ELECTRONIC SUPLEMENTARY MATERIAL

New Journal of Chemistry

Structural, Spectroscopic and Theoretical Study of an *o*-vanillin Schiff base derivative involved in enol-imine and keto-amine tautomerism.

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Figure S1. Drawings of the molecular orbitals of the enol-imine form involved in the electronic transitions

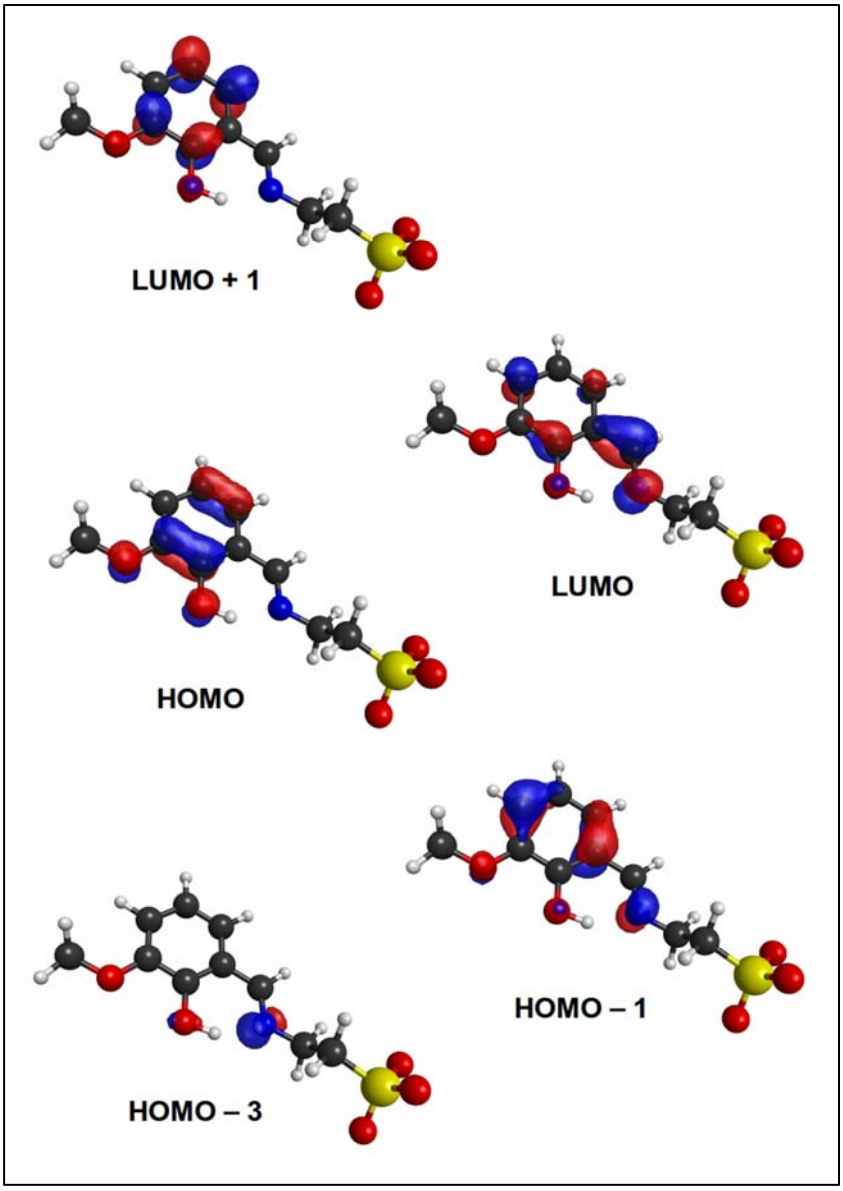

Figure S2. Drawings of the molecular orbitals of the keto-amine form involved in the electronic transitions

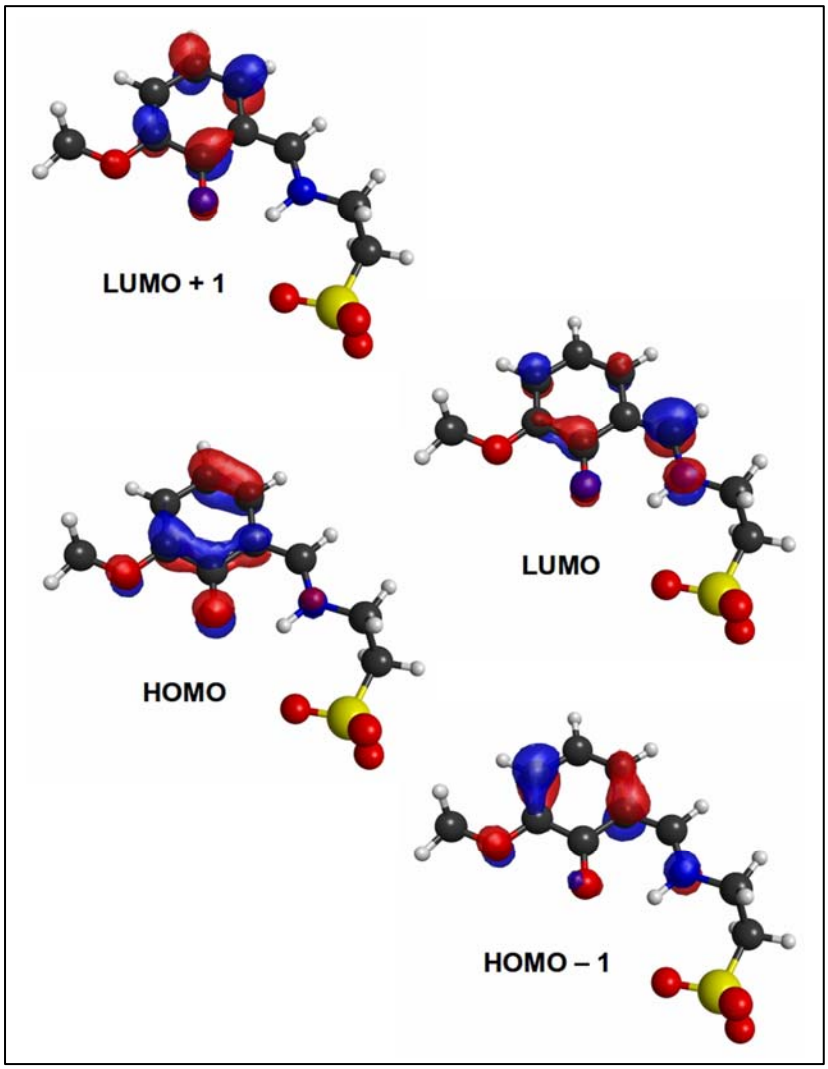

Figure S3. ^{1}H NMR full spectrum

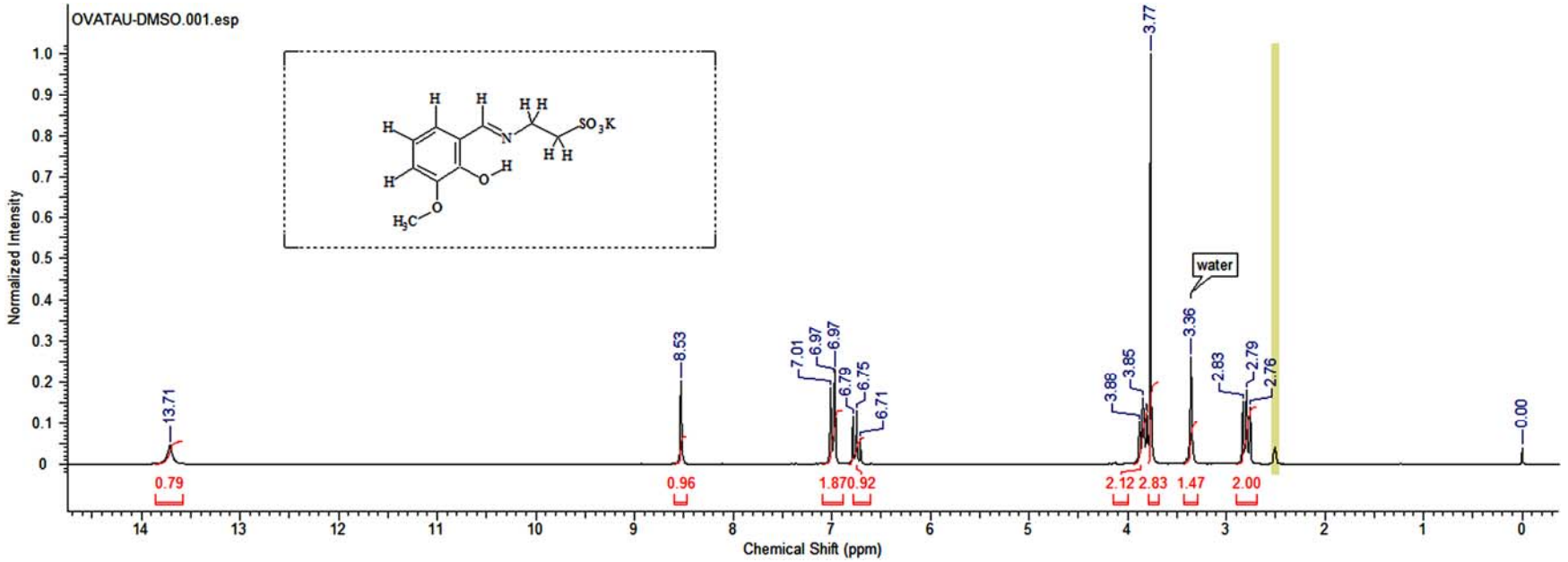

Figure S4. ^{1}H NMR expanded spectrum, 2.7 – 7.2 ppm zone.

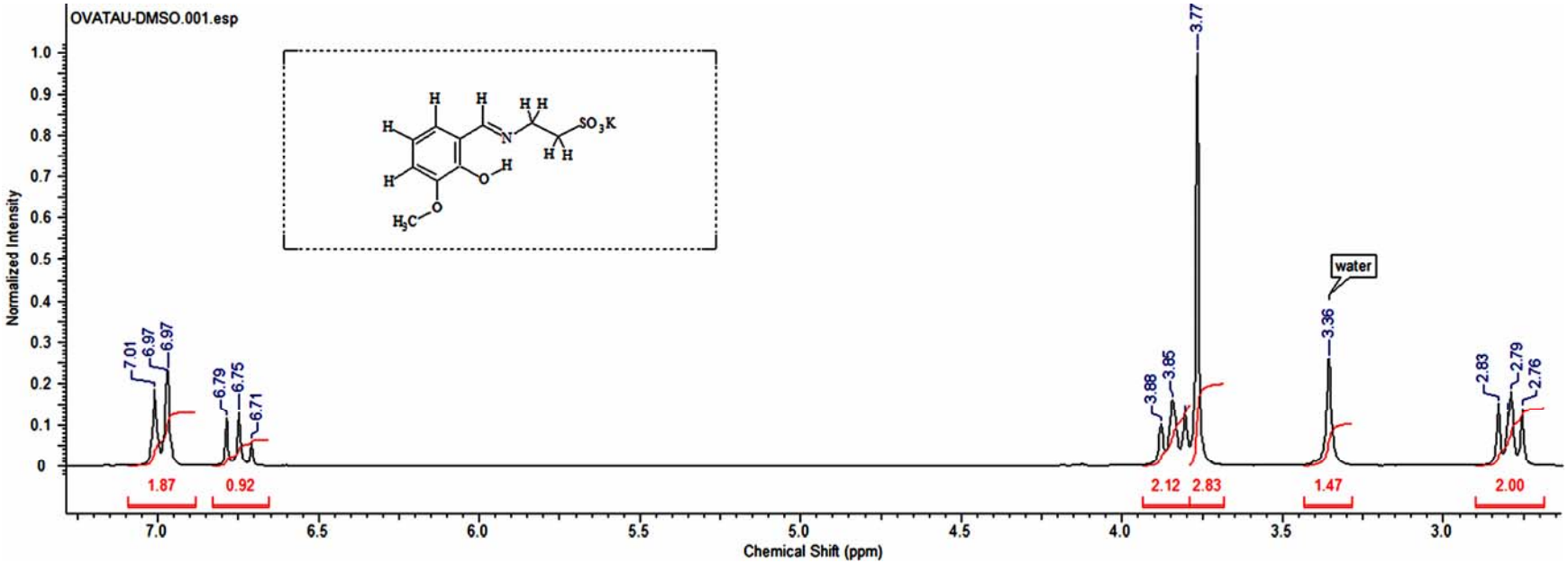

Figure S5: ^{13}C NMR full spectrum

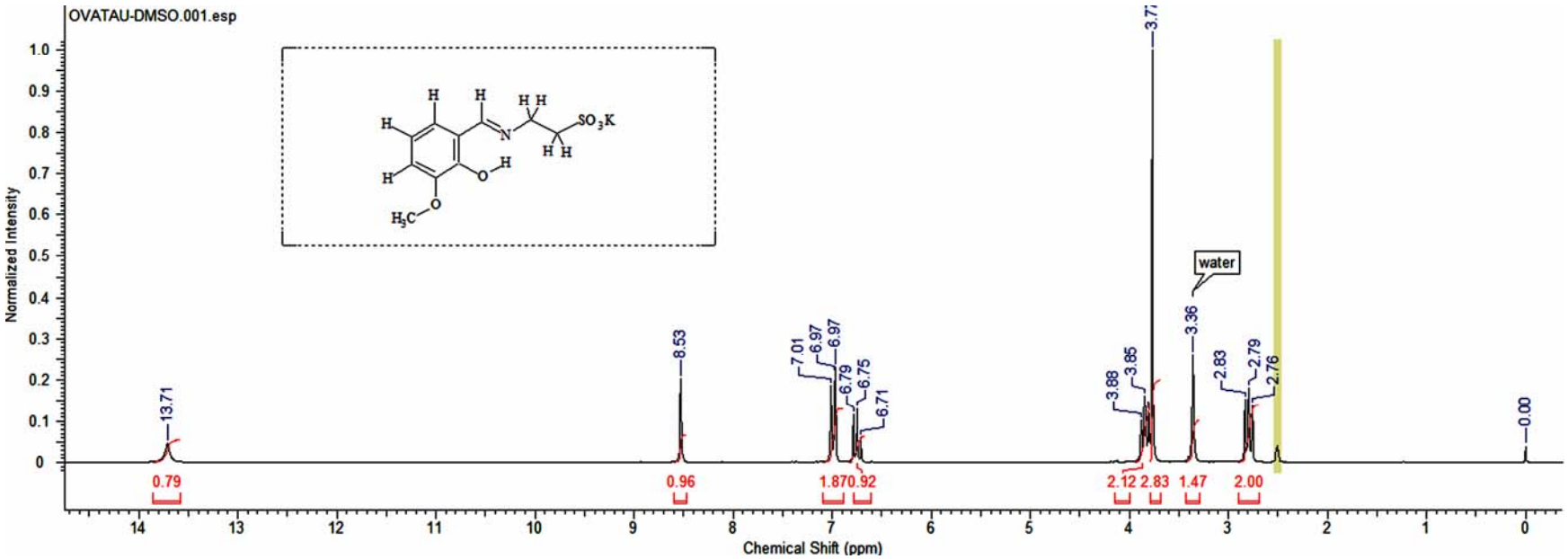

Figure S6: ^{13}C NMR expanded spectrum, 45 – 175 ppm zone.

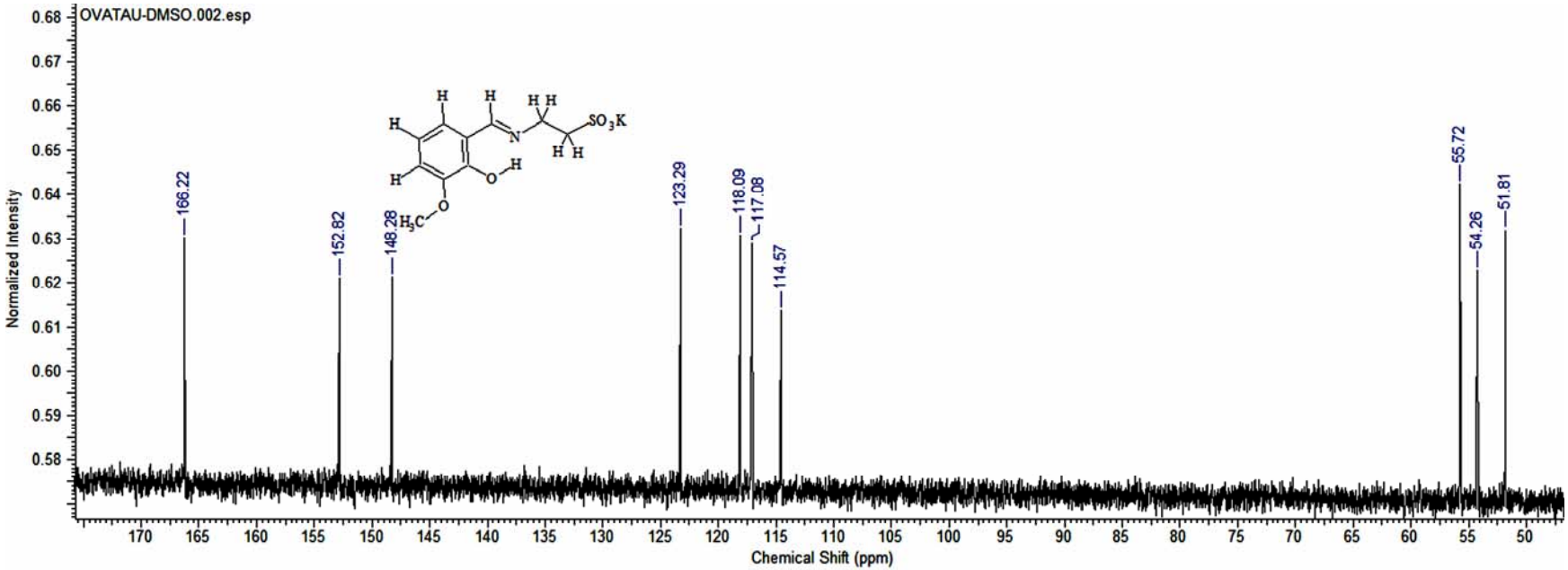

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for *o*-VaTau U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. To be deposited

Atom	x	y	z	U(eq)
C(11)	2347(1)	1732(6)	8239(2)	43(1)
C(12)	2677(1)	781(6)	8762(2)	46(1)
C(13)	3064(1)	1790(7)	9032(2)	53(1)
C(14)	3126(1)	3737(8)	8798(2)	56(1)
C(15)	2804(1)	4752(7)	8314(2)	50(1)
C(16)	2406(1)	3778(6)	8029(1)	41(1)
C(17)	2055(1)	4908(6)	7536(2)	43(1)
C(18)	1342(1)	5217(7)	6783(2)	47(1)
C(19)	1184(1)	3873(7)	6220(2)	42(1)
C(21)	1139(1)	5087(5)	3744(1)	37(1)
C(22)	1256(1)	7023(6)	4130(1)	39(1)
C(23)	1634(1)	8026(7)	4348(2)	50(1)
C(24)	1931(1)	7176(7)	4223(2)	58(1)
C(25)	1845(1)	5304(7)	3892(2)	52(1)
C(26)	1453(1)	4222(6)	3646(1)	41(1)
C(27)	1378(1)	2263(6)	3303(2)	45(1)
C(28)	957(1)	-884(7)	2689(2)	54(1)
C(29)	739(1)	-458(7)	2025(2)	50(1)
C(110)	2876(2)	-1982(10)	9522(2)	79(2)
C(210)	1018(2)	9771(8)	4553(2)	59(1)
N(1)	1693(1)	4037(5)	7271(1)	46(1)
N(2)	1025(1)	1187(5)	3029(1)	47(1)
O(1A)	604(1)	3270(5)	5144(1)	72(1)
O(1B)	732(1)	7080(4)	5509(1)	73(1)
O(1C)	410(1)	4423(5)	5835(1)	72(1)
O(2A)	30(1)	286(4)	1067(1)	58(1)
O(2B)	198(1)	2363(4)	1947(1)	61(1)
O(2C)	37(1)	-1616(4)	1871(1)	61(1)
O(11)	1979(1)	646(4)	7968(1)	54(1)
O(12)	2575(1)	-1119(4)	8955(1)	64(1)
O(21)	777(1)	4234(4)	3511(1)	47(1)
O(22)	955(1)	7716(4)	4236(1)	55(1)
S(1)	691(1)	4774(2)	5629(1)	44(1)
S(2)	208(1)	203(1)	1699(1)	39(1)
K(1)	272(1)	5158(1)	4067(1)	43(1)
K(2)	0	5159(2)	2500	41(1)
K(3)	0	0	0	45(1)

Table S2. Full bond lengths [Å] and angles [°] for s97.

C(11)-O(11)	1.346(4)	K(1)-O(1C)#3	2.714(3)
C(11)-C(16)	1.395(5)	K(1)-O(2B)#1	2.845(3)
C(11)-C(12)	1.409(5)	K(1)-O(2C)#2	2.850(3)
C(12)-O(12)	1.366(4)	K(1)-O(2A)#1	3.048(3)
C(12)-C(13)	1.380(5)	K(1)-O(2A)#2	3.193(3)
C(13)-C(14)	1.381(6)	K(1)-S(2)#1	3.4842(12)
C(14)-C(15)	1.362(5)	K(1)-S(2)#2	3.5299(12)
C(15)-C(16)	1.404(5)	K(1)-K(2)	3.7006(11)
C(16)-C(17)	1.448(5)	K(2)-O(2B)#1	2.556(2)
C(17)-N(1)	1.273(4)	K(2)-O(2C)#2	2.576(3)
C(18)-N(1)	1.458(4)	K(2)-O(2C)#6	2.576(3)
C(18)-C(19)	1.506(5)	K(2)-O(21)#1	2.805(2)
C(19)-S(1)	1.775(4)	K(2)-K(1)#1	3.7006(11)
C(21)-O(21)	1.271(4)	K(3)-O(2A)#7	2.756(2)
C(21)-C(26)	1.427(5)	K(3)-O(1A)#8	2.854(3)
C(21)-C(22)	1.441(4)	K(3)-O(1A)#1	2.854(3)
C(22)-O(22)	1.359(4)	K(3)-O(1B)#9	2.920(3)
C(22)-C(23)	1.363(5)	K(3)-O(1B)#4	2.920(3)
C(23)-C(24)	1.405(5)	K(3)-O(1C)#1	3.247(3)
C(24)-C(25)	1.341(5)	K(3)-O(1C)#8	3.247(3)
C(25)-C(26)	1.416(5)	K(3)-S(1)#1	3.6064(10)
C(26)-C(27)	1.404(5)	K(3)-S(1)#8	3.6064(10)
C(27)-N(2)	1.302(4)	K(3)-K(1)#9	4.2274(8)
C(28)-N(2)	1.459(5)	K(3)-K(1)#4	4.2274(8)
C(28)-C(29)	1.520(5)		
C(29)-S(2)	1.759(4)	O(11)-C(11)-C(16)	122.2(3)
C(110)-O(12)	1.423(5)	O(11)-C(11)-C(12)	118.2(3)
C(210)-O(22)	1.423(5)	C(16)-C(11)-C(12)	119.5(3)
O(1A)-S(1)	1.449(3)	O(12)-C(12)-C(13)	125.9(3)
O(1A)-K(1)	2.680(3)	O(12)-C(12)-C(11)	114.6(3)
O(1A)-K(3)#1	2.854(3)	C(13)-C(12)-C(11)	119.5(4)
O(1B)-S(1)	1.426(3)	C(12)-C(13)-C(14)	120.4(4)
O(1B)-K(3)#2	2.920(3)	C(15)-C(14)-C(13)	120.7(4)
O(1C)-S(1)	1.430(3)	C(14)-C(15)-C(16)	120.4(4)
O(1C)-K(1)#3	2.714(3)	C(11)-C(16)-C(15)	119.2(3)
O(1C)-K(3)#1	3.247(3)	C(11)-C(16)-C(17)	119.9(3)
O(2A)-S(2)	1.439(2)	C(15)-C(16)-C(17)	120.9(3)
O(2A)-K(3)	2.756(2)	N(1)-C(17)-C(16)	121.5(3)
O(2A)-K(1)#1	3.049(3)	N(1)-C(18)-C(19)	109.4(3)
O(2A)-K(1)#4	3.193(3)	C(18)-C(19)-S(1)	114.0(3)
O(2B)-S(2)	1.443(2)	O(21)-C(21)-C(26)	123.3(3)
O(2B)-K(2)	2.556(2)	O(21)-C(21)-C(22)	121.0(3)
O(2B)-K(1)#1	2.845(3)	C(26)-C(21)-C(22)	115.7(3)
O(2C)-S(2)	1.440(3)	O(22)-C(22)-C(23)	125.4(3)
O(2C)-K(2)#5	2.576(3)	O(22)-C(22)-C(21)	113.7(3)
O(2C)-K(1)#4	2.849(3)	C(23)-C(22)-C(21)	120.9(3)
O(21)-K(2)	2.805(2)	C(22)-C(23)-C(24)	121.6(4)
O(21)-K(1)	2.983(2)	C(25)-C(24)-C(23)	119.6(4)
O(22)-K(1)	2.806(2)	C(24)-C(25)-C(26)	121.0(4)
S(1)-K(1)	3.5718(15)	C(27)-C(26)-C(25)	119.0(3)
S(1)-K(3)#1	3.6064(10)	C(27)-C(26)-C(21)	120.0(3)
S(2)-K(1)#1	3.4842(11)	C(25)-C(26)-C(21)	121.0(3)
S(2)-K(1)#4	3.5298(12)	N(2)-C(27)-C(26)	124.7(4)

N(2)-C(28)-C(29)	112.7(3)	O(2C)-S(2)-K(1)#4	50.89(11)
C(28)-C(29)-S(2)	113.4(3)	O(2B)-S(2)-K(1)#4	151.79(12)
C(17)-N(1)-C(18)	120.8(3)	C(29)-S(2)-K(1)#4	101.92(14)
C(27)-N(2)-C(28)	123.8(3)	K(1)#1-S(2)-K(1)#4	114.92(3)
S(1)-O(1A)-K(1)	116.57(15)	O(1A)-K(1)-O(1C)#3	83.34(9)
S(1)-O(1A)-K(3)#1	109.52(16)	O(1A)-K(1)-O(22)	99.70(9)
K(1)-O(1A)-K(3)#1	103.78(9)	O(1C)#3-K(1)-O(22)	139.87(9)
S(1)-O(1B)-K(3)#2	118.94(15)	O(1A)-K(1)-O(2B)#1	118.29(8)
S(1)-O(1C)-K(1)#3	160.19(17)	O(1C)#3-K(1)-O(2B)#1	89.02(9)
S(1)-O(1C)-K(3)#1	92.57(14)	O(22)-K(1)-O(2B)#1	122.39(8)
K(1)#3-O(1C)-K(3)#1	89.86(8)	O(1A)-K(1)-O(2C)#2	162.50(8)
S(2)-O(2A)-K(3)	157.83(17)	O(1C)#3-K(1)-O(2C)#2	92.21(8)
S(2)-O(2A)-K(1)#1	95.07(11)	O(22)-K(1)-O(2C)#2	72.97(8)
K(3)-O(2A)-K(1)#1	97.12(7)	O(2B)#1-K(1)-O(2C)#2	78.40(7)
S(2)-O(2A)-K(1)#4	91.21(11)	O(1A)-K(1)-O(21)	112.10(8)
K(3)-O(2A)-K(1)#4	90.26(7)	O(1C)#3-K(1)-O(21)	158.92(8)
K(1)#1-O(2A)-K(1)#4	142.65(10)	O(22)-K(1)-O(21)	54.34(7)
S(2)-O(2B)-K(2)	155.92(18)	O(2B)#1-K(1)-O(21)	71.21(7)
S(2)-O(2B)-K(1)#1	103.84(12)	O(2C)#2-K(1)-O(21)	77.03(7)
K(2)-O(2B)-K(1)#1	86.33(7)	O(1A)-K(1)-O(2A)#1	70.76(8)
S(2)-O(2C)-K(2)#5	159.42(16)	O(1C)#3-K(1)-O(2A)#1	77.54(8)
S(2)-O(2C)-K(1)#4	106.03(14)	O(22)-K(1)-O(2A)#1	141.48(8)
K(2)#5-O(2C)-K(1)#4	85.86(8)	O(2B)#1-K(1)-O(2A)#1	47.91(6)
C(12)-O(12)-C(110)	117.5(4)	O(2C)#2-K(1)-O(2A)#1	124.88(7)
C(21)-O(21)-K(2)	135.2(2)	O(21)-K(1)-O(2A)#1	93.64(7)
C(21)-O(21)-K(1)	118.8(2)	O(1A)-K(1)-O(2A)#2	117.15(8)
K(2)-O(21)-K(1)	79.43(6)	O(1C)#3-K(1)-O(2A)#2	67.96(8)
C(22)-O(22)-C(210)	118.2(3)	O(22)-K(1)-O(2A)#2	75.45(7)
C(22)-O(22)-K(1)	126.36(19)	O(2B)#1-K(1)-O(2A)#2	115.82(7)
C(210)-O(22)-K(1)	114.6(3)	O(2C)#2-K(1)-O(2A)#2	46.08(7)
O(1B)-S(1)-O(1C)	114.08(18)	O(21)-K(1)-O(2A)#2	113.55(7)
O(1B)-S(1)-O(1A)	113.08(18)	O(2A)#1-K(1)-O(2A)#2	142.65(10)
O(1C)-S(1)-O(1A)	111.80(19)	O(1A)-K(1)-S(2)#1	94.64(7)
O(1B)-S(1)-C(19)	107.38(18)	O(1C)#3-K(1)-S(2)#1	84.27(7)
O(1C)-S(1)-C(19)	105.27(18)	O(22)-K(1)-S(2)#1	134.61(6)
O(1A)-S(1)-C(19)	104.31(17)	O(2B)#1-K(1)-S(2)#1	23.71(5)
O(1B)-S(1)-K(1)	73.59(13)	O(2C)#2-K(1)-S(2)#1	101.78(6)
O(1C)-S(1)-K(1)	118.25(12)	O(21)-K(1)-S(2)#1	80.35(5)
O(1A)-S(1)-K(1)	42.16(11)	O(2A)#1-K(1)-S(2)#1	24.30(4)
C(19)-S(1)-K(1)	131.93(13)	O(2A)#2-K(1)-S(2)#1	133.38(5)
O(1B)-S(1)-K(3)#1	141.34(12)	O(1A)-K(1)-S(2)#2	141.00(7)
O(1C)-S(1)-K(3)#1	64.10(13)	O(1C)#3-K(1)-S(2)#2	75.42(6)
O(1A)-S(1)-K(3)#1	48.23(13)	O(22)-K(1)-S(2)#2	77.90(6)
C(19)-S(1)-K(3)#1	110.16(14)	O(2B)#1-K(1)-S(2)#2	93.96(6)
K(1)-S(1)-K(3)#1	74.71(3)	O(2C)#2-K(1)-S(2)#2	23.09(5)
O(2A)-S(2)-O(2C)	111.90(16)	O(21)-K(1)-S(2)#2	98.11(5)
O(2A)-S(2)-O(2B)	112.77(14)	O(2A)#1-K(1)-S(2)#2	133.08(6)
O(2C)-S(2)-O(2B)	113.57(17)	O(2A)#2-K(1)-S(2)#2	24.06(4)
O(2A)-S(2)-C(29)	107.73(18)	S(2)#1-K(1)-S(2)#2	114.92(3)
O(2C)-S(2)-C(29)	104.88(18)	O(1A)-K(1)-S(1)	21.27(6)
O(2B)-S(2)-C(29)	105.27(17)	O(1C)#3-K(1)-S(1)	76.85(7)
O(2A)-S(2)-K(1)#1	60.64(10)	O(22)-K(1)-S(1)	91.62(6)
O(2C)-S(2)-K(1)#1	128.95(12)	O(2B)#1-K(1)-S(1)	137.17(5)
O(2B)-S(2)-K(1)#1	52.45(10)	O(2C)#2-K(1)-S(1)	141.27(6)
C(29)-S(2)-K(1)#1	125.90(15)	O(21)-K(1)-S(1)	122.66(5)
O(2A)-S(2)-K(1)#4	64.73(10)	O(2A)#1-K(1)-S(1)	89.36(5)

O(2A)#2-K(1)-S(1)	96.14(5)	O(1A)#8-K(3)-O(1B)#4	98.95(8)
S(2)#1-K(1)-S(1)	113.65(3)	O(1A)#1-K(3)-O(1B)#4	81.05(8)
S(2)#2-K(1)-S(1)	120.16(3)	O(1B)#9-K(3)-O(1B)#4	180.00(9)
O(1A)-K(1)-K(2)	152.67(7)	O(2A)#7-K(3)-O(1C)#1	66.69(7)
O(1C)#3-K(1)-K(2)	112.03(7)	O(2A)-K(3)-O(1C)#1	113.31(7)
O(22)-K(1)-K(2)	83.14(6)	O(1A)#8-K(3)-O(1C)#1	134.56(7)
O(2B)#1-K(1)-K(2)	43.57(5)	O(1A)#1-K(3)-O(1C)#1	45.44(7)
O(2C)#2-K(1)-K(2)	43.96(5)	O(1B)#9-K(3)-O(1C)#1	80.73(7)
O(21)-K(1)-K(2)	48.16(5)	O(1B)#4-K(3)-O(1C)#1	99.27(7)
O(2A)#1-K(1)-K(2)	90.00(5)	O(2A)#7-K(3)-O(1C)#8	113.31(7)
O(2A)#2-K(1)-K(2)	89.97(5)	O(2A)-K(3)-O(1C)#8	66.69(7)
S(2)#1-K(1)-K(2)	66.00(3)	O(1A)#8-K(3)-O(1C)#8	45.44(7)
S(2)#2-K(1)-K(2)	66.30(3)	O(1A)#1-K(3)-O(1C)#8	134.56(7)
S(1)-K(1)-K(2)	170.72(3)	O(1B)#9-K(3)-O(1C)#8	99.27(7)
O(2B)-K(2)-O(2B)#1	99.38(13)	O(1B)#4-K(3)-O(1C)#8	80.73(7)
O(2B)-K(2)-O(2C)#2	166.87(9)	O(1C)#1-K(3)-O(1C)#8	180.00(18)
O(2B)#1-K(2)-O(2C)#2	89.08(9)	O(2A)#7-K(3)-S(1)#1	86.52(6)
O(2B)-K(2)-O(2C)#6	89.08(9)	O(2A)-K(3)-S(1)#1	93.48(6)
O(2B)#1-K(2)-O(2C)#6	166.87(9)	O(1A)#8-K(3)-S(1)#1	157.75(6)
O(2C)#2-K(2)-O(2C)#6	84.50(13)	O(1A)#1-K(3)-S(1)#1	22.25(6)
O(2B)-K(2)-O(21)	87.02(7)	O(1B)#9-K(3)-S(1)#1	91.80(6)
O(2B)#1-K(2)-O(21)	78.45(8)	O(1B)#4-K(3)-S(1)#1	88.20(6)
O(2C)#2-K(2)-O(21)	84.85(7)	O(1C)#1-K(3)-S(1)#1	23.34(5)
O(2C)#6-K(2)-O(21)	112.24(8)	O(1C)#8-K(3)-S(1)#1	156.66(5)
O(2B)-K(2)-O(21)#1	78.44(8)	O(2A)#7-K(3)-S(1)#8	93.48(6)
O(2B)#1-K(2)-O(21)#1	87.02(7)	O(2A)-K(3)-S(1)#8	86.52(6)
O(2C)#2-K(2)-O(21)#1	112.24(8)	O(1A)#8-K(3)-S(1)#8	22.25(6)
O(2C)#6-K(2)-O(21)#1	84.85(7)	O(1A)#1-K(3)-S(1)#8	157.75(6)
O(21)-K(2)-O(21)#1	157.51(10)	O(1B)#9-K(3)-S(1)#8	88.20(6)
O(2B)-K(2)-K(1)#1	50.11(6)	O(1B)#4-K(3)-S(1)#8	91.80(6)
O(2B)#1-K(2)-K(1)#1	129.87(6)	O(1C)#1-K(3)-S(1)#8	156.66(5)
O(2C)#2-K(2)-K(1)#1	129.86(7)	O(1C)#8-K(3)-S(1)#8	23.34(5)
O(2C)#6-K(2)-K(1)#1	50.18(6)	S(1)#1-K(3)-S(1)#8	180.00(5)
O(21)-K(2)-K(1)#1	127.59(5)	O(2A)#7-K(3)-K(1)#9	49.05(5)
O(21)#1-K(2)-K(1)#1	52.40(5)	O(2A)-K(3)-K(1)#9	130.95(5)
O(2B)-K(2)-K(1)	129.87(6)	O(1A)#8-K(3)-K(1)#9	96.99(6)
O(2B)#1-K(2)-K(1)	50.10(6)	O(1A)#1-K(3)-K(1)#9	83.01(6)
O(2C)#2-K(2)-K(1)	50.17(6)	O(1B)#9-K(3)-K(1)#9	54.08(7)
O(2C)#6-K(2)-K(1)	129.86(7)	O(1B)#4-K(3)-K(1)#9	125.92(7)
O(21)-K(2)-K(1)	52.41(5)	O(1C)#1-K(3)-K(1)#9	39.95(5)
O(21)#1-K(2)-K(1)	127.59(5)	O(1C)#8-K(3)-K(1)#9	140.05(5)
K(1)#1-K(2)-K(1)	179.97(4)	S(1)#1-K(3)-K(1)#9	62.331(19)
O(2A)#7-K(3)-O(2A)	180.00(12)	S(1)#8-K(3)-K(1)#9	117.669(19)
O(2A)#7-K(3)-O(1A)#8	72.82(8)	O(2A)#7-K(3)-K(1)#4	130.95(5)
O(2A)-K(3)-O(1A)#8	107.18(8)	O(2A)-K(3)-K(1)#4	49.05(5)
O(2A)#7-K(3)-O(1A)#1	107.18(8)	O(1A)#8-K(3)-K(1)#4	83.01(6)
O(2A)-K(3)-O(1A)#1	72.82(8)	O(1A)#1-K(3)-K(1)#4	96.99(6)
O(1A)#8-K(3)-O(1A)#1	180.0	O(1B)#9-K(3)-K(1)#4	125.92(7)
O(2A)#7-K(3)-O(1B)#9	92.12(9)	O(1B)#4-K(3)-K(1)#4	54.08(7)
O(2A)-K(3)-O(1B)#9	87.88(9)	O(1C)#1-K(3)-K(1)#4	140.05(5)
O(1A)#8-K(3)-O(1B)#9	81.05(8)	O(1C)#8-K(3)-K(1)#4	39.95(5)
O(1A)#1-K(3)-O(1B)#9	98.95(8)	S(1)#1-K(3)-K(1)#4	117.669(19)
O(2A)#7-K(3)-O(1B)#4	87.88(9)	S(1)#8-K(3)-K(1)#4	62.331(19)
O(2A)-K(3)-O(1B)#4	92.12(9)	K(1)#9-K(3)-K(1)#4	180.00(2)

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

(#3) -x,-y+1,-z+1; (#4) -x,y-1,-z+1/2; (#5) x,y-1,z; (#6) x,y+1,z; (#7) -x,-y,-z; (#8) x,-y,z-1/2; (#9) x,-y+1,z-1/2

Table S3. Anisotropic displacement parameters ($Å^2$ x 10^3) for s97. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(11)	43(2)	49(2)	35(2)	-3(2)	19(2)	2(2)
C(12)	54(2)	45(2)	38(2)	4(2)	24(2)	13(2)
C(13)	46(2)	67(3)	34(2)	-2(2)	13(2)	15(2)
C(14)	42(2)	75(3)	41(2)	-10(2)	14(2)	-7(2)
C(15)	53(2)	55(3)	42(2)	-5(2)	25(2)	-10(2)
C(16)	45(2)	47(2)	32(2)	0(2)	20(2)	0(2)
C(17)	53(2)	40(2)	38(2)	1(2)	25(2)	0(2)
C(18)	46(2)	44(2)	43(2)	7(2)	17(2)	7(2)
C(19)	39(2)	48(2)	38(2)	8(2)	19(2)	11(2)
C(21)	36(2)	43(2)	25(2)	4(2)	11(1)	-2(2)
C(22)	37(2)	46(2)	30(2)	1(2)	14(2)	-4(2)
C(23)	53(2)	53(2)	41(2)	-10(2)	23(2)	-15(2)
C(24)	43(2)	77(3)	53(3)	-13(2)	23(2)	-21(2)
C(25)	41(2)	72(3)	48(2)	-2(2)	26(2)	0(2)
C(26)	36(2)	47(2)	33(2)	2(2)	14(2)	0(2)
C(27)	39(2)	52(2)	37(2)	4(2)	16(2)	6(2)
C(28)	44(2)	46(2)	49(2)	-9(2)	9(2)	6(2)
C(29)	57(2)	46(2)	51(2)	-14(2)	30(2)	0(2)
C(110)	93(4)	71(4)	45(3)	15(3)	15(3)	15(3)
C(210)	64(3)	51(3)	55(3)	-12(2)	26(3)	-1(2)
N(1)	43(2)	49(2)	37(2)	6(1)	14(1)	0(1)
N(2)	40(2)	50(2)	38(2)	-4(2)	12(2)	7(2)
O(1A)	80(2)	78(2)	34(2)	-2(1)	13(1)	9(2)
O(1B)	67(2)	54(2)	84(2)	30(2)	28(2)	11(1)
O(1C)	43(2)	105(2)	72(2)	21(2)	33(2)	14(1)
O(2A)	77(2)	66(2)	29(1)	1(1)	24(1)	4(1)
O(2B)	72(2)	53(2)	42(2)	-8(1)	18(1)	19(1)
O(2C)	61(2)	68(2)	48(2)	7(1)	23(1)	-13(1)
O(11)	50(2)	54(2)	45(2)	11(1)	15(1)	-5(1)
O(12)	71(2)	56(2)	48(2)	16(1)	18(2)	13(1)
O(21)	32(1)	53(1)	46(2)	-10(1)	14(1)	-6(1)
O(22)	50(2)	55(2)	62(2)	-19(1)	31(1)	-10(1)
S(1)	39(1)	50(1)	38(1)	13(1)	16(1)	7(1)
S(2)	48(1)	38(1)	26(1)	0(1)	17(1)	3(1)
K(1)	44(1)	49(1)	34(1)	2(1)	19(1)	0(1)
K(2)	51(1)	42(1)	36(1)	0	25(1)	0
K(3)	53(1)	52(1)	32(1)	-2(1)	22(1)	-4(1)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for s97.

Atom	x	y	z	U(eq)
H(2)	824(12)	1830(60)	3054(17)	61(13)
H(11)	1808(13)	1600(70)	7670(20)	79(15)
H(11A)	2970(12)	-850(70)	9826(19)	67(13)
H(11B)	3127(15)	-2490(70)	9520(20)	94(18)
H(11C)	2738(14)	-3300(80)	9570(20)	96(18)
H(13)	3278(11)	1030(60)	9386(16)	53(10)
H(14)	3378(12)	4500(60)	8998(16)	54(11)
H(15)	2828(11)	6070(60)	8159(16)	56(12)
H(17)	2108(10)	6360(60)	7441(15)	47(10)
H(18A)	1120(10)	5420(50)	6876(14)	41(9)
H(18B)	1410(9)	6700(50)	6725(14)	38(9)
H(19A)	1153(9)	2330(50)	6268(14)	39(9)
H(19B)	1373(11)	3920(60)	6080(16)	61(11)
H(21A)	1040(13)	11000(70)	4350(20)	83(16)
H(21B)	804(14)	9980(70)	4590(20)	78(16)
H(21C)	1286(12)	9750(60)	4954(19)	67(12)
H(23)	1696(11)	9270(60)	4581(16)	50(11)
H(24)	2194(11)	7930(60)	4388(16)	61(11)
H(25)	2029(11)	4660(60)	3816(15)	52(11)
H(27)	1602(11)	1590(60)	3274(16)	63(12)
H(28A)	791(13)	-1900(70)	2776(18)	75(14)
H(28B)	1237(13)	-1520(60)	2839(18)	77(13)
H(29A)	744(10)	-1700(60)	1845(15)	45(10)
H(29B)	868(13)	760(70)	1901(19)	85(14)

Table S5. Torsion angles [°] for s97.

O(11)-C(11)-C(12)-O(12)	-3.6(5)	K(1)#3-O(1C)-S(1)-O(1B)	40.5(6)
C(16)-C(11)-C(12)-O(12)	174.7(3)	K(3)#1-O(1C)-S(1)-O(1B)	137.20(15)
O(11)-C(11)-C(12)-C(13)	176.5(3)	K(1)#3-O(1C)-S(1)-O(1A)	-89.4(6)
C(16)-C(11)-C(12)-C(13)	-5.3(5)	K(3)#1-O(1C)-S(1)-O(1A)	7.33(16)
O(12)-C(12)-C(13)-C(14)	-178.9(3)	K(1)#3-O(1C)-S(1)-C(19)	157.9(5)
C(11)-C(12)-C(13)-C(14)	1.1(6)	K(3)#1-O(1C)-S(1)-C(19)	-105.34(15)
C(12)-C(13)-C(14)-C(15)	3.0(6)	K(1)#3-O(1C)-S(1)-K(1)	-43.2(6)
C(13)-C(14)-C(15)-C(16)	-2.7(6)	K(3)#1-O(1C)-S(1)-K(1)	53.58(11)
O(11)-C(11)-C(16)-C(15)	-176.3(3)	K(1)#3-O(1C)-S(1)-K(3)#1	-96.7(6)
C(12)-C(11)-C(16)-C(15)	5.5(5)	K(1)-O(1A)-S(1)-O(1B)	-21.9(2)
O(11)-C(11)-C(16)-C(17)	5.8(5)	K(3)#1-O(1A)-S(1)-O(1B)	-139.24(14)
C(12)-C(11)-C(16)-C(17)	-172.3(3)	K(1)-O(1A)-S(1)-O(1C)	108.53(18)
C(14)-C(15)-C(16)-C(11)	-1.5(5)	K(3)#1-O(1A)-S(1)-O(1C)	-8.85(19)
C(14)-C(15)-C(16)-C(17)	176.3(4)	K(1)-O(1A)-S(1)-C(19)	-138.22(18)
C(11)-C(16)-C(17)-N(1)	-2.7(5)	K(3)#1-O(1A)-S(1)-C(19)	104.41(17)
C(15)-C(16)-C(17)-N(1)	179.6(3)	K(3)#1-O(1A)-S(1)-K(1)	-117.4(2)
N(1)-C(18)-C(19)-S(1)	166.8(3)	K(1)-O(1A)-S(1)-K(3)#1	117.4(2)
O(21)-C(21)-C(22)-O(22)	3.3(4)	C(18)-C(19)-S(1)-O(1B)	59.6(3)
C(26)-C(21)-C(22)-O(22)	-176.7(3)	C(18)-C(19)-S(1)-O(1C)	-62.3(3)
O(21)-C(21)-C(22)-C(23)	-175.6(3)	C(18)-C(19)-S(1)-O(1A)	179.9(3)
C(26)-C(21)-C(22)-C(23)	4.4(5)	C(18)-C(19)-S(1)-K(1)	142.9(2)
O(22)-C(22)-C(23)-C(24)	179.0(3)	C(18)-C(19)-S(1)-K(3)#1	-129.8(3)
C(21)-C(22)-C(23)-C(24)	-2.2(6)	K(3)-O(2A)-S(2)-O(2C)	-113.4(4)
C(22)-C(23)-C(24)-C(25)	-1.5(6)	K(1)#1-O(2A)-S(2)-O(2C)	123.46(14)
C(23)-C(24)-C(25)-C(26)	2.7(6)	K(1)#4-O(2A)-S(2)-O(2C)	-19.68(16)
C(24)-C(25)-C(26)-C(27)	-179.8(4)	K(3)-O(2A)-S(2)-O(2B)	117.1(4)
C(24)-C(25)-C(26)-C(21)	-0.3(6)	K(1)#1-O(2A)-S(2)-O(2B)	-6.03(17)
O(21)-C(21)-C(26)-C(27)	-3.6(5)	K(1)#4-O(2A)-S(2)-O(2B)	-149.18(13)
C(22)-C(21)-C(26)-C(27)	176.4(3)	K(3)-O(2A)-S(2)-C(29)	1.4(4)
O(21)-C(21)-C(26)-C(25)	176.8(3)	K(1)#1-O(2A)-S(2)-C(29)	-121.76(16)
C(22)-C(21)-C(26)-C(25)	-3.2(5)	K(1)#4-O(2A)-S(2)-C(29)	95.09(16)
C(25)-C(26)-C(27)-N(2)	-176.4(4)	K(3)-O(2A)-S(2)-K(1)#1	123.2(4)
C(21)-C(26)-C(27)-N(2)	4.0(5)	K(1)#4-O(2A)-S(2)-K(1)#1	-143.14(11)
N(2)-C(28)-C(29)-S(2)	-73.2(4)	K(3)-O(2A)-S(2)-K(1)#4	-93.7(4)
C(16)-C(17)-N(1)-C(18)	178.9(3)	K(1)#1-O(2A)-S(2)-K(1)#4	143.14(11)
C(19)-C(18)-N(1)-C(17)	115.5(4)	K(2)#5-O(2C)-S(2)-O(2A)	146.6(5)
C(26)-C(27)-N(2)-C(28)	-178.2(3)	K(1)#4-O(2C)-S(2)-O(2A)	23.11(18)
C(29)-C(28)-N(2)-C(27)	-99.7(4)	K(2)#5-O(2C)-S(2)-O(2B)	-84.3(5)
C(13)-C(12)-O(12)-C(110)	8.6(6)	K(1)#4-O(2C)-S(2)-O(2B)	152.19(12)
C(11)-C(12)-O(12)-C(110)	-171.3(4)	K(2)#5-O(2C)-S(2)-C(29)	30.1(5)
C(26)-C(21)-O(21)-K(2)	-96.0(4)	K(1)#4-O(2C)-S(2)-C(29)	-93.40(17)
C(22)-C(21)-O(21)-K(2)	84.0(4)	K(2)#5-O(2C)-S(2)-K(1)#1	-144.2(4)
C(26)-C(21)-O(21)-K(1)	159.1(2)	K(1)#4-O(2C)-S(2)-K(1)#1	92.34(14)
C(22)-C(21)-O(21)-K(1)	-20.9(4)	K(2)#5-O(2C)-S(2)-K(1)#4	123.5(5)
C(23)-C(22)-O(22)-C(210)	6.3(5)	K(2)-O(2B)-S(2)-O(2A)	119.6(4)
C(21)-C(22)-O(22)-C(210)	-172.6(3)	K(1)#1-O(2B)-S(2)-O(2A)	6.63(19)
C(23)-C(22)-O(22)-K(1)	-162.5(3)	K(2)-O(2B)-S(2)-O(2C)	-9.1(4)
C(21)-C(22)-O(22)-K(1)	18.7(4)	K(1)#1-O(2B)-S(2)-O(2C)	-121.99(14)
K(3)#2-O(1B)-S(1)-O(1C)	-36.5(2)	K(2)-O(2B)-S(2)-C(29)	-123.2(4)
K(3)#2-O(1B)-S(1)-O(1A)	92.7(2)	K(1)#1-O(2B)-S(2)-C(29)	123.83(16)
K(3)#2-O(1B)-S(1)-C(19)	-152.74(17)	K(2)-O(2B)-S(2)-K(1)#1	112.9(4)
K(3)#2-O(1B)-S(1)-K(1)	77.64(14)	K(2)-O(2B)-S(2)-K(1)#4	40.9(5)
K(3)#2-O(1B)-S(1)-K(3)#1	41.5(3)	K(1)#1-O(2B)-S(2)-K(1)#4	-72.0(3)

C(28)-C(29)-S(2)-O(2A)	-173.0(3)
C(28)-C(29)-S(2)-O(2C)	-53.6(3)
C(28)-C(29)-S(2)-O(2B)	66.5(3)
C(28)-C(29)-S(2)-K(1)#1	120.9(3)
C(28)-C(29)-S(2)-K(1)#4	-106.0(3)
S(1)-O(1A)-K(1)-O(1C)#3	-70.65(19)
K(3)#1-O(1A)-K(1)-O(1C)#3	49.82(10)
S(1)-O(1A)-K(1)-O(22)	68.90(19)
K(3)#1-O(1A)-K(1)-O(22)	-170.62(8)
S(1)-O(1A)-K(1)-O(2B)#1	-155.93(16)
K(3)#1-O(1A)-K(1)-O(2B)#1	-35.45(13)
S(1)-O(1A)-K(1)-O(2C)#2	5.4(4)
K(3)#1-O(1A)-K(1)-O(2C)#2	125.9(3)
S(1)-O(1A)-K(1)-O(21)	124.22(17)
K(3)#1-O(1A)-K(1)-O(21)	-115.30(9)
S(1)-O(1A)-K(1)-O(2A)#1	-149.7(2)
K(3)#1-O(1A)-K(1)-O(2A)#1	-29.27(8)
S(1)-O(1A)-K(1)-O(2A)#2	-9.6(2)
K(3)#1-O(1A)-K(1)-O(2A)#2	110.84(9)
S(1)-O(1A)-K(1)-S(2)#1	-154.32(17)
K(3)#1-O(1A)-K(1)-S(2)#1	-33.84(8)
S(1)-O(1A)-K(1)-S(2)#2	-13.8(3)
K(3)#1-O(1A)-K(1)-S(2)#2	106.67(10)
K(3)#1-O(1A)-K(1)-S(1)	120.5(2)
S(1)-O(1A)-K(1)-K(2)	162.73(9)
K(3)#1-O(1A)-K(1)-K(2)	-76.79(18)
C(22)-O(22)-K(1)-O(1A)	90.7(2)
C(210)-O(22)-K(1)-O(1A)	-78.4(3)
C(22)-O(22)-K(1)-O(1C)#3	-178.2(2)
C(210)-O(22)-K(1)-O(1C)#3	12.8(3)
C(22)-O(22)-K(1)-O(2B)#1	-42.0(3)
C(210)-O(22)-K(1)-O(2B)#1	148.9(3)
C(22)-O(22)-K(1)-O(2C)#2	-105.7(3)
C(210)-O(22)-K(1)-O(2C)#2	85.3(3)
C(22)-O(22)-K(1)-O(21)	-19.6(2)
C(210)-O(22)-K(1)-O(21)	171.3(3)
C(22)-O(22)-K(1)-O(2A)#1	19.5(3)
C(210)-O(22)-K(1)-O(2A)#1	-149.6(3)
C(22)-O(22)-K(1)-O(2A)#2	-153.6(3)
C(210)-O(22)-K(1)-O(2A)#2	37.3(3)
C(22)-O(22)-K(1)-S(2)#1	-15.8(3)
C(210)-O(22)-K(1)-S(2)#1	175.1(2)
C(22)-O(22)-K(1)-S(2)#2	-129.0(2)
C(210)-O(22)-K(1)-S(2)#2	61.9(3)
C(22)-O(22)-K(1)-S(1)	110.5(2)
C(210)-O(22)-K(1)-S(1)	-58.6(3)
C(22)-O(22)-K(1)-K(2)	-61.9(2)
C(210)-O(22)-K(1)-K(2)	129.1(3)
C(21)-O(21)-K(1)-O(1A)	-66.4(2)
K(2)-O(21)-K(1)-O(1A)	157.43(8)
C(21)-O(21)-K(1)-O(1C)#3	158.7(3)
K(2)-O(21)-K(1)-O(1C)#3	22.6(2)
C(21)-O(21)-K(1)-O(22)	19.7(2)
K(2)-O(21)-K(1)-O(22)	-116.44(9)
C(21)-O(21)-K(1)-O(2B)#1	179.8(2)
K(2)-O(21)-K(1)-O(2B)#1	43.72(6)
C(21)-O(21)-K(1)-O(2C)#2	97.9(2)
K(2)-O(21)-K(1)-O(2C)#2	-38.25(7)
C(21)-O(21)-K(1)-O(2A)#1	-137.1(2)
K(2)-O(21)-K(1)-O(2A)#1	86.74(7)
C(21)-O(21)-K(1)-O(2A)#2	69.1(2)
K(2)-O(21)-K(1)-O(2A)#2	-66.99(7)
C(21)-O(21)-K(1)-S(2)#1	-157.6(2)
K(2)-O(21)-K(1)-S(2)#1	66.32(5)
C(21)-O(21)-K(1)-S(2)#2	88.4(2)
K(2)-O(21)-K(1)-S(2)#2	-47.72(5)
C(21)-O(21)-K(1)-S(1)	-45.6(2)
K(2)-O(21)-K(1)-S(1)	178.31(4)
C(21)-O(21)-K(1)-K(2)	136.1(2)
O(1B)-S(1)-K(1)-O(1A)	159.1(2)
O(1C)-S(1)-K(1)-O(1A)	-92.0(2)
C(19)-S(1)-K(1)-O(1A)	60.2(3)
K(3)#1-S(1)-K(1)-O(1A)	-43.36(18)
O(1B)-S(1)-K(1)-O(1C)#3	-95.17(14)
O(1C)-S(1)-K(1)-O(1C)#3	13.8(2)
O(1A)-S(1)-K(1)-O(1C)#3	105.8(2)
C(19)-S(1)-K(1)-O(1C)#3	166.0(2)
K(3)#1-S(1)-K(1)-O(1C)#3	62.40(7)
O(1B)-S(1)-K(1)-O(22)	45.99(13)
O(1C)-S(1)-K(1)-O(22)	154.93(15)
O(1A)-S(1)-K(1)-O(22)	-113.08(19)
C(19)-S(1)-K(1)-O(22)	-52.87(19)
K(3)#1-S(1)-K(1)-O(22)	-156.44(5)
O(1B)-S(1)-K(1)-O(2B)#1	-169.04(15)
O(1C)-S(1)-K(1)-O(2B)#1	-60.10(17)
O(1A)-S(1)-K(1)-O(2B)#1	31.9(2)
C(19)-S(1)-K(1)-O(2B)#1	92.1(2)
K(3)#1-S(1)-K(1)-O(2B)#1	-11.47(9)
O(1B)-S(1)-K(1)-O(2C)#2	-18.34(16)
O(1C)-S(1)-K(1)-O(2C)#2	90.60(17)
O(1A)-S(1)-K(1)-O(2C)#2	-177.4(2)
C(19)-S(1)-K(1)-O(2C)#2	-117.2(2)
K(3)#1-S(1)-K(1)-O(2C)#2	139.22(10)
O(1B)-S(1)-K(1)-O(21)	93.56(14)
O(1C)-S(1)-K(1)-O(21)	-157.50(15)
O(1A)-S(1)-K(1)-O(21)	-65.51(19)
C(19)-S(1)-K(1)-O(21)	-5.3(2)
K(3)#1-S(1)-K(1)-O(21)	-108.87(6)
O(1B)-S(1)-K(1)-O(2A)#1	-172.52(13)
O(1C)-S(1)-K(1)-O(2A)#1	-63.58(16)
O(1A)-S(1)-K(1)-O(2A)#1	28.41(19)
C(19)-S(1)-K(1)-O(2A)#1	88.61(19)
K(3)#1-S(1)-K(1)-O(2A)#1	-14.96(5)
O(1B)-S(1)-K(1)-O(2A)#2	-29.54(13)
O(1C)-S(1)-K(1)-O(2A)#2	79.39(15)
O(1A)-S(1)-K(1)-O(2A)#2	171.39(19)
C(19)-S(1)-K(1)-O(2A)#2	-128.41(19)
K(3)#1-S(1)-K(1)-O(2A)#2	128.02(5)
O(1B)-S(1)-K(1)-S(2)#1	-172.80(12)
O(1C)-S(1)-K(1)-S(2)#1	-63.86(15)
O(1A)-S(1)-K(1)-S(2)#1	28.13(19)
C(19)-S(1)-K(1)-S(2)#1	88.34(19)

K(3)#1-S(1)-K(1)-S(2)#1	-15.23(3)
O(1B)-S(1)-K(1)-S(2)#2	-30.94(13)
O(1C)-S(1)-K(1)-S(2)#2	78.00(15)
O(1A)-S(1)-K(1)-S(2)#2	169.99(19)
C(19)-S(1)-K(1)-S(2)#2	-129.80(19)
K(3)#1-S(1)-K(1)-S(2)#2	126.63(3)
O(1B)-S(1)-K(1)-K(2)	101.4(2)
O(1C)-S(1)-K(1)-K(2)	-149.7(2)
O(1A)-S(1)-K(1)-K(2)	-57.7(3)
C(19)-S(1)-K(1)-K(2)	2.5(3)
K(3)#1-S(1)-K(1)-K(2)	-101.04(19)
S(2)-O(2B)-K(2)-O(2B)#1	18.8(3)
K(1)#1-O(2B)-K(2)-O(2B)#1	135.13(9)
S(2)-O(2B)-K(2)-O(2C)#2	148.3(4)
K(1)#1-O(2B)-K(2)-O(2C)#2	-95.3(4)
S(2)-O(2B)-K(2)-O(2C)#6	-151.1(4)
K(1)#1-O(2B)-K(2)-O(2C)#6	-34.78(8)
S(2)-O(2B)-K(2)-O(21)	96.5(4)
K(1)#1-O(2B)-K(2)-O(21)	-147.10(8)
S(2)-O(2B)-K(2)-O(21)#1	-66.2(4)
K(1)#1-O(2B)-K(2)-O(21)#1	50.16(7)
S(2)-O(2B)-K(2)-K(1)#1	-116.4(4)
S(2)-O(2B)-K(2)-K(1)	63.6(4)
K(1)#1-O(2B)-K(2)-K(1)	179.98(3)
C(21)-O(21)-K(2)-O(2B)	91.2(3)
K(1)-O(21)-K(2)-O(2B)	-148.23(8)
C(21)-O(21)-K(2)-O(2B)#1	-168.6(3)
K(1)-O(21)-K(2)-O(2B)#1	-48.02(7)
C(21)-O(21)-K(2)-O(2C)#2	-78.5(3)
K(1)-O(21)-K(2)-O(2C)#2	42.08(7)
C(21)-O(21)-K(2)-O(2C)#6	3.4(3)
K(1)-O(21)-K(2)-O(2C)#6	123.99(8)
C(21)-O(21)-K(2)-O(21)#1	140.7(3)
K(1)-O(21)-K(2)-O(21)#1	-98.79(4)
C(21)-O(21)-K(2)-K(1)#1	59.5(3)
K(1)-O(21)-K(2)-K(1)#1	-179.96(5)
C(21)-O(21)-K(2)-K(1)	-120.6(3)
O(1A)-K(1)-K(2)-O(2B)	-7.52(18)
O(1C)#3-K(1)-K(2)-O(2B)	-128.19(11)
O(22)-K(1)-K(2)-O(2B)	90.35(10)
O(2B)#1-K(1)-K(2)-O(2B)	-65.07(16)
O(2C)#2-K(1)-K(2)-O(2B)	162.88(11)
O(21)-K(1)-K(2)-O(2B)	43.24(10)
O(2A)#1-K(1)-K(2)-O(2B)	-51.65(10)
O(2A)#2-K(1)-K(2)-O(2B)	165.70(10)
S(2)#1-K(1)-K(2)-O(2B)	-55.54(9)
S(2)#2-K(1)-K(2)-O(2B)	170.11(9)
S(1)-K(1)-K(2)-O(2B)	34.4(2)
O(1A)-K(1)-K(2)-O(2B)#1	57.56(17)
O(1C)#3-K(1)-K(2)-O(2B)#1	-63.12(11)
O(22)-K(1)-K(2)-O(2B)#1	155.43(10)
O(2C)#2-K(1)-K(2)-O(2B)#1	-132.05(11)
O(21)-K(1)-K(2)-O(2B)#1	108.31(10)
O(2A)#1-K(1)-K(2)-O(2B)#1	13.42(10)
O(2A)#2-K(1)-K(2)-O(2B)#1	-129.23(10)
S(2)#1-K(1)-K(2)-O(2B)#1	9.54(8)
S(2)#2-K(1)-K(2)-O(2B)#1	-124.82(8)
S(1)-K(1)-K(2)-O(2B)#1	99.5(2)
O(1A)-K(1)-K(2)-O(2C)#2	-170.39(18)
O(1C)#3-K(1)-K(2)-O(2C)#2	68.93(11)
O(22)-K(1)-K(2)-O(2C)#2	-72.53(9)
O(2B)#1-K(1)-K(2)-O(2C)#2	132.05(11)
O(21)-K(1)-K(2)-O(2C)#2	-119.64(10)
O(2A)#1-K(1)-K(2)-O(2C)#2	145.47(10)
O(2A)#2-K(1)-K(2)-O(2C)#2	2.82(9)
S(2)#1-K(1)-K(2)-O(2C)#2	141.59(8)
S(2)#2-K(1)-K(2)-O(2C)#2	7.23(8)
S(1)-K(1)-K(2)-O(2C)#2	-128.5(2)
O(1A)-K(1)-K(2)-O(2C)#6	-139.57(17)
O(1C)#3-K(1)-K(2)-O(2C)#6	99.75(11)
O(22)-K(1)-K(2)-O(2C)#6	-41.71(10)
O(2B)#1-K(1)-K(2)-O(2C)#6	162.87(11)
O(2C)#2-K(1)-K(2)-O(2C)#6	30.82(16)
O(21)-K(1)-K(2)-O(2C)#6	-88.82(10)
O(2A)#1-K(1)-K(2)-O(2C)#6	176.29(9)
O(2A)#2-K(1)-K(2)-O(2C)#6	33.64(10)
S(2)#1-K(1)-K(2)-O(2C)#6	172.41(8)
S(2)#2-K(1)-K(2)-O(2C)#6	38.05(8)
S(1)-K(1)-K(2)-O(2C)#6	-97.7(2)
O(1A)-K(1)-K(2)-O(21)	-50.75(16)
O(1C)#3-K(1)-K(2)-O(21)	-171.43(9)
O(22)-K(1)-K(2)-O(21)	47.11(8)
O(2B)#1-K(1)-K(2)-O(21)	-108.31(10)
O(2C)#2-K(1)-K(2)-O(21)	119.64(10)
O(2A)#1-K(1)-K(2)-O(21)	-94.89(8)
O(2A)#2-K(1)-K(2)-O(21)	122.46(8)
S(2)#1-K(1)-K(2)-O(21)	-98.77(6)
S(2)#2-K(1)-K(2)-O(21)	126.87(6)
S(1)-K(1)-K(2)-O(21)	-8.9(2)
O(1A)-K(1)-K(2)-O(21)#1	100.75(16)
O(1C)#3-K(1)-K(2)-O(21)#1	-19.92(10)
O(22)-K(1)-K(2)-O(21)#1	-161.38(9)
O(2B)#1-K(1)-K(2)-O(21)#1	43.20(10)
O(2C)#2-K(1)-K(2)-O(21)#1	-88.85(10)
O(21)-K(1)-K(2)-O(21)#1	151.51(13)
O(2A)#1-K(1)-K(2)-O(21)#1	56.62(9)
O(2A)#2-K(1)-K(2)-O(21)#1	-86.03(9)
S(2)#1-K(1)-K(2)-O(21)#1	52.74(7)
S(2)#2-K(1)-K(2)-O(21)#1	-81.62(7)
S(1)-K(1)-K(2)-O(21)#1	142.65(18)
O(1A)-K(1)-K(2)-K(1)#1	29(100)
O(1C)#3-K(1)-K(2)-K(1)#1	-92(100)
O(22)-K(1)-K(2)-K(1)#1	126(100)
O(2B)#1-K(1)-K(2)-K(1)#1	-29(100)
O(2C)#2-K(1)-K(2)-K(1)#1	-161(100)
O(21)-K(1)-K(2)-K(1)#1	79(100)
O(2A)#1-K(1)-K(2)-K(1)#1	-16(100)
O(2A)#2-K(1)-K(2)-K(1)#1	-158(100)
S(2)#1-K(1)-K(2)-K(1)#1	-19(100)
S(2)#2-K(1)-K(2)-K(1)#1	-154(100)
S(1)-K(1)-K(2)-K(1)#1	70(100)
S(2)-O(2A)-K(3)-O(2A)#7	83(6)

K(1)#1-O(2A)-K(3)-O(2A)#7	-154(6)
K(1)#4-O(2A)-K(3)-O(2A)#7	-11(6)
S(2)-O(2A)-K(3)-O(1A)#8	29.8(4)
K(1)#1-O(2A)-K(3)-O(1A)#8	152.62(7)
K(1)#4-O(2A)-K(3)-O(1A)#8	-64.09(8)
S(2)-O(2A)-K(3)-O(1A)#1	-150.2(4)
K(1)#1-O(2A)-K(3)-O(1A)#1	-27.38(7)
K(1)#4-O(2A)-K(3)-O(1A)#1	115.91(8)
S(2)-O(2A)-K(3)-O(1B)#9	-50.2(4)
K(1)#1-O(2A)-K(3)-O(1B)#9	72.67(8)
K(1)#4-O(2A)-K(3)-O(1B)#9	-144.04(7)
S(2)-O(2A)-K(3)-O(1B)#4	129.8(4)
K(1)#1-O(2A)-K(3)-O(1B)#4	-107.33(8)
K(1)#4-O(2A)-K(3)-O(1B)#4	35.96(7)
S(2)-O(2A)-K(3)-O(1C)#1	-129.1(4)
K(1)#1-O(2A)-K(3)-O(1C)#1	-6.30(10)
K(1)#4-O(2A)-K(3)-O(1C)#1	137.00(6)
S(2)-O(2A)-K(3)-O(1C)#8	50.9(4)
K(1)#1-O(2A)-K(3)-O(1C)#8	173.70(10)
K(1)#4-O(2A)-K(3)-O(1C)#8	-43.00(6)
S(2)-O(2A)-K(3)-S(1)#1	-141.9(4)
K(1)#1-O(2A)-K(3)-S(1)#1	-19.01(6)
K(1)#4-O(2A)-K(3)-S(1)#1	124.28(5)
S(2)-O(2A)-K(3)-S(1)#8	38.1(4)
K(1)#1-O(2A)-K(3)-S(1)#8	160.99(6)
K(1)#4-O(2A)-K(3)-S(1)#8	-55.72(5)
S(2)-O(2A)-K(3)-K(1)#9	-86.1(4)
K(1)#1-O(2A)-K(3)-K(1)#9	36.71(11)
K(1)#4-O(2A)-K(3)-K(1)#9	180.0
S(2)-O(2A)-K(3)-K(1)#4	93.9(4)
K(1)#1-O(2A)-K(3)-K(1)#4	-143.29(11)

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