1)-C(58)-H(58B)	111.1	O(12)#3-Sm(5)-C(30)#14	93.14(17)
C(59)-C(58)-H(58B)	111.1	O(23)#13-Sm(5)-C(30)#14	102.33(17)
H(58A)-C(58)-H(58B)	109.0	O(33)-Sm(5)-C(30)#14	71.04(16)
C(58)-C(59)-H(59A)	109.5	O(15)-Sm(5)-C(30)#14	74.23(16)
C(58)-C(59)-H(59B)	109.5	O(8)#13-Sm(5)-C(30)#14	144.00(17)
H(59A)-C(59)-H(59B)	109.5	O(41)-Sm(5)-C(30)#14	141.3(2)
C(58)-C(59)-H(59C)	109.5	O(43)#14-Sm(5)-C(30)#14	24.16(16)
H(59A)-C(59)-H(59C)	109.5	O(20)#14-Sm(5)-C(30)#14	24.64(15)
H(59B)-C(59)-H(59C)	109.5	O(32)-Sm(6)-O(34)	138.44(18)
C(55')-N(1')-C(56')	119.6(18)	O(32)-Sm(6)-O(20)#14	148.80(18)
C(55')-N(1')-C(58')	116.6(17)	O(34)-Sm(6)-O(20)#14	71.87(16)
C(56')-N(1')-C(58')	119(2)	O(32)-Sm(6)-O(27)#14	90.39(18)
O(37)-C(55')-N(1')	123(2)	O(34)-Sm(6)-O(27)#14	77.80(18)
O(37)-C(55')-H(55')	118.7	O(20)#14-Sm(6)-O(27)#14	90.30(15)
N(1')-C(55')-H(55')	118.7	O(32)-Sm(6)-O(40)	75.43(19)
N(1')-C(56')-C(57')	116(2)	O(34)-Sm(6)-O(40)	133.96(16)
N(1')-C(56')-H(56C)	108.2	O(20)#14-Sm(6)-O(40)	75.37(16)

C(57')-C(56')-H(56C)	108.2	O(27)#14-Sm(6)-O(40)	70.88(17)
N(1')-C(56')-H(56D)	108.2	O(32)-Sm(6)-O(24)#13	73.74(18)
C(57')-C(56')-H(56D)	108.2	O(34)-Sm(6)-O(24)#13	89.68(19)
H(56C)-C(56')-H(56D)	107.3	O(20)#14-Sm(6)-O(24)#13	122.43(16)
C(56')-C(57')-H(57D)	109.5	O(27)#14-Sm(6)-O(24)#13	139.46(17)
C(56')-C(57')-H(57E)	109.5	O(40)-Sm(6)-O(24)#13	135.67(18)
H(57D)-C(57')-H(57E)	109.5	O(32)-Sm(6)-O(16)	84.63(16)
C(56')-C(57')-H(57F)	109.5	O(34)-Sm(6)-O(16)	127.96(15)
H(57D)-C(57')-H(57F)	109.5	O(20)#14-Sm(6)-O(16)	75.95(14)
H(57E)-C(57')-H(57F)	109.5	O(27)#14-Sm(6)-O(16)	142.22(16)
N(1')-C(58')-C(59')	110.0(19)	O(40)-Sm(6)-O(16)	71.62(16)
N(1')-C(58')-H(58C)	109.7	O(24)#13-Sm(6)-O(16)	74.47(16)
C(59')-C(58')-H(58C)	109.7	O(32)-Sm(6)-O(42)	69.4(2)
N(1')-C(58')-H(58D)	109.6	O(34)-Sm(6)-O(42)	69.04(18)
C(59')-C(58')-H(58D)	109.7	O(20)#14-Sm(6)-O(42)	139.30(18)
H(58C)-C(58')-H(58D)	108.2	O(27)#14-Sm(6)-O(42)	70.96(18)
C(58')-C(59')-H(59D)	109.5	O(40)-Sm(6)-O(42)	126.97(18)
C(58')-C(59')-H(59E)	109.5	O(24)#13-Sm(6)-O(42)	68.55(19)
H(59D)-C(59')-H(59E)	109.5	O(16)-Sm(6)-O(42)	139.31(18)
C(58')-C(59')-H(59F)	109.5	O(39)-C(65)-N(3)	120(2)
H(59D)-C(59')-H(59F)	109.5	O(39)-C(65)-H(65)	119.9
H(59E)-C(59')-H(59F)	109.5	N(3)-C(65)-H(65)	119.9
C(60)-O(38)-Sm(3)	127.7(5)	N(3)-C(66)-C(67)	112.2(19)
C(60)-N(2)-C(63)	120.3(9)	N(3)-C(66)-H(66A)	109.2
C(60)-N(2)-C(61)	119.0(10)	C(67)-C(66)-H(66A)	109.2
C(63)-N(2)-C(61)	119.8(10)	N(3)-C(66)-H(66B)	109.2
O(38)-C(60)-N(2)	124.1(9)	C(67)-C(66)-H(66B)	109.2
O(38)-C(60)-H(60)	118.0	H(66A)-C(66)-H(66B)	107.9
N(2)-C(60)-H(60)	118.0	C(66)-C(67)-H(67A)	109.5
C(62)-C(61)-N(2)	112.7(14)	C(66)-C(67)-H(67B)	109.5
C(62)-C(61)-H(61A)	109.1	H(67A)-C(67)-H(67B)	109.5
N(2)-C(61)-H(61A)	109.1	C(66)-C(67)-H(67C)	109.5
C(62)-C(61)-H(61B)	109.1	H(67A)-C(67)-H(67C)	109.5
N(2)-C(61)-H(61B)	109.1	H(67B)-C(67)-H(67C)	109.5
H(61A)-C(61)-H(61B)	107.8	N(3)-C(68)-C(69)	112.3(18)
C(61)-C(62)-H(62A)	109.5	N(3)-C(68)-H(68A)	109.1

C(61)-C(62)-H(62B)	109.5	C(69)-C(68)-H(68A)	109.1
H(62A)-C(62)-H(62B)	109.5	N(3)-C(68)-H(68B)	109.1
C(61)-C(62)-H(624)	109.5	C(69)-C(68)-H(68B)	109.1
H(62A)-C(62)-H(624)	109.5	H(68A)-C(68)-H(68B)	107.9
H(62B)-C(62)-H(624)	109.5	C(68)-C(69)-H(69A)	109.5
N(2)-C(63)-C(64)	111.0(13)	C(68)-C(69)-H(69B)	109.5
N(2)-C(63)-H(63A)	109.4	H(69A)-C(69)-H(69B)	109.5
C(64)-C(63)-H(63A)	109.4	C(68)-C(69)-H(69C)	109.5
N(2)-C(63)-H(63B)	109.4	H(69A)-C(69)-H(69C)	109.5
C(64)-C(63)-H(63B)	109.4	H(69B)-C(69)-H(69C)	109.5
H(63A)-C(63)-H(63B)	108.0	C(65')-N(3')-C(68')	121.2(14)
C(63)-C(64)-H(64A)	109.5	C(65')-N(3')-C(66')	119.2(13)
C(63)-C(64)-H(64B)	109.5	C(68')-N(3')-C(66')	118.9(14)
H(64A)-C(64)-H(64B)	109.5	O(39)-C(65')-N(3')	118.6(16)
C(63)-C(64)-H(64C)	109.5	O(39)-C(65')-H(65')	120.7
H(64A)-C(64)-H(64C)	109.5	N(3')-C(65')-H(65')	120.7
H(64B)-C(64)-H(64C)	109.5	N(3')-C(66')-C(67')	110.9(15)
C(65)-N(3)-C(66)	119.9(16)	N(3')-C(66')-H(66C)	109.5
C(65)-N(3)-C(68)	120.1(15)	C(67')-C(66')-H(66C)	109.5
C(66)-N(3)-C(68)	118.8(17)	N(3')-C(66')-H(66D)	109.5
H(78A)-C(78)-H(78B)	109.6	C(67')-C(66')-H(66D)	109.5
C(78)-C(79)-H(79A)	109.5	H(66C)-C(66')-H(66D)	108.0
C(78)-C(79)-H(79B)	109.5	C(66')-C(67')-H(67D)	109.5
H(79A)-C(79)-H(79B)	109.5	C(66')-C(67')-H(67E)	109.5
C(78)-C(79)-H(79C)	109.4	H(67D)-C(67')-H(67E)	109.5
H(79A)-C(79)-H(79C)	109.5	C(66')-C(67')-H(67F)	109.5
H(79B)-C(79)-H(79C)	109.5	H(67D)-C(67')-H(67F)	109.5
C(75')-N(5')-C(76')	124.6(18)	H(67E)-C(67')-H(67F)	109.5
C(75')-N(5')-C(78')	120.8(19)	N(3')-C(68')-C(69')	113.2(17)
C(76')-N(5')-C(78')	97.9(18)	N(3')-C(68')-H(68C)	108.9
O(41)-C(75')-N(5')	131.1(19)	C(69')-C(68')-H(68C)	108.9
O(41)-C(75')-H(75')	114.4	N(3')-C(68')-H(68D)	108.9
N(5')-C(75')-H(75')	114.4	C(69')-C(68')-H(68D)	108.9
C(77')-C(76')-N(5')	115(2)	H(68C)-C(68')-H(68D)	107.7
C(77')-C(76')-H(76C)	108.5	C(68')-C(69')-H(69D)	109.5
N(5')-C(76')-H(76C)	108.5	C(68')-C(69')-H(69E)	109.5

C(77')-C(76')-H(76D)	108.5	H(69D)-C(69')-H(69E)	109.5
N(5')-C(76')-H(76D)	108.5	C(68')-C(69')-H(69F)	109.5
H(76C)-C(76')-H(76D)	107.5	H(69D)-C(69')-H(69F)	109.5
C(76')-C(77')-H(77D)	109.5	H(69E)-C(69')-H(69F)	109.5
C(76')-C(77')-H(77E)	109.5	C(70)-O(40)-Sm(6)	126.0(5)
H(77D)-C(77')-H(77E)	109.5	C(70)-N(4)-C(71)	124.3(9)
C(76')-C(77')-H(77F)	109.5	C(70)-N(4)-C(73)	119.8(8)
H(77D)-C(77')-H(77F)	109.5	C(71)-N(4)-C(73)	115.8(9)
H(77E)-C(77')-H(77F)	109.5	O(40)-C(70)-N(4)	123.8(8)
N(5')-C(78')-C(79')	100(2)	O(40)-C(70)-H(70)	118.1
N(5')-C(78')-H(78C)	111.8	N(4)-C(70)-H(70)	118.1
C(79')-C(78')-H(78C)	111.8	C(72)-C(71)-N(4)	116.0(11)
N(5')-C(78')-H(78D)	111.8	C(72)-C(71)-H(71A)	108.3
C(79')-C(78')-H(78D)	111.8	N(4)-C(71)-H(71A)	108.3
H(78C)-C(78')-H(78D)	109.5	C(72)-C(71)-H(71B)	108.3
C(78')-C(79')-H(79D)	109.5	N(4)-C(71)-H(71B)	108.3
C(78')-C(79')-H(79E)	109.5	H(71A)-C(71)-H(71B)	107.4
H(79D)-C(79')-H(79E)	109.5	C(71)-C(72)-H(72A)	109.5
C(78')-C(79')-H(79F)	109.5	C(71)-C(72)-H(72B)	109.5
H(79D)-C(79')-H(79F)	109.5	H(72A)-C(72)-H(72B)	109.5
H(79E)-C(79')-H(79F)	109.5	C(71)-C(72)-H(72C)	109.5
C(55')-O(37)-Sm(1)	132.9(13)	H(72A)-C(72)-H(72C)	109.5
C(55)-O(37)-Sm(1)	125.2(12)	H(72B)-C(72)-H(72C)	109.5
C(65)-O(39)-Sm(4)	128.1(11)	N(4)-C(73)-C(74)	109.6(11)
C(65')-O(39)-Sm(4)	125.4(10)	N(4)-C(73)-H(73A)	109.7
C(75)-O(41)-Sm(5)	149(2)	C(74)-C(73)-H(73A)	109.7
C(75')-O(41)-Sm(5)	134.1(12)	N(4)-C(73)-H(73B)	109.7
O(41)-C(75)-N(5)	115(3)	C(74)-C(73)-H(73B)	109.7
O(41)-C(75)-H(75)	122.4	H(73A)-C(73)-H(73B)	108.2
N(5)-C(75)-H(75)	122.4	C(73)-C(74)-H(74A)	109.5
N(5)-C(76)-C(77)	115(3)	C(73)-C(74)-H(74B)	109.5
N(5)-C(76)-H(76A)	108.6	H(74A)-C(74)-H(74B)	109.5
C(77)-C(76)-H(76A)	108.6	C(73)-C(74)-H(74C)	109.5
N(5)-C(76)-H(76B)	108.6	H(74A)-C(74)-H(74C)	109.5
C(77)-C(76)-H(76B)	108.6	H(74B)-C(74)-H(74C)	109.5
H(76A)-C(76)-H(76B)	107.6	C(75)-N(5)-C(76)	119(3)

C(76)-C(77)-H(77A)	109.5	C(75)-N(5)-C(78)	115(3)
C(76)-C(77)-H(77B)	109.5	C(76)-N(5)-C(78)	98(2)
H(77A)-C(77)-H(77B)	109.5	N(5)-C(78)-H(78A)	111.9
C(76)-C(77)-H(77C)	109.5	C(79)-C(78)-H(78A)	111.9
H(77A)-C(77)-H(77C)	109.5	N(5)-C(78)-H(78B)	112.0
H(77B)-C(77)-H(77C)	109.5	C(79)-C(78)-H(78B)	112.0
N(5)-C(78)-C(79)	99(2)		

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z+1 #2 x,y+1,z #3 x,y-1,z-1 #4 -x+1,-y+1,z-1/2 #5 -x+1,-y+2,z-1/2 #6 -x+1,-y+2,z+1/2 #7 x,y+1,z+1 #8 -x+3/2,y-1/2,z+1/2 #9 -x+3/2,y-1/2,z-1/2 #10 -x+1,-y+1,z+1/2 #11 -x+3/2,y+1/2,z-1/2 #12 -x+3/2,y+1/2,z+1/2 #13 x,y-1,z #14 x,y,z-1

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C(1)-O(2)	1.247(17)	C(47)-O(28)	1.23(3)
C(1)-O(1)	1.255(16)	C(47)-N(3)	1.33(2)
C(1)-C(2)	1.473(18)	C(47)-H(47)	0.9300
C(2)-C(3)	1.363(18)	C(47')-O(28)	1.110(19)
C(2)-S(1)	1.718(12)	C(47')-N(3)	1.40(2)
C(3)-C(4)	1.421(18)	C(47')-H(47')	0.9300
C(3)-H(3)	0.9300	C(48)-N(3)	1.45(2)
C(4)-C(5)	1.349(19)	C(48)-C(49)	1.53(3)
C(4)-H(4)	0.9300	C(48)-H(48A)	0.9700
C(5)-C(6)	1.490(17)	C(48)-H(48B)	0.9700
C(5)-S(1)	1.705(12)	C(49)-H(49A)	0.9600
C(6)-O(4)	1.224(17)	C(49)-H(49B)	0.9600
C(6)-O(3)	1.278(16)	C(49)-H(49C)	0.9600
C(7)-O(6)	1.244(15)	C(50)-N(3)	1.48(2)
C(7)-O(5)	1.278(16)	C(50)-C(51)	1.50(3)
C(7)-C(8)	1.465(17)	C(50)-H(50A)	0.9700
C(7)-Eu(1)#1	3.150(13)	C(50)-H(50B)	0.9700
C(8)-C(9)	1.343(18)	C(51)-H(51A)	0.9600
C(8)-S(2)	1.717(11)	C(51)-H(51B)	0.9600

C(9)-C(10)	1.417(18)	C(51)-H(51C)	0.9600
C(9)-H(9)	0.9300	O(1)-Eu(2)#3	2.327(8)
C(10)-C(11)	1.357(17)	O(2)-Eu(1)#3	2.454(8)
C(10)-H(10)	0.9300	O(3)-Eu(4)#4	2.286(8)
C(11)-C(12)	1.481(16)	O(4)-Eu(1)	2.424(9)
C(11)-S(2)	1.699(12)	O(5)-Eu(2)#1	2.277(8)
C(12)-O(8)	1.250(15)	O(6)-Eu(1)#1	2.376(8)
C(12)-O(7)	1.275(15)	O(7)-Eu(1)	2.318(8)
C(13)-O(9)	1.232(15)	O(8)-Eu(2)	2.382(8)
C(13)-O(10)	1.235(15)	O(9)-Eu(1)#3	2.332(9)
C(13)-C(14)	1.496(17)	O(10)-Eu(4)#5	2.378(8)
C(14)-C(15)	1.342(18)	O(11)-Eu(1)	2.458(8)
C(14)-S(3)	1.717(13)	O(11)-Eu(2)	2.782(9)
C(15)-C(16)	1.414(18)	O(12)-Eu(2)	2.422(9)
C(15)-H(15)	0.9300	O(13)-Eu(4)#2	2.459(8)
C(16)-C(17)	1.355(19)	O(14)-Eu(3)#2	2.353(7)
C(16)-H(16)	0.9300	O(14)-Eu(4)#2	2.833(8)
C(17)-C(18)	1.489(17)	O(15)-Eu(2)	2.414(8)
C(17)-S(3)	1.710(13)	O(16)-Eu(3)	2.298(8)
C(18)-O(12)	1.249(16)	O(17)-Eu(3)#6	2.392(7)
C(18)-O(11)	1.255(15)	O(18)-Eu(4)#6	2.376(7)
C(18)-Eu(2)	2.951(13)	O(19)-Eu(4)	2.311(8)
C(19)-O(13)	1.253(14)	O(19)-Eu(3)	2.890(8)
C(19)-O(14)	1.264(14)	O(20)-Eu(3)	2.485(8)
C(19)-C(20)	1.478(16)	O(21)-Eu(3)#2	2.390(8)
C(19)-Eu(4)#2	2.999(12)	O(22)-Eu(2)#2	2.302(8)
C(20)-C(21)	1.371(17)	O(23)-Eu(3)	2.449(8)
C(20)-S(4)	1.726(12)	O(24)-Eu(4)	2.367(7)
C(21)-C(22)	1.382(17)	O(25)-Eu(3)	2.657(5)
C(21)-H(21)	0.9300	O(25)-Eu(2)	2.677(6)
C(22)-C(23)	1.357(18)	O(26)-Eu(3)	2.444(8)
C(22)-H(22)	0.9300	O(27)-Eu(1)	2.420(8)
C(23)-C(24)	1.509(17)	O(28)-Eu(4)	2.402(8)
C(23)-S(4)	1.728(13)	O(29)-Eu(1)	2.560(7)
C(24)-O(16)	1.218(16)	O(29)-H(29A)	0.85(3)
C(24)-O(15)	1.257(16)	O(29)-H(29B)	0.85(3)

C(25)-O(18)	1.254(14)	Eu(1)-O(9)#7	2.332(9)
C(25)-O(17)	1.258(14)	Eu(1)-O(6)#8	2.376(8)
C(25)-C(26)	1.484(15)	Eu(1)-O(2)#7	2.454(8)
C(26)-C(27)	1.348(17)	Eu(1)-C(7)#8	3.150(13)
C(26)-S(5)	1.713(11)	Eu(1)-Eu(2)	4.2233(6)
C(27)-C(28)	1.421(17)	Eu(2)-O(5)#8	2.277(8)
C(27)-H(27)	0.9300	Eu(2)-O(22)#9	2.302(8)
C(28)-C(29)	1.353(17)	Eu(2)-O(1)#7	2.327(8)
C(28)-H(28)	0.9300	Eu(3)-O(14)#9	2.353(7)
C(29)-C(30)	1.492(16)	Eu(3)-O(21)#9	2.390(8)
C(29)-S(5)	1.711(11)	Eu(3)-O(17)#5	2.392(7)
C(30)-O(20)	1.245(15)	Eu(3)-Eu(4)	4.0915(6)
C(30)-O(19)	1.257(14)	Eu(4)-O(3)#10	2.286(8)
C(30)-Eu(3)	3.036(12)	Eu(4)-O(18)#5	2.376(7)
C(31)-O(22)	1.249(16)	Eu(4)-O(10)#6	2.378(8)
C(31)-O(21)	1.273(17)	Eu(4)-O(13)#9	2.459(8)
C(31)-C(32)	1.469(18)	Eu(4)-O(14)#9	2.833(8)
C(32)-C(33)	1.378(17)	Eu(4)-C(19)#9	2.999(12)
C(32)-S(6)	1.697(13)	C(38)-H(38B)	0.9700
C(33)-C(34)	1.396(17)	C(39)-H(39A)	0.9600
C(33)-H(33)	0.9300	C(39)-H(39B)	0.9600
C(34)-C(35)	1.375(17)	C(39)-H(39C)	0.9600
C(34)-H(34)	0.9300	C(40)-N(1)	1.48(2)
C(35)-C(36)	1.485(16)	C(40)-C(41)	1.48(2)
C(35)-S(6)	1.705(12)	C(40)-H(40A)	0.9700
C(36)-O(23)	1.246(14)	C(40)-H(40B)	0.9700
C(36)-O(24)	1.286(14)	C(41)-H(41A)	0.9600
C(37)-O(26)	1.204(13)	C(41)-H(41B)	0.9600
C(37)-N(1)	1.332(15)	C(41)-H(41C)	0.9600
C(37)-H(37)	0.9300	C(42)-O(27)	1.189(17)
C(38)-N(1)	1.463(19)	C(42)-N(2)	1.35(2)
C(38)-C(39)	1.50(2)	C(42)-H(42)	0.9300
C(38)-H(38A)	0.9700	C(43)-N(2)	1.47(2)
C(45)-N(2)	1.45(2)	C(43)-C(44)	1.50(3)
C(45)-C(46)	1.54(2)	C(43)-H(43A)	0.9700
C(45)-H(45A)	0.9700	C(43)-H(43B)	0.9700

C(45)-H(45B)	0.9700	C(44)-H(44A)	0.9600
C(46)-H(46A)	0.9600	C(44)-H(44B)	0.9600
C(46)-H(46B)	0.9600	C(44)-H(44C)	0.9600
C(46)-H(46C)	0.9600	O(8)-C(12)-C(11)	119.6(11)
(2)-C(1)-O(1)	127.4(12)	O(7)-C(12)-C(11)	114.9(11)
O(2)-C(1)-C(2)	118.1(11)	O(9)-C(13)-O(10)	126.1(12)
O(1)-C(1)-C(2)	114.5(13)	O(9)-C(13)-C(14)	116.1(12)
C(3)-C(2)-C(1)	128.0(12)	O(10)-C(13)-C(14)	117.8(11)
C(3)-C(2)-S(1)	111.0(10)	C(15)-C(14)-C(13)	126.7(12)
C(1)-C(2)-S(1)	120.8(10)	C(15)-C(14)-S(3)	111.7(10)
C(2)-C(3)-C(4)	112.0(13)	C(13)-C(14)-S(3)	121.6(10)
C(2)-C(3)-H(3)	124.0	C(14)-C(15)-C(16)	113.0(13)
C(4)-C(3)-H(3)	124.0	C(14)-C(15)-H(15)	123.5
C(5)-C(4)-C(3)	113.3(13)	C(16)-C(15)-H(15)	123.5
C(5)-C(4)-H(4)	123.3	C(17)-C(16)-C(15)	112.2(13)
C(3)-C(4)-H(4)	123.3	C(17)-C(16)-H(16)	123.9
C(4)-C(5)-C(6)	128.4(12)	C(15)-C(16)-H(16)	123.9
C(4)-C(5)-S(1)	111.3(10)	C(16)-C(17)-C(18)	128.7(12)
C(6)-C(5)-S(1)	120.1(10)	C(16)-C(17)-S(3)	111.8(10)
O(4)-C(6)-O(3)	125.7(12)	C(18)-C(17)-S(3)	119.4(10)
O(4)-C(6)-C(5)	120.5(12)	O(12)-C(18)-O(11)	123.1(12)
O(3)-C(6)-C(5)	113.7(12)	O(12)-C(18)-C(17)	117.9(11)
O(6)-C(7)-O(5)	125.3(12)	O(11)-C(18)-C(17)	119.0(12)
O(6)-C(7)-C(8)	118.3(12)	O(12)-C(18)-Eu(2)	53.4(6)
O(5)-C(7)-C(8)	116.4(11)	O(11)-C(18)-Eu(2)	69.9(7)
O(6)-C(7)-Eu(1)#1	42.0(6)	C(17)-C(18)-Eu(2)	169.4(10)
O(5)-C(7)-Eu(1)#1	84.7(7)	O(13)-C(19)-O(14)	122.6(11)
C(8)-C(7)-Eu(1)#1	156.9(9)	O(13)-C(19)-C(20)	118.9(11)
C(9)-C(8)-C(7)	128.1(11)	O(14)-C(19)-C(20)	118.5(11)
C(9)-C(8)-S(2)	111.1(9)	O(13)-C(19)-Eu(4)#2	53.1(6)
C(7)-C(8)-S(2)	120.8(9)	O(14)-C(19)-Eu(4)#2	70.2(6)
C(8)-C(9)-C(10)	113.4(12)	C(20)-C(19)-Eu(4)#2	167.9(8)
C(8)-C(9)-H(9)	123.3	C(21)-C(20)-C(19)	127.5(11)
C(10)-C(9)-H(9)	123.3	C(21)-C(20)-S(4)	111.5(9)
C(11)-C(10)-C(9)	111.6(12)	C(19)-C(20)-S(4)	121.0(9)
C(11)-C(10)-H(10)	124.2	C(20)-C(21)-C(22)	112.1(11)

C(9)-C(10)-H(10)	124.2	C(20)-C(21)-H(21)	123.9
C(10)-C(11)-C(12)	126.2(11)	C(22)-C(21)-H(21)	123.9
C(10)-C(11)-S(2)	112.1(9)	C(23)-C(22)-C(21)	114.7(12)
C(12)-C(11)-S(2)	121.7(9)	C(23)-C(22)-H(22)	122.7
O(8)-C(12)-O(7)	125.5(11)	C(21)-C(22)-H(22)	122.7
C(38)-C(39)-H(39C)	109.5	C(22)-C(23)-C(24)	124.8(12)
H(39A)-C(39)-H(39C)	109.5	C(22)-C(23)-S(4)	110.6(10)
H(39B)-C(39)-H(39C)	109.5	C(24)-C(23)-S(4)	124.6(11)
N(1)-C(40)-C(41)	115(2)	O(16)-C(24)-O(15)	126.4(12)
N(1)-C(40)-H(40A)	108.5	O(16)-C(24)-C(23)	114.2(12)
C(41)-C(40)-H(40A)	108.5	O(15)-C(24)-C(23)	119.4(12)
N(1)-C(40)-H(40B)	108.5	O(18)-C(25)-O(17)	125.8(10)
C(41)-C(40)-H(40B)	108.5	O(18)-C(25)-C(26)	117.7(10)
H(40A)-C(40)-H(40B)	107.5	O(17)-C(25)-C(26)	116.6(11)
C(40)-C(41)-H(41A)	109.5	C(27)-C(26)-C(25)	127.9(11)
C(40)-C(41)-H(41B)	109.5	C(27)-C(26)-S(5)	111.7(9)
H(41A)-C(41)-H(41B)	109.5	C(25)-C(26)-S(5)	120.5(9)
C(40)-C(41)-H(41C)	109.5	C(26)-C(27)-C(28)	113.3(11)
H(41A)-C(41)-H(41C)	109.5	C(26)-C(27)-H(27)	123.3
H(41B)-C(41)-H(41C)	109.5	C(28)-C(27)-H(27)	123.3
O(27)-C(42)-N(2)	126(2)	C(29)-C(28)-C(27)	111.1(11)
O(27)-C(42)-H(42)	116.9	C(29)-C(28)-H(28)	124.5
N(2)-C(42)-H(42)	116.9	C(27)-C(28)-H(28)	124.5
N(2)-C(43)-C(44)	142(4)	C(28)-C(29)-C(30)	126.8(11)
N(2)-C(43)-H(43A)	101.4	C(28)-C(29)-S(5)	112.8(9)
C(44)-C(43)-H(43A)	101.4	C(30)-C(29)-S(5)	120.3(9)
N(2)-C(43)-H(43B)	101.4	O(20)-C(30)-O(19)	123.1(11)
C(44)-C(43)-H(43B)	101.4	O(20)-C(30)-C(29)	118.5(10)
H(43A)-C(43)-H(43B)	104.6	O(19)-C(30)-C(29)	118.4(11)
C(43)-C(44)-H(44A)	109.5	O(20)-C(30)-Eu(3)	52.6(6)
C(43)-C(44)-H(44B)	109.5	O(19)-C(30)-Eu(3)	71.3(6)
H(44A)-C(44)-H(44B)	109.5	C(29)-C(30)-Eu(3)	167.0(8)
C(43)-C(44)-H(44C)	109.5	O(22)-C(31)-O(21)	124.3(12)
H(44A)-C(44)-H(44C)	109.5	O(22)-C(31)-C(32)	117.7(13)
H(44B)-C(44)-H(44C)	109.5	O(21)-C(31)-C(32)	118.0(12)
N(2)-C(45)-C(46)	101(3)	C(33)-C(32)-C(31)	125.7(12)

N(2)-C(45)-H(45A)	111.7	C(33)-C(32)-S(6)	111.7(9)
C(46)-C(45)-H(45A)	111.7	C(31)-C(32)-S(6)	122.4(11)
N(2)-C(45)-H(45B)	111.7	C(32)-C(33)-C(34)	112.7(11)
C(46)-C(45)-H(45B)	111.7	C(32)-C(33)-H(33)	123.6
H(45A)-C(45)-H(45B)	109.4	C(34)-C(33)-H(33)	123.6
C(45)-C(46)-H(46A)	109.5	C(35)-C(34)-C(33)	111.8(11)
C(45)-C(46)-H(46B)	109.5	C(35)-C(34)-H(34)	124.1
H(46A)-C(46)-H(46B)	109.5	C(33)-C(34)-H(34)	124.1
C(45)-C(46)-H(46C)	109.5	C(34)-C(35)-C(36)	128.2(11)
H(46A)-C(46)-H(46C)	109.5	C(34)-C(35)-S(6)	112.1(9)
H(46B)-C(46)-H(46C)	109.5	C(36)-C(35)-S(6)	119.6(9)
O(28)-C(47)-N(3)	123(3)	O(23)-C(36)-O(24)	125.8(10)
O(28)-C(47)-H(47)	118.3	O(23)-C(36)-C(35)	118.4(10)
N(3)-C(47)-H(47)	118.3	O(24)-C(36)-C(35)	115.7(11)
O(28)-C(47')-N(3)	127(3)	O(26)-C(37)-N(1)	124.6(14)
O(28)-C(47')-H(47')	116.3	O(26)-C(37)-H(37)	117.7
N(3)-C(47')-H(47')	116.3	N(1)-C(37)-H(37)	117.7
N(3)-C(48)-C(49)	113(3)	N(1)-C(38)-C(39)	113(2)
N(3)-C(48)-H(48A)	108.9	N(1)-C(38)-H(38A)	109.0
C(49)-C(48)-H(48A)	108.9	C(39)-C(38)-H(38A)	109.0
N(3)-C(48)-H(48B)	108.9	N(1)-C(38)-H(38B)	109.0
C(49)-C(48)-H(48B)	108.9	C(39)-C(38)-H(38B)	109.0
H(48A)-C(48)-H(48B)	107.7	H(38A)-C(38)-H(38B)	107.8
C(48)-C(49)-H(49A)	109.5	C(38)-C(39)-H(39A)	109.5
C(48)-C(49)-H(49B)	109.5	C(38)-C(39)-H(39B)	109.5
H(49A)-C(49)-H(49B)	109.5	H(39A)-C(39)-H(39B)	109.5
C(48)-C(49)-H(49C)	109.5	C(36)-O(23)-Eu(3)	138.6(7)
H(49A)-C(49)-H(49C)	109.5	C(36)-O(24)-Eu(4)	132.3(7)
H(49B)-C(49)-H(49C)	109.5	Eu(3)-O(25)-Eu(2)	124.0(2)
N(3)-C(50)-C(51)	110(3)	C(37)-O(26)-Eu(3)	126.6(8)
N(3)-C(50)-H(50A)	109.8	C(42)-O(27)-Eu(1)	131.9(12)
C(51)-C(50)-H(50A)	109.8	C(47')-O(28)-Eu(4)	147(2)
N(3)-C(50)-H(50B)	109.8	C(47)-O(28)-Eu(4)	130(3)
C(51)-C(50)-H(50B)	109.8	Eu(1)-O(29)-H(29A)	118(10)
H(50A)-C(50)-H(50B)	108.2	Eu(1)-O(29)-H(29B)	118(10)
C(50)-C(51)-H(51A)	109.5	H(29A)-O(29)-H(29B)	112(5)

C(50)-C(51)-H(51B)	109.5	C(5)-S(1)-C(2)	92.2(6)
H(51A)-C(51)-H(51B)	109.5	C(11)-S(2)-C(8)	91.7(5)
C(50)-C(51)-H(51C)	109.5	C(17)-S(3)-C(14)	91.2(6)
H(51A)-C(51)-H(51C)	109.5	C(20)-S(4)-C(23)	91.1(6)
H(51B)-C(51)-H(51C)	109.5	C(29)-S(5)-C(26)	91.0(5)
C(37)-N(1)-C(38)	121.2(17)	C(32)-S(6)-C(35)	91.6(6)
C(37)-N(1)-C(40)	120.9(15)	O(7)-Eu(1)-O(9)#7	137.9(4)
C(38)-N(1)-C(40)	117.7(15)	O(7)-Eu(1)-O(6)#8	81.4(3)
C(42)-N(2)-C(45)	120(3)	O(9)#7-Eu(1)-O(6)#8	75.5(3)
C(42)-N(2)-C(43)	114(3)	O(7)-Eu(1)-O(27)	137.3(4)
C(45)-N(2)-C(43)	126(3)	O(9)#7-Eu(1)-O(27)	79.1(4)
C(47)-N(3)-C(48)	125(3)	O(6)#8-Eu(1)-O(27)	138.1(4)
C(47')-N(3)-C(48)	122(3)	O(7)-Eu(1)-O(4)	81.8(3)
C(47)-N(3)-C(50)	120(3)	O(9)#7-Eu(1)-O(4)	97.3(4)
C(47')-N(3)-C(50)	116(2)	O(6)#8-Eu(1)-O(4)	144.7(3)
C(48)-N(3)-C(50)	115(2)	O(27)-Eu(1)-O(4)	70.9(4)
C(1)-O(1)-Eu(2)#3	133.8(9)	O(7)-Eu(1)-O(2)#7	119.4(3)
C(1)-O(2)-Eu(1)#3	143.1(8)	O(9)#7-Eu(1)-O(2)#7	87.0(3)
C(6)-O(3)-Eu(4)#4	142.4(8)	O(6)#8-Eu(1)-O(2)#7	73.3(3)
C(6)-O(4)-Eu(1)	126.7(9)	O(27)-Eu(1)-O(2)#7	72.7(3)
C(7)-O(5)-Eu(2)#1	164.3(9)	O(4)-Eu(1)-O(2)#7	141.7(3)
C(7)-O(6)-Eu(1)#1	117.5(8)	O(7)-Eu(1)-O(11)	68.7(3)
C(12)-O(7)-Eu(1)	147.4(8)	O(9)#7-Eu(1)-O(11)	153.3(4)
C(12)-O(8)-Eu(2)	129.0(7)	O(6)#8-Eu(1)-O(11)	114.1(3)
C(13)-O(9)-Eu(1)#3	169.7(10)	O(27)-Eu(1)-O(11)	78.0(3)
C(13)-O(10)-Eu(4)#5	133.0(8)	O(4)-Eu(1)-O(11)	88.0(3)
C(18)-O(11)-Eu(1)	166.8(9)	O(2)#7-Eu(1)-O(11)	73.2(3)
C(18)-O(11)-Eu(2)	85.0(8)	O(7)-Eu(1)-O(29)	68.2(3)
Eu(1)-O(11)-Eu(2)	107.3(3)	O(9)#7-Eu(1)-O(29)	71.0(4)
C(18)-O(12)-Eu(2)	102.2(8)	O(6)#8-Eu(1)-O(29)	70.6(3)
C(19)-O(13)-Eu(4)#2	102.9(7)	O(27)-Eu(1)-O(29)	130.2(3)
C(19)-O(14)-Eu(3)#2	171.2(8)	O(4)-Eu(1)-O(29)	74.4(4)
C(19)-O(14)-Eu(4)#2	85.0(7)	O(2)#7-Eu(1)-O(29)	141.3(4)
Eu(3)#2-O(14)-Eu(4)#2	103.8(3)	O(11)-Eu(1)-O(29)	135.2(3)
C(24)-O(15)-Eu(2)	129.7(8)	O(7)-Eu(1)-C(7)#8	73.4(3)
C(24)-O(16)-Eu(3)	163.9(9)	O(9)#7-Eu(1)-C(7)#8	93.5(4)

C(25)-O(17)-Eu(3)#6	135.8(7)	O(6)#8-Eu(1)-C(7)#8	20.5(3)
C(25)-O(18)-Eu(4)#6	136.1(7)	O(27)-Eu(1)-C(7)#8	136.2(4)
C(30)-O(19)-Eu(4)	169.8(8)	O(4)-Eu(1)-C(7)#8	152.6(4)
C(30)-O(19)-Eu(3)	84.4(7)	O(2)#7-Eu(1)-C(7)#8	63.8(3)
Eu(4)-O(19)-Eu(3)	103.2(3)	O(11)-Eu(1)-C(7)#8	93.6(3)
C(30)-O(20)-Eu(3)	103.9(7)	O(29)-Eu(1)-C(7)#8	85.6(3)
C(31)-O(21)-Eu(3)#2	133.4(8)	O(7)-Eu(1)-Eu(2)	58.8(2)
C(31)-O(22)-Eu(2)#2	143.2(9)	O(9)#7-Eu(1)-Eu(2)	142.1(2)
O(24)-Eu(4)-O(10)#6	75.6(3)	O(6)#8-Eu(1)-Eu(2)	75.2(2)
O(18)#5-Eu(4)-O(10)#6	145.7(3)	O(27)-Eu(1)-Eu(2)	108.4(2)
O(3)#10-Eu(4)-O(28)	79.2(4)	O(4)-Eu(1)-Eu(2)	120.5(2)
O(19)-Eu(4)-O(28)	84.7(4)	O(2)#7-Eu(1)-Eu(2)	61.73(19)
O(24)-Eu(4)-O(28)	144.2(5)	O(11)-Eu(1)-Eu(2)	39.0(2)
O(18)#5-Eu(4)-O(28)	72.8(4)	O(29)-Eu(1)-Eu(2)	119.86(16)
O(10)#6-Eu(4)-O(28)	73.5(4)	C(7)#8-Eu(1)-Eu(2)	54.8(2)
O(3)#10-Eu(4)-O(13)#9	70.7(3)	O(5)#8-Eu(2)-O(22)#9	136.3(3)
O(19)-Eu(4)-O(13)#9	125.8(3)	O(5)#8-Eu(2)-O(1)#7	78.8(3)
O(24)-Eu(4)-O(13)#9	78.4(3)	O(22)#9-Eu(2)-O(1)#7	138.6(3)
O(18)#5-Eu(4)-O(13)#9	80.9(3)	O(5)#8-Eu(2)-O(8)	80.2(3)
O(10)#6-Eu(4)-O(13)#9	129.5(3)	O(22)#9-Eu(2)-O(8)	79.1(3)
O(28)-Eu(4)-O(13)#9	136.2(4)	O(1)#7-Eu(2)-O(8)	137.9(3)
O(3)#10-Eu(4)-O(14)#9	118.4(3)	O(5)#8-Eu(2)-O(15)	78.3(3)
O(19)-Eu(4)-O(14)#9	77.4(2)	O(22)#9-Eu(2)-O(15)	82.2(3)
O(24)-Eu(4)-O(14)#9	68.6(3)	O(1)#7-Eu(2)-O(15)	86.5(3)
O(18)#5-Eu(4)-O(14)#9	66.0(2)	O(8)-Eu(2)-O(15)	124.0(3)
O(10)#6-Eu(4)-O(14)#9	143.6(3)	O(5)#8-Eu(2)-O(12)	133.8(3)
O(28)-Eu(4)-O(14)#9	136.9(3)	O(22)#9-Eu(2)-O(12)	80.5(3)
O(13)#9-Eu(4)-O(14)#9	48.7(2)	O(1)#7-Eu(2)-O(12)	86.4(4)
O(3)#10-Eu(4)-C(19)#9	93.8(3)	O(8)-Eu(2)-O(12)	82.4(3)
O(19)-Eu(4)-C(19)#9	102.2(3)	O(15)-Eu(2)-O(12)	144.6(3)
O(24)-Eu(4)-C(19)#9	74.1(3)	O(5)#8-Eu(2)-O(25)	139.9(3)
O(18)#5-Eu(4)-C(19)#9	70.0(3)	O(22)#9-Eu(2)-O(25)	73.0(3)
O(10)#6-Eu(4)-C(19)#9	144.2(3)	O(1)#7-Eu(2)-O(25)	65.9(3)
O(28)-Eu(4)-C(19)#9	140.7(4)	O(8)-Eu(2)-O(25)	139.3(3)
O(13)#9-Eu(4)-C(19)#9	24.0(3)	O(15)-Eu(2)-O(25)	80.9(3)
O(14)#9-Eu(4)-C(19)#9	24.8(3)	O(12)-Eu(2)-O(25)	64.6(3)

O(3)#10-Eu(4)-Eu(3)	151.9(2)	O(5)#8-Eu(2)-O(11)	84.4(3)
O(19)-Eu(4)-Eu(3)	43.4(2)	O(22)#9-Eu(2)-O(11)	123.7(3)
O(24)-Eu(4)-Eu(3)	67.91(19)	O(1)#7-Eu(2)-O(11)	70.6(3)
O(18)#5-Eu(4)-Eu(3)	67.83(19)	O(8)-Eu(2)-O(11)	71.3(3)
O(10)#6-Eu(4)-Eu(3)	124.3(2)	O(15)-Eu(2)-O(11)	153.6(3)
O(28)-Eu(4)-Eu(3)	117.1(2)	O(12)-Eu(2)-O(11)	49.5(3)
O(13)#9-Eu(4)-Eu(3)	82.55(19)	O(25)-Eu(2)-O(11)	100.6(2)
O(14)#9-Eu(4)-Eu(3)	33.96(14)	O(5)#8-Eu(2)-C(18)	109.3(4)
C(19)#9-Eu(4)-Eu(3)	58.8(2)	O(22)#9-Eu(2)-C(18)	101.5(3)
O(16)-Eu(3)-O(20)	73.8(3)	O(1)#7-Eu(2)-C(18)	78.7(4)
O(14)#9-Eu(3)-O(20)	123.2(3)	O(8)-Eu(2)-C(18)	74.5(3)
O(21)#9-Eu(3)-O(20)	136.3(3)	O(15)-Eu(2)-C(18)	161.4(4)
O(17)#5-Eu(3)-O(20)	85.8(3)	O(12)-Eu(2)-C(18)	24.4(3)
O(26)-Eu(3)-O(20)	137.1(3)	O(25)-Eu(2)-C(18)	82.8(3)
O(23)-Eu(3)-O(20)	76.3(3)	O(11)-Eu(2)-C(18)	25.1(3)
O(16)-Eu(3)-O(25)	68.7(3)	O(5)#8-Eu(2)-Eu(1)	50.6(2)
O(14)#9-Eu(3)-O(25)	138.6(3)	O(22)#9-Eu(2)-Eu(1)	146.7(2)
O(21)#9-Eu(3)-O(25)	70.9(3)	O(1)#7-Eu(2)-Eu(1)	68.4(2)
O(17)#5-Eu(3)-O(25)	66.6(3)	O(8)-Eu(2)-Eu(1)	70.0(2)
O(26)-Eu(3)-O(25)	125.9(3)	O(15)-Eu(2)-Eu(1)	125.5(2)
O(23)-Eu(3)-O(25)	137.8(3)	O(12)-Eu(2)-Eu(1)	83.2(2)
O(20)-Eu(3)-O(25)	65.4(3)	O(25)-Eu(2)-Eu(1)	124.59(12)
O(16)-Eu(3)-O(19)	117.3(3)	O(11)-Eu(2)-Eu(1)	33.76(16)
O(14)#9-Eu(3)-O(19)	75.6(2)	C(18)-Eu(2)-Eu(1)	58.8(3)
O(21)#9-Eu(3)-O(19)	144.7(3)	O(16)-Eu(3)-O(14)#9	150.4(3)
O(17)#5-Eu(3)-O(19)	68.4(3)	O(16)-Eu(3)-O(21)#9	91.1(3)
O(26)-Eu(3)-O(19)	133.3(3)	O(14)#9-Eu(3)-O(21)#9	89.9(3)
O(23)-Eu(3)-O(19)	64.3(3)	O(16)-Eu(3)-O(17)#5	135.3(3)
O(20)-Eu(3)-O(19)	47.6(3)	O(14)#9-Eu(3)-O(17)#5	73.5(3)
O(25)-Eu(3)-O(19)	98.9(2)	O(21)#9-Eu(3)-O(17)#5	76.7(3)
O(16)-Eu(3)-C(30)	94.4(3)	O(16)-Eu(3)-O(26)	74.3(3)
O(14)#9-Eu(3)-C(30)	99.7(3)	O(14)#9-Eu(3)-O(26)	77.9(3)
O(21)#9-Eu(3)-C(30)	149.3(3)	O(21)#9-Eu(3)-O(26)	71.8(3)
O(17)#5-Eu(3)-C(30)	78.2(3)	O(17)#5-Eu(3)-O(26)	137.0(3)
O(26)-Eu(3)-C(30)	138.6(3)	O(16)-Eu(3)-O(23)	84.6(3)
O(23)-Eu(3)-C(30)	66.5(3)	O(14)#9-Eu(3)-O(23)	77.5(3)

O(20)-Eu(3)-C(30)	23.5(3)	O(21)#9-Eu(3)-O(23)	144.2(3)
O(25)-Eu(3)-C(30)	83.0(3)	O(17)#5-Eu(3)-O(23)	129.0(3)
O(19)-Eu(3)-C(30)	24.3(3)	O(26)-Eu(3)-O(23)	72.8(3)
O(16)-Eu(3)-Eu(4)	144.7(2)	O(14)#9-Eu(3)-Eu(4)	42.25(19)
O(19)-Eu(4)-O(24)	77.3(3)	O(21)#9-Eu(3)-Eu(4)	124.1(2)
O(3)#10-Eu(4)-O(18)#5	98.6(3)	O(17)#5-Eu(3)-Eu(4)	64.8(2)
O(19)-Eu(4)-O(18)#5	81.6(3)	O(26)-Eu(3)-Eu(4)	111.3(2)
O(24)-Eu(4)-O(18)#5	133.0(3)	O(23)-Eu(3)-Eu(4)	65.41(19)
O(3)#10-Eu(4)-O(10)#6	81.1(3)	O(20)-Eu(3)-Eu(4)	81.0(2)
O(19)-Eu(4)-O(10)#6	89.1(3)	O(25)-Eu(3)-Eu(4)	121.87(12)
O(3)#10-Eu(4)-O(19)	163.0(3)	O(19)-Eu(3)-Eu(4)	33.36(15)
O(3)#10-Eu(4)-O(24)	113.3(3)	C(30)-Eu(3)-Eu(4)	57.6(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y-1/2,-z+1 #2 -x,y+1/2,-z+2 #3 -x+1,y-1/2,-z+1 #4 x,y,z-1 #5 -x+1,y-1/2,-z+2 #6 -x+1,y+1/2,-z+2 #7 -x+1,y+1/2,-z+1 #8 -x,y+1/2,-z+1 #9 -x,y-1/2,-z+2 #10 x,y,z+1

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Gd1	$Gd1^{1}$	3.9863(4)	C30	O32	1.253(6)
Gd1	$O35^{2}$	2.417(3)	C30	C26	1.482(6)
Gd1	O36	2.368(3)	C30	O31	1.253(5)
Gd1	O13	2.384(3)	C6	C7	1.375(6)
Gd1	$O34^{1}$	2.679(3)	C6	C5	1.407(6)
Gd1	O34	2.371(3)	C16	C17	1.415(6)
Gd1	O21	2.306(3)	O9	$Gd2^{5}$	2.283(3)
Gd1	$O20^{3}$	2.324(3)	O9	C8	1.266(5)
Gd1	$O12^{1}$	2.366(3)	O23	$Gd2^{4}$	2.827(3)
Gd1	$C33^{2}$	2.923(4)	O23	$C22^{4}$	1.267(5)
Gd2	$Gd2^{4}$	4.0556(4)	C22	$O23^{4}$	1.267(5)
Gd2	O10	2.308(3)	C22	C18	1.476(6)
Gd2	O24	2.365(3)	O34	$Gd1^{1}$	2.679(3)
Gd2	$O9^{5}$	2.283(3)	O34	$C33^{6}$	1.274(5)

Gd2	O23	2.360(3)	C18	C17	1.373(6)
Gd2	O23^{4}	2.827(3)	C26	C27	1.362(6)
Gd2	C22	2.956(4)	C28	C27	1.416(6)
Gd2	O32	2.356(3)	C11	C7	1.491(6)
Gd2	O43	2.446(3)	C11	O12	1.258(5)
Gd2	O31^{4}	2.344(3)	O43	C44	1.241(8)
S3	C7	1.726(4)	O31	Gd2^{4}	2.344(3)
S3	C4	1.725(4)	N38	C37	1.318(6)
S14	C15	1.717(4)	N38	C39	1.462(6)
S14	C18	1.724(4)	N38	C41	1.470(6)
S25	C29	1.725(4)	C4	C5	1.368(6)
S25	C26	1.725(4)	C4	C8	1.484(6)
O10	C8	1.253(5)	C39	C40	1.505(7)
O35	Gd1^{2}	2.417(3)	C41	C42	1.518(7)
O35	C33	1.259(5)	N45	C44	1.333(9)
C19	C15	1.487(6)	N45	C46	1.532(10)
C19	O21	1.280(5)	N45	C48	1.459(10)
C19	O20	1.234(5)	O20	Gd1^{3}	2.324(3)
O24	C22	1.259(5)	O12	Gd1^{1}	2.366(3)
O36	C37	1.230(6)	C33	Gd1^{2}	2.923(4)
O13	C11	1.251(5)	C33	O34^{7}	1.274(5)
C29	C28	1.353(6)	C46	C47	1.463(11)
C29	C33	1.472(6)	C49	C48	1.482(13)
C15	C16	1.374(6)			

O35^{1}	Gd1	Gd1^{2}	85.91(7)	O31^{4}	Gd2	O23	74.17(11)
O35^{1}	Gd1	O34^{2}	50.83(10)	O31^{4}	Gd2	C22	75.70(11)
O35^{1}	Gd1	C33^{1}	25.04(11)	O31^{4}	Gd2	O32	134.20(11)
O36	Gd1	Gd1^{2}	137.74(8)	O31^{4}	Gd2	O43	72.47(12)
O36	Gd1	O35^{1}	74.36(11)	C4	S3	C7	90.9(2)
O36	Gd1	O13	73.52(11)	C15	S14	C18	91.1(2)
O36	Gd1	O34	137.67(11)	C26	S25	C29	90.9(2)
O36	Gd1	O34^{2}	116.55(11)	C8	O10	Gd2	161.8(3)
O36	Gd1	C33^{1}	95.90(12)	C33	O35	Gd1^{1}	100.6(3)
O13	Gd1	Gd1^{2}	69.09(8)	O21	C19	C15	116.0(4)
O13	Gd1	O35^{1}	89.10(11)	O20	C19	C15	119.0(4)
O13	Gd1	O34^{2}	76.04(10)	O20	C19	O21	125.0(4)
O13	Gd1	C33^{1}	82.97(11)	C22	O24	Gd2	105.1(3)

O34^{2}	Gd1	Gd1^{2}	35.23(6)	C37	O36	Gd1	133.8(3)
O34	Gd1	Gd1^{2}	40.69(7)	C11	O13	Gd1	135.4(3)
O34	Gd1	O35^{1}	126.43(10)	C28	C29	S25	112.6(3)
O34	Gd1	O13	70.89(11)	C28	C29	C33	127.8(4)
O34	Gd1	O34^{2}	75.91(10)	C33	C29	S25	119.6(3)
O34^{2}	Gd1	C33^{1}	25.83(10)	C19	C15	S14	119.6(3)
O34	Gd1	C33^{1}	101.69(11)	C16	C15	S14	112.3(3)
O21	Gd1	Gd1^{2}	124.88(8)	C16	C15	C19	128.1(4)
O21	Gd1	O35^{1}	148.75(11)	O32	C30	C26	117.2(4)
O21	Gd1	O36	77.99(11)	O32	C30	O31	127.3(4)
O21	Gd1	O13	96.82(11)	O31	C30	C26	115.5(4)
O21	Gd1	O34	84.20(11)	C7	C6	C5	113.1(4)
O21	Gd1	O34^{2}	160.09(10)	C15	C16	C17	112.2(4)
O21	Gd1	O20^{3}	79.91(10)	C8	O9	Gd2^{5}	137.8(3)
O21	Gd1	O12^{2}	103.51(11)	Gd2	O23	Gd2^{4}	102.49(10)
O21	Gd1	C33^{1}	173.63(12)	C22^{4}	O23	Gd2^{4}	83.1(3)
O20^{3}	Gd1	Gd1^{2}	137.41(8)	C22^{4}	O23	Gd2	173.2(3)
O20^{3}	Gd1	O35^{1}	79.42(11)	O24	C22	Gd2	50.6(2)
O20^{3}	Gd1	O36	75.67(11)	O24	C22	O23^{4}	121.9(4)
O20^{3}	Gd1	O13	149.01(11)	O24	C22	C18	117.5(4)
O20^{3}	Gd1	O34	138.28(11)	O23^{4}	C22	Gd2	71.7(2)
O20^{3}	Gd1	O34^{2}	115.78(10)	O23^{4}	C22	C18	120.6(4)
O20^{3}	Gd1	O12^{2}	73.32(11)	C18	C22	Gd2	166.0(3)
O20^{3}	Gd1	C33^{1}	96.97(11)	C30	O32	Gd2	137.6(3)
O12^{2}	Gd1	Gd1^{2}	67.65(8)	Gd1	O34	Gd1^{2}	104.09(10)
O12^{2}	Gd1	O35^{1}	92.66(12)	C33^{6}	O34	Gd1^{2}	87.8(2)
O12^{2}	Gd1	O36	148.09(11)	C33^{6}	O34	Gd1	167.6(3)
O12^{2}	Gd1	O13	136.45(11)	C22	C18	S14	117.3(3)
O12^{2}	Gd1	O34^{2}	71.80(11)	C17	C18	S14	112.1(3)
O12^{2}	Gd1	O34	73.36(11)	C17	C18	C22	130.6(4)
O12^{2}	Gd1	C33^{1}	80.72(12)	C30	C26	S25	121.2(4)
C33^{1}	Gd1	Gd1^{2}	61.02(9)	C27	C26	S25	111.4(3)
O10	Gd2	Gd2^{4}	136.51(8)	C27	C26	C30	127.2(4)
O10	Gd2	O24	77.70(11)	C29	C28	C27	111.9(4)
O10	Gd2	O23	140.72(12)	O13	C11	C7	117.6(4)
O10	Gd2	O23^{4}	113.25(10)	O13	C11	O12	127.0(4)
O10	Gd2	C22	94.29(11)	O12	C11	C7	115.4(4)

O10	Gd2	O32	73.22(12)	C44	O43	Gd2	126.2(4)
O10	Gd2	O43	75.82(12)	C30	O31	Gd2^{4}	139.2(3)
O10	Gd2	O31^{4}	144.95(12)	C37	N38	C39	119.1(4)
O24	Gd2	Gd2^{4}	83.77(8)	C37	N38	C41	121.5(4)
O24	Gd2	O23^{4}	49.38(10)	C39	N38	C41	119.4(4)
O24	Gd2	C22	24.28(12)	C6	C7	S3	111.5(3)
O24	Gd2	O43	76.47(12)	C6	C7	C11	127.2(4)
O9^{5}	Gd2	Gd2^{4}	123.29(8)	C11	C7	S3	121.3(3)
O9^{5}	Gd2	O10	87.97(11)	C5	C4	S3	112.4(3)
O9^{5}	Gd2	O24	150.05(11)	C5	C4	C8	127.0(4)
O9^{5}	Gd2	O23	80.71(11)	C8	C4	S3	120.5(3)
O9^{5}	Gd2	O23^{4}	157.22(10)	O36	C37	N38	124.2(4)
O9^{5}	Gd2	C22	171.09(12)	C4	C5	C6	112.1(4)
O9^{5}	Gd2	O32	111.12(12)	C26	C27	C28	113.3(4)
O9^{5}	Gd2	O43	74.56(12)	C18	C17	C16	112.3(4)
O9^{5}	Gd2	O31^{4}	97.56(11)	N38	C39	C40	111.3(4)
O23	Gd2	Gd2^{4}	42.89(8)	N38	C41	C42	111.4(4)
O23^{4}	Gd2	Gd2^{4}	34.62(6)	C44	N45	C46	119.6(6)
O23	Gd2	O24	126.40(11)	C44	N45	C48	121.4(8)
O23	Gd2	O23^{4}	77.51(10)	C48	N45	C46	118.6(7)
O23^{4}	Gd2	C22	25.19(10)	C19	O21	Gd1	135.8(3)
O23	Gd2	C22	102.64(12)	C19	O20	Gd1^{3}	171.0(3)
O23	Gd2	O43	134.89(11)	C11	O12	Gd1^{2}	137.0(3)
C22	Gd2	Gd2^{4}	59.77(9)	O10	C8	O9	124.6(4)
O32	Gd2	Gd2^{4}	67.73(8)	O10	C8	C4	118.6(4)
O32	Gd2	O24	89.93(12)	O9	C8	C4	116.8(4)
O32	Gd2	O23^{4}	69.91(11)	O35	C33	Gd1^{1}	54.4(2)
O32	Gd2	O23	76.12(11)	O35	C33	C29	119.3(4)
O32	Gd2	C22	77.77(12)	O35	C33	O34^{7}	120.6(4)
O32	Gd2	O43	148.19(12)	C29	C33	Gd1^{1}	172.8(3)
O43	Gd2	Gd2^{4}	136.91(9)	O34^{7}	C33	Gd1^{1}	66.4(2)
O43	Gd2	O23^{4}	117.29(11)	O34^{7}	C33	C29	120.2(4)
O43	Gd2	C22	97.61(12)	O43	C44	N45	127.2(7)
O31^{4}	Gd2	Gd2^{4}	66.73(8)	C47	C46	N45	115.1(9)
O31^{4}	Gd2	O24	80.70(11)	N45	C48	C49	113.0(8)
O31^{4}	Gd2	O23^{4}	70.18(10)				

[1]2-X,2-Y,1-Z; [2]2-X,1-Y,1-Z; [3]2-X,+Y,3/2-Z; [4]1-X,2-Y,1-Z; [5]1-X,+Y,1/2-Z; [6]+X,-1+Y,+Z; [7]+X,1+Y,+Z[1]2-X,1-Y,1-Z; [2]2-X,2-Y,1-Z; [3]2-X,+Y,3/2-Z; [4]1-X,2-Y,1-Z; [5]1-X,+Y,1/2-Z; [6]+X,-1+Y,+Z; [7]+X,1+Y,+Z

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Tb1	Tb1[1]	3.9846(3)	C8	O9[4]	1.235(4)
Tb1	O10	2.288(3)	C8	C4	1.482(5)
Tb1	O9	2.312(2)	O36	C37	1.237(4)
Tb1	O32	2.348(2)	O12	C11	1.261(4)
Tb1	O32[1]	2.696(3)	C19	O20[3]	1.268(4)
Tb1	O24	2.348(3)	C19	C15	1.478(5)
Tb1	O23	2.363(2)	O43	C44	1.239(5)
Tb1	O36	2.358(3)	C4	C5	1.366(5)
Tb1	O31	2.399(2)	O31	C30	1.260(4)
Tb1	C30	2.918(4)	N38	C37	1.322(5)
Tb2	O21	2.293(3)	N38	C39	1.459(5)
Tb2	O35	2.339(2)	N38	C41	1.472(5)
Tb2	O20	2.264(2)	C33	O34[2]	1.261(4)
Tb2	O13	2.333(3)	C33	C29	1.481(5)
Tb2	O13[2]	2.883(3)	C15	C16	1.369(5)
Tb2	O34	2.330(2)	C26	C30[5]	1.470(5)
Tb2	O12	2.349(2)	C26	C27	1.376(5)
Tb2	O43	2.431(3)	C17	C16	1.413(5)
Tb2	C11	2.970(3)	C17	C18	1.363(5)
S3	C4	1.720(3)	C22	O23[1]	1.267(4)
S3	C7	1.719(4)	C22	C18[1]	1.493(5)
S14	C15	1.727(4)	C29	C28	1.375(5)
S14	C18	1.725(4)	C18	C22[1]	1.494(5)
S25	C26	1.729(4)	C30	O32[1]	1.273(4)
S25	C29	1.721(4)	C30	C26[5]	1.470(5)
O10	C8	1.283(4)	C27	C28	1.402(5)
O21	C19	1.244(4)	C11	O13[2]	1.269(4)
O35	C33	1.253(4)	C11	C7	1.477(5)

O20	C19[3]	1.268(4)	C6	C7	1.364(5)
O9	C8[4]	1.235(4)	C6	C5	1.420(5)
O32	Tb1[1]	2.696(3)	C39	C40	1.510(6)
O32	C30[1]	1.273(4)	N45	C44	1.317(6)
O24	C22	1.255(4)	N45	C46	1.502(7)
O13	Tb2[2]	2.883(3)	N45	C48	1.465(7)
O13	C11[2]	1.269(4)	C41	C42	1.518(6)
O34	C33[2]	1.261(4)	C46	C47	1.478(7)
O23	C22[1]	1.267(4)	C49	C48	1.495(8)

O10	Tb1	Tb1[1]	124.96(6)	C7	S3	C4	91.15(18)
O10	Tb1	O9	79.77(9)	C18	S14	C15	90.95(17)
O10	Tb1	O32[1]	159.77(8)	C29	S25	C26	91.10(18)
O10	Tb1	O32	83.98(9)	C8	O10	Tb1	136.2(2)
O10	Tb1	O24	104.17(9)	C19	O21	Tb2	161.7(3)
O10	Tb1	O23	96.60(9)	C33	O35	Tb2	138.3(2)
O10	Tb1	O36	78.20(9)	C19[3]	O20	Tb2	137.7(2)
O10	Tb1	O31	148.93(8)	C8[4]	O9	Tb1	170.1(2)
O10	Tb1	C30	173.59(9)	Tb1	O32	Tb1[1]	104.16(9)
O9	Tb1	Tb1[1]	137.59(6)	C30[1]	O32	Tb1	168.3(2)
O9	Tb1	O32[1]	116.46(8)	C30[1]	O32	Tb1[1]	86.9(2)
O9	Tb1	O32	137.86(9)	C22	O24	Tb1	137.7(2)
O9	Tb1	O24	73.36(9)	Tb2	O13	Tb2[2]	102.19(8)
O9	Tb1	O23	149.09(9)	C11[2]	O13	Tb2	176.0(2)
O9	Tb1	O36	75.67(9)	C11[2]	O13	Tb2[2]	81.3(2)
O9	Tb1	O31	80.02(9)	C33[2]	O34	Tb2	139.7(2)
O9	Tb1	C30	97.82(9)	C22[1]	O23	Tb1	135.7(2)
O32[1]	Tb1	Tb1[1]	34.84(5)	O10	C8	C4	116.1(3)
O32	Tb1	Tb1[1]	41.00(6)	O9[4]	C8	O10	124.6(3)
O32	Tb1	O32[1]	75.84(9)	O9[4]	C8	C4	119.3(3)
O32	Tb1	O23	71.06(9)	C37	O36	Tb1	132.7(2)
O32	Tb1	O36	137.94(9)	C11	O12	Tb2	106.8(2)
O32	Tb1	O31	126.41(9)	O21	C19	O20[3]	125.0(3)
O32	Tb1	C30	101.60(9)	O21	C19	C15	118.1(3)
O32[1]	Tb1	C30	25.81(8)	O20[3]	C19	C15	116.8(3)
O24	Tb1	Tb1[1]	67.59(6)	C44	O43	Tb2	126.7(3)
O24	Tb1	O32	73.43(9)	C8	C4	S3	119.6(3)

O24	Tb1	O32[1]	71.63(9)	C5	C4	S3	112.2(3)
O24	Tb1	O23	136.32(9)	C5	C4	C8	128.2(3)
O24	Tb1	O36	147.90(9)	C30	O31	Tb1	101.2(2)
O24	Tb1	O31	92.29(10)	C37	N38	C39	119.3(3)
O24	Tb1	C30	80.63(10)	C37	N38	C41	120.8(3)
O23	Tb1	Tb1[1]	68.98(6)	C39	N38	C41	119.9(3)
O23	Tb1	O32[1]	75.67(8)	O35	C33	O34[2]	126.9(3)
O23	Tb1	O31	88.85(9)	O35	C33	C29	117.8(3)
O23	Tb1	C30	82.39(9)	O34[2]	C33	C29	115.4(3)
O36	Tb1	Tb1[1]	137.43(6)	C19	C15	S14	121.2(3)
O36	Tb1	O32[1]	116.23(8)	C16	C15	S14	111.8(3)
O36	Tb1	O23	73.55(9)	C16	C15	C19	126.9(3)
O36	Tb1	O31	74.08(9)	C30[5]	C26	S25	120.0(3)
O36	Tb1	C30	95.47(10)	C27	C26	S25	111.9(3)
O31	Tb1	Tb1[1]	85.55(6)	C27	C26	C30[5]	128.1(3)
O31	Tb1	O32[1]	50.85(8)	C18	C17	C16	112.6(3)
O31	Tb1	C30	25.06(9)	C15	C16	C17	112.5(3)
C30	Tb1	Tb1[1]	60.62(7)	O24	C22	O23[1]	126.3(3)
O21	Tb2	O35	73.42(9)	O24	C22	C18[1]	116.0(3)
O21	Tb2	O13[2]	114.04(8)	O23[1]	C22	C18[1]	117.6(3)
O21	Tb2	O13	140.02(9)	C33	C29	S25	121.3(3)
O21	Tb2	O34	145.28(9)	C28	C29	S25	111.7(3)
O21	Tb2	O12	78.22(9)	C28	C29	C33	126.8(3)
O21	Tb2	O43	76.03(9)	C17	C18	S14	112.1(3)
O21	Tb2	C11	94.83(10)	C17	C18	C22[1]	126.8(3)
O35	Tb2	O13[2]	69.35(8)	C22[1]	C18	S14	121.1(3)
O35	Tb2	O12	88.18(9)	O32[1]	C30	Tb1	67.30(19)
O35	Tb2	O43	148.15(9)	O32[1]	C30	C26[5]	120.0(3)
O35	Tb2	C11	76.37(10)	O31	C30	Tb1	53.75(17)
O20	Tb2	O21	87.97(9)	O31	C30	O32[1]	121.0(3)
O20	Tb2	O35	112.56(9)	O31	C30	C26[5]	119.0(3)
O20	Tb2	O13[2]	156.63(8)	C26[5]	C30	Tb1	171.9(2)
O20	Tb2	O13	80.11(9)	C26	C27	C28	112.2(3)
O20	Tb2	O34	97.20(9)	O13[2]	C11	Tb2	73.67(19)
O20	Tb2	O12	150.80(9)	O13[2]	C11	C7	120.3(3)
O20	Tb2	O43	74.79(9)	O12	C11	Tb2	49.22(17)
O20	Tb2	C11	171.07(9)	O12	C11	O13[2]	122.4(3)

O13	Tb2	O35	76.31(9)	O12	C11	C7	117.3(3)
O13	Tb2	O13[2]	77.82(8)	C7	C11	Tb2	164.1(3)
O13	Tb2	O12	126.35(9)	C7	C6	C5	112.6(3)
O13	Tb2	O43	134.96(9)	C29	C28	C27	113.1(3)
O13	Tb2	C11	102.80(9)	O36	C37	N38	122.9(4)
O13[2]	Tb2	C11	25.00(8)	C11	C7	S3	117.8(3)
O34	Tb2	O35	133.40(9)	C6	C7	S3	112.0(3)
O34	Tb2	O13[2]	69.54(8)	C6	C7	C11	130.2(3)
O34	Tb2	O13	74.47(9)	N38	C39	C40	111.9(3)
O34	Tb2	O12	80.97(9)	C44	N45	C46	120.2(4)
O34	Tb2	O43	72.37(9)	C44	N45	C48	121.0(5)
O34	Tb2	C11	75.72(9)	C48	N45	C46	118.5(4)
O12	Tb2	O13[2]	48.85(8)	N38	C41	C42	111.0(3)
O12	Tb2	O43	76.95(9)	C4	C5	C6	112.0(3)
O12	Tb2	C11	23.98(9)	O43	C44	N45	126.5(5)
O43	Tb2	O13[2]	116.67(8)	C47	C46	N45	114.2(6)
O43	Tb2	C11	97.64(9)	N45	C48	C49	114.1(5)

[1]-X,2-Y,1-Z; [2]1-X,1-Y,1-Z; [3]1-X,+Y,3/2-Z; [4]-X,+Y,1/2-Z; [5]-X,1-Y,1-Z[1]-X,2-Y,1-Z; [2]1-X,1-Y,1-Z; [3]1-X,+Y,3/2-Z; [4]-X,+Y,1/2-Z; [5]-X,1-Y,1-Z

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Dy1	Dy1[1]	3.9815(4)	C19	C15	1.481(6)
Dy1	O21	2.278(3)	C8	O10[4]	1.235(5)
Dy1	O20	2.304(3)	C8	C4	1.478(6)
Dy1	O32	2.338(3)	O23	C22[3]	1.266(5)
Dy1	O32[1]	2.708(3)	O31	Dy1[6]	2.379(3)
Dy1	O13	2.333(3)	O31	C30	1.261(5)
Dy1	O36	2.348(3)	O43	C44	1.240(7)
Dy1	O12	2.353(3)	N38	C37	1.322(6)
Dy1	O31[2]	2.379(3)	N38	C39	1.451(6)
Dy1	C30[2]	2.913(4)	N38	C41	1.467(6)
Dy2	O10	2.280(3)	C15	C16	1.365(6)
Dy2	O9	2.249(3)	C4	C5	1.366(6)
Dy2	O35	2.335(3)	C7	C11	1.486(6)
Dy2	O34	2.316(3)	C7	C6	1.366(6)

Dy2	O24[3]	2.881(3)	C26	C30	1.475(6)
Dy2	O24	2.326(3)	C26	C27	1.373(6)
Dy2	O23	2.327(3)	C29	C33	1.485(6)
Dy2	O43	2.420(3)	C29	C28	1.371(6)
Dy2	C22[3]	2.966(4)	C5	C6	1.417(6)
S3	C4	1.734(4)	C11	O12[1]	1.262(5)
S3	C7	1.729(4)	C33	O35[3]	1.252(5)
S14	C15	1.725(4)	C18	C22[7]	1.471(6)
S14	C18	1.722(4)	C18	C17	1.366(6)
S25	C26	1.730(4)	C22	Dy2[3]	2.966(4)
S25	C29	1.721(4)	C22	O23[3]	1.266(5)
O10	C8[4]	1.235(5)	C22	C18[8]	1.471(6)
O21	C19[5]	1.266(5)	C30	Dy1[6]	2.913(4)
O9	C8	1.277(5)	C30	O32[5]	1.268(5)
O20	C19	1.247(5)	C27	C28	1.403(6)
O32	Dy1[1]	2.708(3)	C16	C17	1.409(6)
O32	C30[5]	1.269(5)	C39	C40	1.511(7)
O35	C33[3]	1.252(5)	C41	C42	1.515(7)
O13	C11	1.256(5)	N45	C44	1.328(8)
O34	C33	1.254(5)	N45	C46	1.507(9)
O36	C37	1.240(5)	N45	C48	1.471(9)
O24	Dy2[3]	2.881(3)	C46	C47	1.463(10)
O24	C22	1.263(5)	C49	C48	1.474(12)
O12	C11[1]	1.262(5)	O2	O2[4]	0.0(2)
C19	O21[5]	1.266(5)			

O21	Dy1	Dy1[1]	124.98(7)	C7	S3	C4	91.3(2)
O21	Dy1	O20	79.63(10)	C18	S14	C15	91.1(2)
O21	Dy1	O32[1]	159.66(10)	C29	S25	C26	90.9(2)
O21	Dy1	O32	83.69(11)	C8[4]	O10	Dy2	161.8(3)
O21	Dy1	O13	104.65(11)	C19[5]	O21	Dy1	136.4(3)
O21	Dy1	O36	78.38(11)	C8	O9	Dy2	138.0(3)
O21	Dy1	O12	96.47(11)	C19	O20	Dy1	170.4(3)
O21	Dy1	O31[2]	149.05(10)	Dy1	O32	Dy1[1]	103.94(10)
O21	Dy1	C30[2]	173.67(11)	C30[5]	O32	Dy1	169.5(3)
O20	Dy1	Dy1[1]	137.60(8)	C30[5]	O32	Dy1[1]	86.2(3)
O20	Dy1	O32	137.21(11)	C33[3]	O35	Dy2	137.9(3)

O20	Dy1	O32[1]	116.87(10)	C11	O13	Dy1	137.8(3)
O20	Dy1	O13	73.21(11)	C33	O34	Dy2	139.9(3)
O20	Dy1	O36	75.74(11)	C37	O36	Dy1	132.8(3)
O20	Dy1	O12	149.34(10)	Dy2	O24	Dy2[3]	102.14(10)
O20	Dy1	O31[2]	80.16(11)	C22	O24	Dy2[3]	81.3(3)
O20	Dy1	C30[2]	98.10(11)	C22	O24	Dy2	176.1(3)
O32[1]	Dy1	Dy1[1]	34.75(6)	C11[1]	O12	Dy1	135.7(3)
O32	Dy1	Dy1[1]	41.31(8)	O21[5]	C19	C15	117.3(4)
O32	Dy1	O32[1]	76.06(11)	O20	C19	O21[5]	125.0(4)
O32	Dy1	O36	138.31(11)	O20	C19	C15	117.7(4)
O32	Dy1	O12	71.33(11)	O10[4]	C8	O9	125.4(4)
O32	Dy1	O31[2]	126.65(11)	O10[4]	C8	C4	118.8(4)
O32[1]	Dy1	C30[2]	25.75(10)	O9	C8	C4	115.8(4)
O32	Dy1	C30[2]	101.78(11)	C22[3]	O23	Dy2	107.6(3)
O13	Dy1	Dy1[1]	67.52(8)	C30	O31	Dy1[6]	101.9(3)
O13	Dy1	O32	73.42(11)	C44	O43	Dy2	126.6(4)
O13	Dy1	O32[1]	71.60(11)	C37	N38	C39	119.6(4)
O13	Dy1	O36	147.60(11)	C37	N38	C41	120.6(4)
O13	Dy1	O12	136.22(11)	C39	N38	C41	119.8(4)
O13	Dy1	O31[2]	91.58(12)	C19	C15	S14	118.7(3)
O13	Dy1	C30[2]	80.16(12)	C16	C15	S14	111.6(3)
O36	Dy1	Dy1[1]	137.34(8)	C16	C15	C19	129.7(4)
O36	Dy1	O32[1]	115.88(10)	C8	C4	S3	120.5(3)
O36	Dy1	O12	73.70(10)	C5	C4	S3	111.4(3)
O36	Dy1	O31[2]	74.07(11)	C5	C4	C8	128.0(4)
O36	Dy1	C30[2]	95.35(12)	C11	C7	S3	121.4(3)
O12	Dy1	Dy1[1]	68.91(7)	C6	C7	S3	111.7(3)
O12	Dy1	O32[1]	75.37(10)	C6	C7	C11	126.9(4)
O12	Dy1	O31[2]	89.17(11)	C30	C26	S25	119.8(3)
O12	Dy1	C30[2]	82.45(11)	C27	C26	S25	112.0(3)
O31[2]	Dy1	Dy1[1]	85.44(7)	C27	C26	C30	128.1(4)
O31[2]	Dy1	O32[1]	50.79(9)	C33	C29	S25	121.2(3)
O31[2]	Dy1	C30[2]	25.06(11)	C28	C29	S25	111.8(3)
C30[2]	Dy1	Dy1[1]	60.48(8)	C28	C29	C33	126.9(4)
O10	Dy2	O35	73.28(11)	C4	C5	C6	112.9(4)
O10	Dy2	O34	145.56(11)	O13	C11	O12[1]	126.6(4)
O10	Dy2	O24	139.66(11)	O13	C11	C7	115.8(4)

O10	Dy2	O24^{3}	114.17(10)	O12^{1}	C11	C7	117.5(4)
O10	Dy2	O23	78.46(11)	C7	C6	C5	112.7(4)
O10	Dy2	O43	75.79(11)	O35^{3}	C33	O34	127.0(4)
O10	Dy2	C22^{3}	95.05(12)	O35^{3}	C33	C29	117.5(4)
O9	Dy2	O10	87.52(11)	O34	C33	C29	115.5(4)
O9	Dy2	O35	111.97(11)	C22^{7}	C18	S14	117.7(3)
O9	Dy2	O34	97.91(11)	C17	C18	S14	112.0(3)
O9	Dy2	O24	80.01(11)	C17	C18	C22^{7}	130.3(4)
O9	Dy2	O24^{3}	156.74(10)	O24	C22	Dy2^{3}	73.8(2)
O9	Dy2	O23	151.20(11)	O24	C22	O23^{3}	121.7(4)
O9	Dy2	O43	75.18(11)	O24	C22	C18^{8}	120.6(4)
O9	Dy2	C22^{3}	171.72(12)	O23^{3}	C22	Dy2^{3}	48.4(2)
O35	Dy2	O24^{3}	69.41(10)	O23^{3}	C22	C18^{8}	117.7(4)
O35	Dy2	O43	147.77(12)	C18^{8}	C22	Dy2^{3}	164.3(3)
O35	Dy2	C22^{3}	76.30(12)	O32^{5}	C30	Dy1^{6}	68.1(2)
O34	Dy2	O35	133.24(11)	O32^{5}	C30	C26	119.5(4)
O34	Dy2	O24^{3}	69.32(10)	O31	C30	Dy1^{6}	53.0(2)
O34	Dy2	O24	74.56(11)	O31	C30	O32^{5}	121.0(4)
O34	Dy2	O23	80.89(11)	O31	C30	C26	119.5(4)
O34	Dy2	O43	72.89(11)	C26	C30	Dy1^{6}	171.6(3)
O34	Dy2	C22^{3}	75.56(11)	C26	C27	C28	112.0(4)
O24	Dy2	O35	76.22(11)	C15	C16	C17	112.9(4)
O24	Dy2	O24^{3}	77.87(10)	O36	C37	N38	123.0(4)
O24	Dy2	O23	126.33(11)	C18	C17	C16	112.4(4)
O24	Dy2	O43	135.38(11)	C29	C28	C27	113.2(4)
O24^{3}	Dy2	C22^{3}	24.88(10)	N38	C39	C40	111.6(4)
O24	Dy2	C22^{3}	102.74(12)	N38	C41	C42	111.6(4)
O23	Dy2	O35	88.09(11)	C44	N45	C46	119.7(6)
O23	Dy2	O24^{3}	48.75(10)	C44	N45	C48	120.4(7)
O23	Dy2	O43	77.03(11)	C48	N45	C46	119.7(6)
O23	Dy2	C22^{3}	24.00(11)	O43	C44	N45	126.6(6)
O43	Dy2	O24^{3}	116.80(10)	C47	C46	N45	115.3(8)
O43	Dy2	C22^{3}	97.80(12)	N45	C48	C49	114.3(7)

^{1}-X,2-Y,-Z; ^{2}+X,2-Y,-1/2+Z; ^{3}1-X,1-Y,1-Z; ^{4}1-X,+Y,1/2-Z; ^{5}-X,+Y,1/2-Z; ^{6}+X,2-Y,1/2+Z; ^{7}+X,1+Y,+Z; ^{8}+X,-1+Y,+Z^{1}-X,2-Y,-Z; ^{2}+X,2-Y,-1/2+Z; ^{3}1-X,1-Y,1-Z; ^{4}1-X,+Y,1/2-Z; ^{5}-X,+Y,1/2-Z; ^{6}+X,2-Y,1/2+Z; ^{7}+X,1+Y,+Z; ^{8}+X,-1+Y,+Z

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Yb1	Yb1[1]	4.1121(7)	C17	C16	1.392(12)
Yb1	O13[2]	2.214(6)	C17	C18	1.364(12)
Yb1	O24[3]	2.298(6)	C30	O31	1.278(10)
Yb1	C33[4]	2.995(9)	C30	C26	1.496(11)
Yb1	O34[4]	2.270(6)	O34	Yb1[10]	2.270(6)
Yb1	O35[4]	3.056(7)	C4	C8	1.493(12)
Yb1	O35[5]	2.248(6)	C4	C5	1.370(12)
Yb1	O23[6]	2.263(6)	O36	C37	1.237(11)
Yb1	O43	2.370(7)	C22	O23	1.253(10)
Yb1	O12	2.203(6)	C22	C18	1.492(11)
Yb2	Yb2[7]	4.0162(7)	N38	C39	1.454(12)
Yb2	O32	2.253(6)	N38	C37	1.318(11)
Yb2	O10	2.297(6)	N38	C41	1.466(12)
Yb2	O36	2.289(6)	C19	O21	1.251(10)
Yb2	C19	2.942(8)	C19	O20	1.250(10)
Yb2	O31[8]	2.235(6)	C19	C15	1.481(11)
Yb2	O21	2.831(6)	O35	Yb1[10]	3.056(7)
Yb2	O21[7]	2.271(6)	O35	Yb1[5]	2.248(6)
Yb2	O20	2.321(6)	C27	C26	1.355(12)
Yb2	O9[7]	2.274(6)	C27	C28	1.416(13)
S3	C4	1.716(9)	C39	C40	1.511(15)
S3	C7	1.718(9)	C8	O9	1.250(10)
S14	C18	1.731(9)	O31	Yb2[8]	2.235(6)
S14	C15	1.725(9)	O21	Yb2[7]	2.271(6)
S25	C26	1.724(8)	O23	Yb1[6]	2.263(6)
S25	C29	1.709(9)	O43	C44	1.179(17)
O32	C30	1.237(10)	C7	C6	1.382(12)
N11	O13	1.239(10)	C16	C15	1.362(12)
N11	O12	1.271(11)	C6	C5	1.402(12)
N11	C7	1.482(11)	C29	C28	1.365(12)
O13	Yb1[2]	2.214(6)	C41	C42	1.519(15)
O24	Yb1[9]	2.298(6)	C45	C44	1.37(2)

O24	C22	1.234(10)	C45	C46	1.52(2)
O10	C8	1.263(10)	C45	C48	1.44(2)
C33	Yb1[10]	2.995(9)	O9	Yb2[7]	2.274(6)
C33	O34	1.245(11)	C46	C47	1.46(3)
C33	O35	1.261(11)	C49	C48	1.51(3)
C33	C29	1.493(12)			

O13[1]	Yb1	Yb1[2]	136.10(16)	O9[7] Yb2 O36	147.0(2)
O13[1]	Yb1	O24[3]	73.6(2)	O9[7] Yb2 C19	77.6(2)
O13[1]	Yb1	C33[4]	96.7(2)	O9[7] Yb2 O21	69.6(2)
O13[1]	Yb1	O34[4]	80.4(2)	O9[7] Yb2 O20	88.0(2)
O13[1]	Yb1	O35[4]	115.7(2)	C4 S3 C7	91.5(4)
O13[1]	Yb1	O35[5]	136.7(3)	C15 S14 C18	91.3(4)
O13[1]	Yb1	O23[6]	147.0(2)	C29 S25 C26	91.0(4)
O13[1]	Yb1	O43	76.4(2)	C30 O32 Yb2	168.8(6)
O24[3]	Yb1	Yb1[2]	66.15(16)	O13 N11 O12	124.7(8)
O24[3]	Yb1	C33[4]	74.1(2)	O13 N11 C7	118.3(8)
O24[3]	Yb1	O35[4]	68.7(2)	O12 N11 C7	117.0(8)
O24[3]	Yb1	O43	147.5(2)	N11 O13 Yb1[1]	159.8(6)
C33[4]	Yb1	Yb1[2]	56.53(17)	C22 O24 Yb1[9]	137.9(6)
C33[4]	Yb1	O35[4]	24.0(2)	C8 O10 Yb2	136.2(5)
O34[4]	Yb1	Yb1[2]	78.82(17)	O34 C33 Yb1[10]	44.0(4)
O34[4]	Yb1	O24[3]	84.1(2)	O34 C33 O35	124.3(8)
O34[4]	Yb1	C33[4]	22.4(2)	O34 C33 C29	117.5(8)
O34[4]	Yb1	O35[4]	46.3(2)	O35 C33 Yb1[10]	80.7(5)
O34[4]	Yb1	O43	78.9(2)	O35 C33 C29	118.2(8)
O35[5]	Yb1	Yb1[2]	46.94(18)	C29 C33 Yb1[10]	160.4(6)
O35[4]	Yb1	Yb1[2]	32.51(11)	C18 C17 C16	114.6(9)
O35[5]	Yb1	O24[3]	75.8(2)	O32 C30 O31	126.2(7)
O35[5]	Yb1	C33[4]	103.5(2)	O32 C30 C26	118.3(7)
O35[5]	Yb1	O34[4]	125.8(2)	O31 C30 C26	115.5(7)
O35[5]	Yb1	O35[4]	79.4(2)	C33 O34 Yb1[10]	113.6(6)
O35[5]	Yb1	O23[6]	76.0(2)	C8 C4 S3	121.5(6)
O35[5]	Yb1	O43	136.4(2)	C5 C4 S3	111.2(7)
O23[6]	Yb1	Yb1[2]	65.15(16)	C5 C4 C8	127.2(8)
O23[6]	Yb1	O24[3]	130.9(2)	C37 O36 Yb2	133.0(6)
O23[6]	Yb1	C33[4]	74.5(2)	O24 C22 O23	129.0(8)

O23^{6}	Yb1	O34^{4}	81.0(2)	O24	C22	C18	117.4(8)
O23^{6}	Yb1	O35^{4}	67.2(2)	O23	C22	C18	113.6(8)
O23^{6}	Yb1	O43	73.4(2)	C39	N38	C41	119.6(8)
O43	Yb1	Yb1^{2}	135.31(18)	C37	N38	C39	119.7(8)
O43	Yb1	C33^{4}	97.5(2)	C37	N38	C41	120.7(8)
O43	Yb1	O35^{4}	115.1(2)	O21	C19	Yb2	72.6(5)
O12	Yb1	Yb1^{2}	125.00(18)	O21	C19	C15	119.3(8)
O12	Yb1	O13^{1}	87.1(2)	O20	C19	Yb2	48.9(4)
O12	Yb1	O24^{3}	114.8(2)	O20	C19	O21	121.5(8)
O12	Yb1	C33^{4}	171.1(2)	O20	C19	C15	119.1(7)
O12	Yb1	O34^{4}	153.5(3)	C15	C19	Yb2	167.5(6)
O12	Yb1	O35^{4}	156.1(2)	Yb1^{5}	O35	Yb1^{10}	100.6(2)
O12	Yb1	O35^{5}	78.8(2)	C33	O35	Yb1^{10}	75.3(5)
O12	Yb1	O23^{6}	97.9(2)	C33	O35	Yb1^{5}	175.2(7)
O12	Yb1	O43	75.5(3)	C26	C27	C28	111.0(8)
O32	Yb2	Yb2^{7}	137.06(15)	N38	C39	C40	110.7(9)
O32	Yb2	O10	150.5(2)	O36	C37	N38	123.7(8)
O32	Yb2	O36	76.3(2)	O10	C8	C4	117.5(7)
O32	Yb2	C19	100.0(2)	O9	C8	O10	126.7(8)
O32	Yb2	O21	117.87(19)	O9	C8	C4	115.8(7)
O32	Yb2	O21^{7}	135.4(2)	C30	O31	Yb2^{8}	136.7(5)
O32	Yb2	O20	82.4(2)	Yb2^{7}	O21	Yb2	103.3(2)
O32	Yb2	O9^{7}	73.4(2)	C19	O21	Yb2	82.5(5)
O10	Yb2	Yb2^{7}	68.13(15)	C19	O21	Yb2^{7}	173.8(6)
O10	Yb2	C19	80.7(2)	C22	O23	Yb1^{6}	140.3(6)
O10	Yb2	O21	73.81(19)	C44	O43	Yb1	128.5(8)
O10	Yb2	O20	88.1(2)	C19	O20	Yb2	107.1(5)
O36	Yb2	Yb2^{7}	136.52(15)	N11	O12	Yb1	141.2(6)
O36	Yb2	O10	74.3(2)	N11	C7	S3	120.9(7)
O36	Yb2	C19	95.2(2)	C6	C7	S3	112.0(6)
O36	Yb2	O21	115.1(2)	C6	C7	N11	127.1(8)
O36	Yb2	O20	75.3(2)	C30	C26	S25	119.4(6)
C19	Yb2	Yb2^{7}	58.29(16)	C27	C26	S25	112.9(6)
O31^{8}	Yb2	Yb2^{7}	125.55(15)	C27	C26	C30	127.7(8)
O31^{8}	Yb2	O32	80.0(2)	C15	C16	C17	112.0(8)
O31^{8}	Yb2	O10	96.4(2)	C17	C18	S14	110.1(7)
O31^{8}	Yb2	O36	78.9(2)	C17	C18	C22	127.9(8)

O31[8]	Yb2	C19	174.0(2)	C22	C18	S14	121.8(7)
O31[8]	Yb2	O21[7]	82.3(2)	C7	C6	C5	111.4(8)
O31[8]	Yb2	O21	158.72(19)	C33	C29	S25	118.1(7)
O31[8]	Yb2	O20	151.5(2)	C28	C29	S25	111.5(7)
O31[8]	Yb2	O9[7]	108.0(2)	C28	C29	C33	130.3(8)
O21[7]	Yb2	Yb2[7]	43.31(16)	C4	C5	C6	113.8(8)
O21	Yb2	Yb2[7]	33.38(12)	C29	C28	C27	113.5(8)
O21[7]	Yb2	O10	71.9(2)	N38	C41	C42	111.9(8)
O21[7]	Yb2	O36	138.9(2)	C19	C15	S14	121.2(6)
O21	Yb2	C19	24.9(2)	C16	C15	S14	111.9(6)
O21[7]	Yb2	C19	101.6(2)	C16	C15	C19	126.9(8)
O21[7]	Yb2	O21	76.7(2)	C44	C45	C46	119.4(13)
O21[7]	Yb2	O20	125.5(2)	C44	C45	C48	120.7(17)
O21[7]	Yb2	O9[7]	73.8(2)	C48	C45	C46	119.3(15)
O20	Yb2	Yb2[7]	82.22(15)	C8	O9	Yb2[7]	140.2(6)
O20	Yb2	C19	24.0(2)	O43	C44	C45	125.6(15)
O20	Yb2	O21	48.88(19)	C47	C46	C45	121(2)
O9[7]	Yb2	Yb2[7]	66.22(15)	C45	C48	C49	114.5(18)
O9[7]	Yb2	O10	134.3(2)				

[1]1-X,+Y,1/2-Z; [2]1-X,-Y,-Z; [3]-1+X,-Y,-1/2+Z; [4]-1+X,+Y,-1+Z; [5]2-X,-Y,1-Z; [6]2-X,+Y,1/2-Z; [7]2-X,1-Y,1-Z; [8]2-X,+Y,3/2-Z; [9]1+X,-Y,1/2+Z; [10]1+X,+Y,1+Z[1]1-X,-Y,-Z; [2]1-X,+Y,1/2-Z; [3]-1+X,-Y,-1/2+Z; [4]-1+X,+Y,-1+Z; [5]2-X,-Y,1-Z; [6]2-X,+Y,1/2-Z; [7]2-X,1-Y,1-Z; [8]2-X,+Y,3/2-Z; [9]1+X,-Y,1/2+Z; [10]1+X,+Y,1+Z

Symmetry transformations used to generate equivalent atoms:#1 -x+1,y,-z+2 #2 x,y-1,z+1 #3 x,y-1,z #4 -x+3/2,y-1/2,-z+1 #5 x,y,z+1 #6 -x+1,y,-z+1 #7 -x+3/2,y+1/2,-z+1 #8+3/2,y+1/2,-z #9 x,y+1,z #10 x,y,z-1 #11 x,y+1,z-1 #12 -x+3/2,y-1/2,-z

Table S2. Hydrogen bonds for CPs 1-9 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	(DHA)
		1		
C(4)-H(4)...O(17)#4	0.93	2.48	3.38(2)	163.6
C(4)-H(4)...S(5)#4	0.93	3.00	3.630(17)	126.6
C(9)-H(9)...O(11)#5	0.93	2.65	3.45(2)	144.6
C(21)-H(21)...S(1)	0.93	2.82	3.468(17)	127.6
C(27)-H(27)...S(7)	0.93	2.88	3.344(19)	112.5
C(34)-H(34)...O(8)	0.93	2.54	3.415(19)	155.8
C(40)-H(40)...S(6)#8	0.93	2.89	3.546(18)	128.7
C(45)-H(45)...S(4)	0.93	2.93	3.371(16)	110.4
C(46)-H(46)...S(4)	0.93	2.88	3.350(17)	113.0
C(52)-H(52)...O(31)#9	0.93	2.56	3.43(2)	156.5
O(19)-H(19A)...O(35)#7	0.86(3)	2.33(12)	2.815(17)	115(11)
O(19)-H(19B)...O(6)	0.86(3)	1.92(6)	2.732(17)	156(13)
O(42)-H(42A)...O(30)#9	0.86(3)	2.15(15)	2.815(17)	134(18)
O(42)-H(42B)...O(24)#11	0.86(3)	2.47(15)	2.899(18)	112(13)
O(44)-H(44A)...O(11)#5	0.85(3)	2.35(8)	3.104(18)	147(13)
O(44)-H(44A)...O(12)#5	0.85(3)	2.55(8)	3.321(17)	152(14)
O(44)-H(44B)...O(15)#10	0.85(3)	1.99(7)	2.797(16)	158(16)
C(57')-H(57F)...S(1)#2	0.96	2.88	3.39(9)	114.9
C(59')-H(59D)...O(17)#2	0.96	2.01	2.91(6)	156.0
C(59')-H(59E)...O(1)#2	0.96	2.01	2.95(7)	164.5
C(65)-H(65)...O(22)	0.93	2.58	3.10(4)	115.5
C(69)-H(69A)...S(8)#2	0.96	2.71	3.63(7)	162.0
C(65')-H(65')...O(28)#12	0.93	2.64	3.13(3)	113.5
C(67')-H(67F)...S(8)#13	0.96	2.95	3.51(5)	118.8
C(72)-H(72A)...S(6)	0.96	2.93	3.88(5)	170.5
C(79)-H(79A)...S(2)#11	0.96	2.97	3.60(11)	124.7
C(75')-H(75')...O(8)#11	0.93	2.48	3.05(4)	119.5
C(77')-H(77D)...S(5)#3	0.96	2.84	3.62(8)	139.0

Symmetry transformations used to generate equivalent atoms: #1 x,y,z-1 #2 x,y-1,z #3 x,y+1,z+1 #4 -x+1,-y+1,z+1/2 #5 -x+1,-y,z+1/2 #6 -x+1,-y,z-1/2 #7 x,y-1,z-1

C(4)-H(4)...O(17)#4	0.93	2.49	3.385(12)	161.3
C(4)-H(4)...S(5)#4	0.93	2.96	3.607(10)	127.7
C(4)-H(4)...O(17)#4	0.93	2.49	3.385(12)	161.3
C(4)-H(4)...S(5)#4	0.93	2.96	3.607(10)	127.7
C(9)-H(9)...O(11)#5	0.93	2.64	3.412(13)	141.2
C(16)-H(16)...O(33)#7	0.93	2.62	3.500(12)	158.0
C(21)-H(21)...S(1)	0.93	2.88	3.480(10)	123.3
C(27)-H(27)...S(7)	0.93	2.87	3.337(10)	112.6
C(28)-H(28)...S(7)	0.93	2.93	3.364(11)	110.3
C(34)-H(34)...O(8)	0.93	2.53	3.399(11)	156.2
C(34)-H(34)...S(2)	0.93	3.01	3.566(9)	119.6
C(40)-H(40)...S(6)#8	0.93	2.87	3.537(10)	129.3
C(46)-H(46)...S(4)	0.93	2.88	3.336(10)	111.4
C(52)-H(52)...O(31)#9	0.93	2.53	3.409(12)	158.4
C(59)-H(59A)...S(5)#2	0.96	2.95	3.73(3)	140.0
C(59)-H(59B)...S(3)	0.96	2.77	3.56(5)	139.7
C(57')-H(57D)...S(1)#2	0.96	2.79	3.37(4)	119.3
C(59')-H(59D)...O(17)#2	0.96	2.49	3.39(4)	157.4
C(65)-H(65)...O(28)#11	0.93	2.54	3.05(4)	114.8
C(69)-H(69A)...S(8)#2	0.96	2.76	3.63(4)	151.0
C(67')-H(67E)...S(8)#12	0.96	2.89	3.49(3)	121.3
C(72)-H(72A)...S(6)	0.96	2.91	3.85(2)	170.2
C(76)-H(76A)...O(41)	0.97	2.22	2.72(4)	110.3
C(78)-H(78A)...O(44)#15	0.97	2.66	3.55(4)	152.6
C(75')-H(75')...O(8)#13	0.93	2.25	2.89(3)	126.0
C(77')-H(77D)...S(5)#3	0.96	2.79	3.75(4)	172.2
O(19)-H(19A)...O(35)#7	0.85(3)	2.20(8)	2.773(9)	125(8)
O(19)-H(19B)...O(6)	0.84(3)	2.33(9)	2.755(10)	112(8)
O(42)-H(42B)...O(26)#9	0.86(3)	2.26(11)	2.757(9)	117(10)
O(44)-H(44A)...O(43)#4	0.86(3)	2.20(7)	2.883(10)	137(8)
O(44)-H(44B)...O(15)#10	0.86(3)	2.03(5)	2.818(9)	151(8)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 x,y-1,z #3 x,y+1,z+1 #4 -x-2,-y-1,z+1/2
#5 -x-2,-y-2,z+1/2 #6 -x-2,-y-2,z-1/2 #7 x,y-1,z-1
#8 -x-5/2,y+1/2,z-1/2 #9 -x-5/2,y+1/2,z+1/2
#10 -x-2,-y-1,z-1/2 #11 -x-5/2,y-1/2,z+1/2 #12 -x-5/2,y-1/2,z-1/2
#13 x,y+1,z #14 x,y,z+1 #15 -x-2,-y,z+1/2

3

C(4)-H(4)...O(17)#4	0.93	2.48	3.372(13)	161.1
C(4)-H(4)...S(5)#4	0.93	2.94	3.586(12)	127.5
C(9)-H(9)...O(11)#5	0.93	2.66	3.418(14)	139.6
C(16)-H(16)...O(33)#7	0.93	2.61	3.486(13)	157.5
C(21)-H(21)...S(1)	0.93	2.87	3.471(11)	123.7
C(27)-H(27)...S(7)	0.93	2.88	3.338(12)	111.9
C(28)-H(28)...S(7)	0.93	2.92	3.352(11)	110.0
C(34)-H(34)...O(8)	0.93	2.53	3.400(12)	156.5
C(34)-H(34)...S(2)	0.93	3.00	3.555(11)	119.6
C(40)-H(40)...S(6)#8	0.93	2.85	3.523(11)	129.7
C(46)-H(46)...S(4)	0.93	2.89	3.347(11)	111.7
C(52)-H(52)...O(31)#9	0.93	2.55	3.422(13)	157.2
C(59)-H(59A)...S(5)#2	0.96	2.89	3.68(3)	140.5
C(59)-H(59C)...S(3)	0.96	2.80	3.56(6)	137.5
C(57')-H(57D)...S(1)#2	0.96	2.83	3.40(4)	119.3
C(59')-H(59D)...O(17)#2	0.96	2.51	3.43(4)	159.1
C(65)-H(65)...O(28)#11	0.93	2.48	3.01(4)	116.0
C(69)-H(69A)...S(8)#2	0.96	2.84	3.70(5)	149.5
C(67')-H(67D)...S(7)#2	0.96	2.99	3.63(3)	125.6
C(67')-H(67F)...S(8)#12	0.96	2.85	3.48(3)	123.9
C(72)-H(72A)...S(6)	0.96	2.88	3.83(2)	170.1
C(75')-H(75')...O(8)#13	0.93	2.28	2.90(3)	123.6
C(77')-H(77D)...S(5)#3	0.96	2.77	3.72(4)	171.4
O(19)-H(19A)...O(35)#7	0.85(3)	2.10(7)	2.762(10)	135(8)
O(19)-H(19B)...O(6)	0.85(3)	2.29(8)	2.742(11)	114(7)

O(42)-H(42B)...O(26)#9	0.85(3)	2.21(3)	2.780(10)	124(4)
O(44)-H(44A)...O(43)#4	0.86(3)	2.14(8)	2.892(10)	146(12)
O(44)-H(44B)...O(15)#10	0.85(3)	2.08(8)	2.824(10)	146(11)
C(4)-H(4)...O(17)#4	0.93	2.48	3.372(13)	161.1
C(4)-H(4)...S(5)#4	0.93	2.94	3.586(12)	127.5
C(9)-H(9)...O(11)#5	0.93	2.66	3.418(14)	139.6
C(16)-H(16)...O(33)#7	0.93	2.61	3.486(13)	157.5
C(21)-H(21)...S(1)	0.93	2.87	3.471(11)	123.7
C(27)-H(27)...S(7)	0.93	2.88	3.338(12)	111.9
C(34)-H(34)...O(8)	0.93	2.53	3.400(12)	156.5
C(34)-H(34)...S(2)	0.93	3.00	3.555(11)	119.6
C(40)-H(40)...S(6)#8	0.93	2.85	3.523(11)	129.7
C(46)-H(46)...S(4)	0.93	2.89	3.347(11)	111.7
C(52)-H(52)...O(31)#9	0.93	2.55	3.422(13)	157.2
C(59)-H(59A)...S(5)#2	0.96	2.89	3.68(3)	140.5
C(59)-H(59C)...S(3)	0.96	2.80	3.56(6)	137.5
C(57')-H(57D)...S(1)#2	0.96	2.83	3.40(4)	119.3
C(59')-H(59D)...O(17)#2	0.96	2.51	3.43(4)	159.1
C(69)-H(69A)...S(8)#2	0.96	2.84	3.70(5)	149.5
C(67')-H(67D)...S(7)#2	0.96	2.99	3.63(3)	125.6
C(67')-H(67F)...S(8)#12	0.96	2.85	3.48(3)	123.9
C(72)-H(72A)...S(6)	0.96	2.88	3.83(2)	170.1
C(79)-H(79B)...S(2)#13	0.96	2.71	3.50(7)	140.7
C(75')-H(75')...O(8)#13	0.93	2.28	2.90(3)	123.6
C(77')-H(77D)...S(5)#3	0.96	2.77	3.72(4)	171.4
O(19)-H(19A)...O(35)#7	0.85(3)	2.10(7)	2.762(10)	135(8)
O(19)-H(19B)...O(6)	0.85(3)	2.29(8)	2.742(11)	114(7)
O(42)-H(42B)...O(26)#9	0.85(3)	2.21(3)	2.780(10)	124(4)
O(44)-H(44A)...O(43)#4	0.86(3)	2.14(8)	2.892(10)	146(12)
O(44)-H(44B)...O(15)#10	0.85(3)	2.08(8)	2.824(10)	146(11)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 x,y+1,z #3 x,y-1,z-1 #4 -x+1,-y+1,z-1/2 #5 -x+1,-y+2,z-1/2 #6 -x+1,-y+2,z+1/2 #7 x,y+1,z+1 #8 -x+3/2,y-1/2,z+1/2 #9 -x+3/2,y-1/2,z-1/2 #10 -x+1,-y+1,z+1/2 #11 -x+3/2,y+1/2,z-1/2 #12 -x+3/2,y+1/2,z+1/2 #13 x,y-1,z #14 x,y,z-1

C(4)-H(4)...O(17)#4	0.93	2.49	3.380(9)	159.3
C(4)-H(4)...S(5)#4	0.93	2.92	3.566(8)	128.1
C(16)-H(16)...O(33)#7	0.93	2.56	3.443(9)	159.3
C(21)-H(21)...S(1)	0.93	2.85	3.451(7)	123.5
C(28)-H(28)...O(40)#1	0.93	2.64	3.410(8)	140.1
C(34)-H(34)...O(8)	0.93	2.54	3.404(8)	154.7
C(34)-H(34)...S(2)	0.93	2.97	3.520(7)	119.5
C(40)-H(40)...S(6)#8	0.93	2.83	3.512(7)	130.8
C(46)-H(46)...S(4)	0.93	2.89	3.330(7)	110.0
C(52)-H(52)...O(31)#9	0.93	2.55	3.411(8)	154.4
C(59)-H(59A)...S(5)#2	0.96	2.96	3.67(3)	131.5
C(55')-H(55')...O(9)	0.93	2.36	2.91(2)	116.9
C(57')-H(57D)...S(1)#2	0.96	2.74	3.45(4)	131.3
C(59')-H(59D)...O(17)#2	0.96	2.55	3.40(3)	147.8
C(65)-H(65)...O(22)	0.93	2.49	3.01(2)	115.9
C(69)-H(69A)...S(8)#2	0.96	2.71	3.63(3)	160.9
C(67')-H(67D)...S(7)#2	0.96	3.03	3.68(3)	126.1
C(67')-H(67E)...S(8)#12	0.96	2.83	3.45(3)	122.9
C(72)-H(72A)...S(6)	0.96	2.86	3.811(16)	172.2
C(79)-H(79C)...S(2)#13	0.96	2.79	3.52(7)	133.2
C(75')-H(75')...O(8)#13	0.93	2.38	2.95(2)	119.8
C(77')-H(77D)...S(5)#3	0.96	2.93	3.78(3)	147.9
O(19)-H(19A)...O(35)#7	0.84(3)	2.17(6)	2.750(7)	126(7)
O(19)-H(19B)...O(6)	0.83(3)	2.35(7)	2.745(7)	109(6)
O(42)-H(42B)...O(26)#9	0.84(3)	2.20(3)	2.771(7)	125(3)
O(44)-H(44A)...O(43)#4	0.85(3)	2.24(6)	2.905(7)	135(7)
O(44)-H(44B)...O(15)#10	0.85(3)	2.09(5)	2.852(6)	149(7)
O(42)-H(42A)...O(30)#9	0.86(3)	2.23(3)	2.829(7)	126(4)
C(4)-H(4)...O(17)#4	0.93	2.49	3.380(9)	159.3
C(4)-H(4)...S(5)#4	0.93	2.92	3.566(8)	128.1

C(16)-H(16)...O(33)#7	0.93	2.56	3.443(9)	159.3
C(21)-H(21)...S(1)	0.93	2.85	3.451(7)	123.5
C(28)-H(28)...O(40)#1	0.93	2.64	3.410(8)	140.1
C(34)-H(34)...O(8)	0.93	2.54	3.404(8)	154.7
C(34)-H(34)...S(2)	0.93	2.97	3.520(7)	119.5
C(40)-H(40)...S(6)#8	0.93	2.83	3.512(7)	130.8
C(46)-H(46)...S(4)	0.93	2.89	3.330(7)	110.0
C(52)-H(52)...O(31)#9	0.93	2.55	3.411(8)	154.4
C(59)-H(59A)...S(5)#2	0.96	2.96	3.67(3)	131.5
C(55')-H(55')...O(9)	0.93	2.36	2.91(2)	116.9
C(57')-H(57D)...S(1)#2	0.96	2.74	3.45(4)	131.3
C(59')-H(59D)...O(17)#2	0.96	2.55	3.40(3)	147.8
C(65)-H(65)...O(22)	0.93	2.49	3.01(2)	115.9
C(69)-H(69A)...S(8)#2	0.96	2.71	3.63(3)	160.9
C(67')-H(67D)...S(7)#2	0.96	3.03	3.68(3)	126.1
C(67')-H(67E)...S(8)#12	0.96	2.83	3.45(3)	122.9
C(72)-H(72A)...S(6)	0.96	2.86	3.811(16)	172.2
C(79)-H(79C)...S(2)#13	0.96	2.79	3.52(7)	133.2
C(75')-H(75')...O(8)#13	0.93	2.38	2.95(2)	119.8
C(77')-H(77D)...S(5)#3	0.96	2.93	3.78(3)	147.9
O(19)-H(19A)...O(35)#7	0.84(3)	2.17(6)	2.750(7)	126(7)
O(19)-H(19B)...O(6)	0.83(3)	2.35(7)	2.745(7)	109(6)
O(42)-H(42B)...O(26)#9	0.84(3)	2.20(3)	2.771(7)	125(3)
O(44)-H(44A)...O(43)#4	0.85(3)	2.24(6)	2.905(7)	135(7)
O(44)-H(44B)...O(15)#10	0.85(3)	2.09(5)	2.852(6)	149(7)
O(42)-H(42A)...O(30)#9	0.86(3)	2.23(3)	2.829(7)	126(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 x,y+1,z #3 x,y-1,z-1 #4 -x+1,-y+1,z-1/2 #5 -x+1,-y+2,z-1/2 #6 -x+1,-y+2,z+1/2 #7 x,y+1,z+1 #8 -x+3/2,y-1/2,z+1/2 #9 -x+3/2,y-1/2,z-1/2 #10 -x+1,-y+1,z+1/2 #11 -x+3/2,y+1/2,z-1/2 #12 -x+3/2,y+1/2,z+1/2 #13 x,y-1,z #14 x,y,z-1

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C(4)-H(4)...O(18)#3	0.93	2.59	3.473(16)	159.1
C(4)-H(4)...S(5)#3	0.93	3.01	3.581(15)	121.0
C(9)-H(9)...O(15)#1	0.93	2.54	3.419(15)	157.7
C(9)-H(9)...S(4)#1	0.93	2.93	3.588(14)	128.7
C(28)-H(28)...O(10)#6	0.93	2.58	3.412(15)	149.8
C(28)-H(28)...S(3)#6	0.93	3.02	3.533(13)	116.5
C(33)-H(33)...S(2)#2	0.93	2.88	3.461(12)	121.5
C(44)-H(44A)...S(2)#11	0.96	2.65	3.51(5)	149.4
C(47)-H(47)...O(10)#6	0.93	2.49	3.01(3)	115.2
O(29)-H(29A)...O(13)#1	0.85(3)	2.30(10)	2.918(13)	130(10)
O(29)-H(29B)...O(24)#4	0.85(3)	2.05(6)	2.830(12)	153(11)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y-1/2,-z+1 #2 -x,y+1/2,-z+2 #3 -x+1,y-1/2,-z+1 #4 x,y,z-1 #5 -x+1,y-1/2,-z+2
#6 -x+1,y+1/2,-z+2 #7 -x+1,y+1/2,-z+1 #8 -x,y+1/2,-z+1 #9 -x,y-1/2,-z+2 #10 x,y,z+1
#11 x+1,y,z

6

C27 H27 O10[1]	0.93	2.24	3.138(4)	161.3
C6 H6 O20[2]	0.93	2.51	3.382(5)	155.2
C5 H5 O31[3]	0.93	2.41	3.254(4)	151.4

[1]+X,-1+Y,+Z; [2]1-X,-1+Y,1/2-Z

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C49 H49A O2[1]	0.96	2.03	2.67(5)	122.3
C49 H49A O2[2]	0.96	2.03	2.67(5)	122.3

[1]+X,-1+Y,+Z; [2]1-X,-1+Y,1/2-Z

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C49 H49A O2	0.96	2.12	2.74(8)	121.7
C49 H49A O2[1]	0.96	2.12	2.74(8)	121.7

[1]1-X,+Y,1/2-Z