## 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. <sup>1</sup>H NMR full spectrum



**Figure S4.** <sup>1</sup>H NMR expanded spectrum, 2.7 – 7.2 ppm zone.









**Figure S6:** <sup>13</sup>C NMR expanded spectrum, 45 – 175 ppm zone.

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

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$\begin{array}{c} C(1) - C(16) \\ (11) - C(16) \\ (12) - C(12) \\ (14) - C(12) \\ (14) - C(12) \\ (12) - C(12) \\ (12) - C(12) \\ (12) - C(12) \\ (13) - C(13) \\ (12) - C(13) \\ (13) - C(14) \\ (13) - C(16) \\ (14) - C(15) \\ (13) - C(16) \\ (14) - C(15) \\ (13) - C(16) \\ (14) - C(15) \\ (15) - C(16) \\ (14) - C(17) \\ (14) - C(15) \\ (15) - C(16) \\ (15) - C(16) \\ (16) - C(17) \\ (14) - C(15) \\ (16) - C(17) \\ (14) - C(15) \\ (18) - N(1) \\ (12) - C(17) \\ (14) - C(15) \\ (18) - N(1) \\ (12) - C(17) \\ (14) - C(15) \\ (18) - N(1) \\ (12) - C(16) \\ (18) - N(1) \\ (12) - C(17) \\ (14) - C(16) - C(17) \\ (14) - C(18) - N(11) \\ (14) - C(16) - C(12) - C(13) \\ (13) - C(12) - C(12) \\ (13) - C(12) - C(13) \\ (13) - C(11) - C(11) - C(16) \\ (12) - C(12) \\ (12) - C(22) \\ (14) - C(13) - C(11) - C(11) - C(16) \\ (12) - C(12) \\ (12) - C(12) - C(13) \\ (13) - C(11) - C(11) - C(13) \\ (13) - C(12) - C(13) \\ (13) - C(13) - C(13) - C(13) - C(13) \\ (13) - C(13) - C(13) - C(13) - C$	$\overline{C(11)}$ - $O(11)$	1 346(4)	K(1) - O(1C) #3	2 714(3)
$\begin{array}{c} (1) - (21) \\ (11) - (21) \\ (12) \\ (13) - (12) \\ (14) - (01) \\ (12) - (13) \\ (13) - (14) \\ (15) \\ (12) - (13) \\ (13) - (14) \\ (15) \\ (13) - (14) \\ (15) \\ (13) - (14) \\ (15) \\ (13) - (14) \\ (15) \\ (14) - (15) \\ (15) - (16) \\ (14) - (15) \\ (15) - (16) \\ (14) - (15) \\ (15) - (16) \\ (14) - (15) \\ (15) - (16) \\ (16) - (17) \\ (16) - (16) \\ (16) - (17) \\ (16) - (16) \\ (17) - (11) \\ (16) - (17) \\ (16) - (17) \\ (16) - (17) \\ (16) - (17) \\ (16) - (16) \\ (17) - (16) \\ (16) - (17) \\ (16) - (17) \\ (16) - (16) \\ (17) - (16) \\ (16) - (17) \\ (16) - (16) \\ (17) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (16) \\ (11) - (16) \\ (11) - (16) \\ (11) - (16) \\ (11) - (16) \\ (11) - (16) \\ (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (11) - (16) \\ (11) - (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (11) - (16) \\ (11) - (16) - (11) - (11) - (16) \\ (11) - (16) - (12) - (11) \\ (11) - (16) - (12) - (11) \\ (11) - (16) - (12) - (11) \\ (11) - (16) - (12) - (11) \\ (11) - (16) - (12) - (11) \\ (11) - (16) - (12) - (11) \\ (11) - (16) - (12) - (11) \\ (11) - (16) - (12) - (16) \\ (11) - (16) - (12) - (16) \\ (11) - (16) - (12) - (16) \\ (11) - (16) - (12$	C(11)-C(16)	1 395(5)	K(1)-O(2B)#1	2.714(3) 2.845(3)
$\begin{array}{c} C(1) = O(12) \\ C(12) = O(12) \\ C(12) = O(12) \\ (13) = C(13) \\ C(12) = O(12) \\ (14) = 1.3810(5) \\ (14) = O(13) \\ C(14) = C(13) \\ C(14) = C(13) \\ C(14) = C(13) \\ C(14) = C(13) \\ C(15) = C(16) \\ (15) = C(17) \\ (14) = C(17) \\ (14) = C(17) \\ (14) = C(17) \\ (15) = C(17) \\ (14) = C(17) \\ (15) = C(17) \\ (15) = C(16) \\ (15) = C(17) \\ (15) = C(16) \\ (15) = C(17) \\ (15) = C(17) \\ (15) = C(16) \\ (15) = C(17) \\ (1$	C(11) - C(10)	1.090(5)	K(1) - O(2D) # 1 K(1) - O(2C) # 2	2.843(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(12) - O(12)	1.409(3) 1 366(4)	$K(1) - O(2C) \pi 2$ K(1) - O(2A) # 1	2.850(3) 3.048(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(12) - O(12) C(12) - O(12)	1.300(4)	K(1) - O(2A) # 2	3.040(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(12) - C(13) C(12) - C(14)	1.380(3) 1.281(6)	K(1) = O(2A) + 2 V(1) = S(2) + 1	3.193(3) 3.4842(12)
$\begin{array}{c} 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)-K(1) & 1.273(4) & K(2)-O(2D)\#1 & 2.556(3) \\ C(18)-K(1) & 1.458(4) & K(2)-O(2D)\#1 & 2.805(2) \\ C(19)-S(1) & 1.775(4) & K(2)-C(1)\#1 & 3.7006(11) \\ C(21)-O(21) & 1.271(4) & K(3)-O(1A)\#8 & 2.854(3) \\ C(21)-C(26) & 1.427(5) & K(3)-O(1A)\#8 & 2.854(3) \\ C(21)-C(26) & 1.427(5) & K(3)-O(1A)\#8 & 2.854(3) \\ C(21)-C(22) & 1.359(4) & K(3)-O(1B)\#4 & 2.920(3) \\ C(22)-C(23) & 1.359(4) & K(3)-O(1B)\#4 & 2.920(3) \\ C(22)-C(23) & 1.359(4) & K(3)-O(1B)\#4 & 2.920(3) \\ C(23)-C(25) & 1.341(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)\#1 & 3.6064(10) \\ C(26)-C(27) & 1.404(5) & K(3)-S(1)\#8 & 3.6064(10) \\ C(26)-C(27) & 1.404(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) \\ O(1A)-S(1) & 1.449(3) & O(12)-C(12)-C(11) & 114.6(3) \\ O(1A)-S(1) & 1.430(3) & C(14)-C(13) & 120.7(4) \\ O(15)-S(1) & 1.430(3) & C(14)-C(13) & 120.7(4) \\ O(15)-S(1) & 1.430(3) & C(14)-C(15) & 119.2(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) & 114.6(3) \\ O(1A)-K(3)\#1 & 2.854(3) & C(13)-C(12)-C(11) & 114.6(3) \\ O(1A)-K(3)\#1 & 2.854(3) & C(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(3) & 2.756(2) & O(11)-C(12)-C(16) & 122.5(3) \\ O(2A)-K(3) & 2.756(2) & O(11)-C(12)-C(16) & 122.5(3) \\ O(2A)-K(3) & 2.756(2) & O(11)-C(12)-C(16) & 123.5(3) \\ O(2A)-K(3) & 2.756(2) & O(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(3) & 2.756(2) & O(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(3) & 2.756(2) & O(21)-C(22) & 115.7(3) \\ O(2A)-K(1)\#1 & 3.248(3) & C(23)-C(22)-C(23) & 125.4(3) \\ O(2A)-K(1)\#1 & 3.6064(10) & C(27)-C(26)-C(21) & 120.9(3) \\ O(21)-K(1) & 2.805(2) & C(24)-C(25)-C(26) & 121.9(3) \\ O(22)-K(1) & 2.806(2) & C(27)-C(26)-C(21) & 120.9(3) \\ O(21)-K(1) & 2.806(2) & C(27)-C(26)-C(21) & 120.9(3) \\ $	C(13)-C(14)	1.361(0)	K(1)-S(2)#1 V(1)-S(2)#2	3.4842(12) 3.5200(12)
$\begin{array}{c} C(15)-C(16) & 1.494(3) & K(1)-K(2) & 5.7006(11) \\ C(16)-C(17) & 1.448(5) & K(2)-O(2B)\#1 & 2.556(2) \\ C(17)-N(1) & 1.273(4) & K(2)-O(2C)\#6 & 2.576(3) \\ C(18)-K(1) & 1.458(4) & K(2)-O(2C)\#6 & 2.576(3) \\ C(18)-K(1) & 1.75(4) & K(2)-O(2L)\#1 & 2.805(2) \\ C(19)-S(1) & 1.775(4) & K(2)-O(2L)\#1 & 2.805(2) \\ C(21)-O(21) & 1.271(4) & K(3)-O(1A)\#8 & 2.854(3) \\ C(21)-O(21) & 1.271(4) & K(3)-O(1A)\#1 & 2.854(3) \\ C(22)-O(22) & 1.459(4) & K(3)-O(1A)\#1 & 2.854(3) \\ C(22)-O(22) & 1.359(4) & K(3)-O(1B)\#9 & 2.920(3) \\ C(22)-C(22) & 1.359(4) & K(3)-O(1B)\#9 & 2.920(3) \\ C(22)-C(23) & 1.363(5) & K(3)-O(1C)\#8 & 3.247(3) \\ C(24)-C(25) & 1.341(5) & K(3)-O(1C)\#8 & 3.247(3) \\ C(26)-C(27) & 1.404(5) & K(3)-O(1C)\#8 & 3.247(3) \\ C(26)-C(27) & 1.404(5) & K(3)-S(1)\#8 & 3.6064(10) \\ C(27)-N(2) & 1.302(4) & K(3)-K(1)\#9 & 4.2274(8) \\ C(28)-N(2) & 1.459(5) & K(3)-K(1)\#4 & 4.2274(8) \\ C(28)-N(2) & 1.459(5) & K(3)-K(1)\#4 & 4.2274(8) \\ C(28)-N(2) & 1.423(5) & O(11)-C(11)-C(16) & 122.2(3) \\ C(110)-O(12) & 1.423(5) & O(11)-C(11)-C(12) & 118.2(3) \\ C(10)-O(12) & 1.423(5) & O(11)-C(11)-C(12) & 118.2(3) \\ C(10)-O(22) & 1.423(5) & O(11)-C(11)-C(12) & 118.2(3) \\ C(10)-O(12) & 1.423(5) & O(11)-C(11)-C(12) & 118.2(3) \\ C(10)-O(22) & 1.423(5) & O(12)-C(21) & 114.4(63) \\ O(1A)-K(1) & 2.680(3) & O(12)-C(12)-C(11) & 114.6(3) \\ O(1A)-K(1) & 2.680(3) & O(12)-C(12)-C(11) & 114.6(3) \\ O(1A)-K(1) & 1.430(3) & C(13)-C(12)-C(11) & 119.5(4) \\ O(1B)-K(3)\#1 & 3.049(3) & N(1)-C(18)-C(16) & 121.2(3) \\ O(1A)-K(1) & 1.430(3) & C(14)-C(15)-C(16) & 121.2(3) \\ O(1A)-K(1) & 1.430(3) & C(14)-C(15)-C(16) & 121.2(3) \\ O(1A)-K(1) & 1.430(3) & O(22)-C(22)-C(23) & 119.6(4) \\ O(22)-K(1) & 2.896(2) & C(23)-C(22)-C(23) & 119.6(4) \\ O(23)-K(1)\#1 & 3.608(4) & O(22)-C(22)-C(23) & 119.6(4) \\ O(23)-K(1)\#1 & 3.608(10) & C(27)-C(26)-C(21) & 120.0(3) \\ S(2)-K(1)\#4 & 3.59$	C(14)-C(15)	1.302(3) 1.404(5)	K(1)-S(2)#2 K(1)-K(2)	5.5299(12)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(15)-C(16)	1.404(5)	K(1)-K(2) K(2) O(2D) = 1	3.7006(11)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(10)-C(17)	1.448(5)	K(2) - O(2B) # 1	2.556(2)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(17) - N(1)	1.2/3(4)	K(2) - O(2C) # 2	2.576(5)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(18) - N(1)	1.458(4)	K(2) - O(2C) # 6	2.5/6(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(18) - C(19)	1.506(5)	K(2)-O(21)#1	2.805(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(19)-S(1)	1.//5(4)	K(2)-K(1)#1	3.7006(11)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(21)-O(21)	1.271(4)	K(3)-O(2A)#/	2.756(2)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(21)-C(26)	1.427(5)	K(3)-O(1A)#8	2.854(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(21)-C(22)	1.441(4)	K(3)-O(1A)#1	2.854(3)
$\begin{array}{ccccc} 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)-S(1)\#1 & 3.6064(10) \\ C(26)-C(27) & 1.404(5) & K(3)-S(1)\#1 & 3.6064(10) \\ C(27)-N(2) & 1.302(4) & K(3)-S(1)\#9 & 4.2274(8) \\ C(28)-N(2) & 1.302(4) & K(3)-K(1)\#9 & 4.2274(8) \\ C(28)-N(2) & 1.302(4) & K(3)-K(1)\#4 & 4.2274(8) \\ C(28)-N(2) & 1.302(4) & K(3)-K(1)\#4 & 4.2274(8) \\ C(28)-N(2) & 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(10)-O(22) & 1.423(5) & C(16)-C(11)-C(12) & 118.2(3) \\ C(10)-O(22) & 1.423(5) & C(16)-C(11)-C(12) & 118.2(3) \\ O(1A)-S(1) & 1.449(3) & O(12)-C(12)-C(11) & 114.6(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) & 114.6(3) \\ O(1B)-K(3)\#1 & 2.854(3) & C(13)-C(12)-C(11) & 119.5(4) \\ O(1B)-K(3)\#2 & 2.920(3) & 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)-S(1) & 1.430(3) & C(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(3)\#1 & 3.247(3) & C(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(3)\#1 & 3.247(3) & C(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(3)\#1 & 3.049(3) & N(1)-C(18)-C(19) & 109.4(3) \\ O(2A)-K(3)\#1 & 3.049(3) & N(1)-C(18)-C(19) & 109.4(3) \\ O(2A)-K(1)\#1 & 3.049(3) & O(22)-C(22)-C(21) & 113.7(3) \\ O(2B)-S(2) & 1.443(2) & O(21)-C(22) & 125.7(3) \\ O(2B)-S(2) & 1.440(3) & O(22)-C(22)-C(21) & 113.7(3) \\ O(2B)-S(2) & 1.440(3) & O(22)-C(22)-C(21) & 113.7(3) \\ O(2B)-K(1)\#1 & 2.845(3) & C(23)-C(22)-C(21) & 120.9(3) \\ O(2D)-K(1)\#4 & 2.849(3) & C(23)-C(22)-C(21) & 120.9(3) \\ O(2D)-K(1)\#4 & 2.849(3) & C(23)-C(22)-C(21) & 120.9(3) \\ O(2D)-K(1)\#4 & 2.849(3) & C(22)-C(22)-C(23) & 125.4(3) \\ 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(21)-C(22) & 119.0(4) \\ S(1)-K(1) & 3.5718(15) & C(27)-C(26)-C(21) & 120.9(3) \\ S(1)-K(3)\#1 & 3.6064(10) & C(27)-C(26)-C(21) & 120.9(3) \\ S(1)-K(3)\#1 & 3.6064(10) & C(27)-C(26)-C(21) & 120.9(3) \\ S(1)-K(3)\#1 & 3.6482(11) & C(25)-$	C(22)-O(22)	1.359(4)	K(3)-O(1B)#9	2.920(3)
$\begin{array}{ccccc} 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)-N(2) & 1.459(5) & K(3)-K(1)\#4 & 4.2274(8) \\ C(29)-C(29) & 1.520(5) & & \\ C(110)-O(12) & 1.423(5) & O(11)-C(11)-C(16) & 122.2(3) \\ C(110)-O(12) & 1.423(5) & O(11)-C(11)-C(12) & 118.5(3) \\ O(1A)-S(1) & 1.449(3) & O(12)-C(12)-C(13) & 125.9(3) \\ O(1A)-S(1) & 1.449(3) & O(12)-C(12)-C(11) & 119.5(3) \\ O(1A)-K(1) & 2.680(3) & O(12)-C(12)-C(11) & 119.5(4) \\ O(1B)-S(1) & 1.426(3) & C(12)-C(13) & 120.7(4) \\ O(1B)-K(3)\#1 & 2.854(3) & 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) & 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) & 119.9(3) \\ O(2A)-K(3) & 2.756(2) & N(1)-C(17)-C(16) & 121.5(3) \\ O(2A)-K(1)\#4 & 3.193(3) & C(18)-C(19)-S(1) & 114.0(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(2A)-K(1)\#4 & 3.193(3) & C(18)-C(19)-S(1) & 114.0(3) \\ O(2B)-K(2) & 2.556(2) & O(21)-C(21)-C(22) & 115.7(3) \\ O(2A)-K(1)\#4 & 3.193(3) & C(26)-C(21)-C(22) & 115.7(3) \\ O(2A)-K(1)\#4 & 2.849(3) & C(22)-C(22)-C(21) & 113.7(3) \\ O(22)-K(1)\#4 & 2.849(3) & C(22)-C(22)-C(21) & 113.7(3) \\ O(22)-K(1)\#4 & 2.849(3) & C(22)-C(22)-C(21) & 113.7(3) \\ O(22)-K(1)\#4 & 2.849(3) & C(22)-C(22)-C(21) & 120.9(3) \\ O(21)-K(1) & 2.983(2) & C(25)-C(24)-C(23) & 119.6(4) \\ O(21)-K(1) & 2.845(2) & C(22)-C(22) & 119.0(3) \\ S(1)-K(3)\#1 & 3.6064(10) & C(27)-C(26) & C21) & 120.0(3) \\ S(1)-K(3)\#1 & 3.6064(10) & C(27)-C(26)-C(21) & 120.0(3) \\ S(2)-K(1)\#4 & 3.5718(15) & C(27)-C(26)-C(21) & 120.0(3) \\ S(2)-K(1)\#4 & 3.5288(12) & N(2)-C(27)-C(26) & 124.7(4) \\ \end{array}$	C(22)-C(23)	1.363(5)	K(3)-O(1B)#4	2.920(3)
$\begin{array}{ccccc} C(24)-C(25) & 1.341(5) & K(3)-O(1C)\#8 & 3.247(3) \\ C(25)-C(26) & 1.416(5) & K(3)-S(1)\#1 & 3.6064(10) \\ C(27)-N(2) & 1.302(4) & K(3)-S(1)\#8 & 3.6064(10) \\ C(27)-N(2) & 1.302(4) & K(3)-S(1)\#8 & 3.6064(10) \\ C(27)-N(2) & 1.459(5) & K(3)-K(1)\#4 & 4.2274(8) \\ C(28)-C(29) & 1.520(5) & & & & & & & & & & & & & & & & & & &$	C(23)-C(24)	1.405(5)	K(3)-O(1C)#1	3.247(3)
$\begin{array}{ccccc} C(25)-C(26) & 1.416(5) & K(3)-S(1)\#1 & 3.6064(10) \\ C(26)-C(27) & 1.404(5) & K(3)-S(1)\#8 & 3.6064(10) \\ C(27)-N(2) & 1.302(4) & K(3)-K(1)\#9 & 4.2274(8) \\ C(28)-N(2) & 1.520(5) & \\ C(29)-S(2) & 1.520(5) & \\ C(29)-S(2) & 1.759(4) & O(11)-C(11)-C(16) & 122.2(3) \\ C(110)-O(12) & 1.423(5) & O(11)-C(11)-C(12) & 118.2(3) \\ C(110)-O(12) & 1.423(5) & C(16)-C(11)-C(12) & 119.5(3) \\ O(1A)-S(1) & 1.449(3) & O(12)-C(12)-C(13) & 125.9(3) \\ O(1A)-K(1) & 2.680(3) & O(12)-C(12)-C(11) & 114.6(3) \\ O(1A)-K(1) & 2.680(3) & O(12)-C(12)-C(11) & 114.6(3) \\ O(1B)-S(1) & 1.426(3) & C(13)-C(12)-C(11) & 119.5(4) \\ O(1B)-S(1) & 1.426(3) & C(13)-C(14)-C(15) & 119.2(3) \\ O(1C)-K(1)\#3 & 2.714(3) & C(11)-C(16)-C(15) & 119.2(3) \\ O(1C)-K(1)\#3 & 2.714(3) & C(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-S(2) & 1.439(2) & C(15)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(3) & 2.756(2) & N(1)-C(16)-C(17) & 119.9(3) \\ O(2A)-K(1)\#1 & 3.049(3) & N(1)-C(18)-C(19) & 109.4(3) \\ O(2B)-S(2) & 1.443(2) & O(21)-C(21)-S(1) & 114.0(3) \\ O(2B)-S(2) & 1.443(2) & O(21)-C(21)-C(22) & 121.0(3) \\ O(2B)-K(1)\#1 & 2.845(3) & C(26)-C(21)-C(22) & 125.4(3) \\ O(2B)-K(1)\#1 & 2.845(3) & C(26)-C(21)-C(22) & 125.4(3) \\ O(2B)-K(1)\#1 & 2.845(3) & C(26)-C(21)-C(22) & 125.4(3) \\ O(2B)-K(1)\#1 & 2.845(3) & C(23)-C(22)-C(23) & 125.4(3) \\ O(2C)-S(2) & 1.440(3) & O(22)-C(22)-C(23) & 125.4(3) \\ O(2D)-K(2)\#5 & 2.576(3) & O(22)-C(22)-C(23) & 125.4(3) \\ O(2D)-K(1)\#4 & 2.849(3) & C(23)-C(22)-C(23) & 125.4(3) \\ O(2D)-K(1)\#4 & 2.849(3) & C(23)-C(22)-C(23) & 125.4(3) \\ O(2D)-K(1)\#1 & 2.845(2) & C(22)-C(23) & 125.4(3) \\ O(22)-K(1)\#1 & 2.845(2) & C(22)-C(23) & 125.4(3) \\ O(22)-K(1)\#1 & 3.6064(10) & C(27)-C(26) & 121.0(4) \\ S(1)-K(1) & 3.5718(15) & C(27)-C(26)-C(21) & 120.0(3) \\ S(1)-K(3)\#1 & 3.6064(10) & C(27)-C(26)-C(21) & 120.0(3) \\ S(1)-K(1)\#4 & 3.5298(12) & N(2)-C(7)-C(26) & 124.7(4) \\ \end{array} \right)$	C(24)-C(25)	1.341(5)	K(3)-O(1C)#8	3.247(3)
$\begin{array}{ccccc} C(26)-C(27) & 1.404(5) & K(3)-S(1)\#8 & 3.6064(10) \\ C(27)-N(2) & 1.302(4) & K(3)-K(1)\#9 & 4.2274(8) \\ C(28)-N(2) & 1.459(5) & K(3)-K(1)\#4 & 4.2274(8) \\ C(29)-S(2) & 1.759(4) & O(11)-C(11)-C(16) & 122.2(3) \\ C(110)-O(12) & 1.423(5) & O(11)-C(11)-C(12) & 118.2(3) \\ O(10)-O(22) & 1.423(5) & O(12)-C(12)-C(13) & 125.9(3) \\ O(1A)-S(1) & 1.449(3) & O(12)-C(12)-C(13) & 125.9(3) \\ O(1A)-K(1) & 2.680(3) & O(12)-C(12)-C(11) & 114.6(3) \\ O(1A)-K(3)\#1 & 2.854(3) & C(13)-C(12)-C(11) & 114.6(3) \\ O(1B)-S(1) & 1.426(3) & C(12)-C(13) & 120.7(4) \\ O(1B)-S(1) & 1.426(3) & C(12)-C(13) & 120.7(4) \\ O(1C)-S(1) & 1.430(3) & C(14)-C(15) & 120.7(4) \\ O(1C)-S(1) & 1.430(3) & C(11)-C(16)-C(17) & 119.9(3) \\ O(2A)-S(2) & 1.439(2) & C(15)-C(16) & 121.5(3) \\ O(2A)-K(3)\#1 & 3.049(3) & N(1)-C(17)-C(16) & 121.5(3) \\ O(2A)-K(1)\#1 & 3.049(3) & N(1)-C(18)-C(19) & 109.4(3) \\ O(2B)-S(2) & 1.443(2) & O(21)-C(21)-C(22) & 121.0(3) \\ O(2B)-S(2) & 1.443(2) & O(21)-C(21)-C(22) & 121.0(3) \\ O(2B)-K(2) & 2.556(2) & O(21)-C(21)-C(22) & 121.0(3) \\ O(2B)-K(1)\#1 & 2.845(3) & C(26)-C(21)-C(22) & 125.4(3) \\ O(2C)-S(2) & 1.440(3) & O(22)-C(22)-C(23) & 125.4(3) \\ O(21)-K(1) & 2.983(2) & C(23)-C(22)-C(23) & 126.4(4) \\ O(21)-K(1) & 3.5718(15) & C(27)-C(26)-C(23) & 119.0(3) \\ S(1)-K(1) & 3.5298(12) & N(2)-C(27)-C(26) & 121.0(3) \\ S(2)-K(1)\#4 & 3.5298(12) & N(2)-C(27)-C(26) & 124.7(4) \\ \end{array}$	C(25)-C(26)	1.416(5)	K(3)-S(1)#1	3.6064(10)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(26)-C(27)	1.404(5)	K(3)-S(1)#8	3.6064(10)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(27)-N(2)	1.302(4)	K(3)-K(1)#9	4.2274(8)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(28)-N(2)	1.459(5)	K(3)-K(1)#4	4.2274(8)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(28)-C(29)	1.520(5)		
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(29)-S(2)	1.759(4)	O(11)-C(11)-C(16)	122.2(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(110)-O(12)	1.423(5)	O(11)-C(11)-C(12)	118.2(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(210)-O(22)	1.423(5)	C(16)-C(11)-C(12)	119.5(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1A)-S(1)	1.449(3)	O(12)-C(12)-C(13)	125.9(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1A)-K(1)	2.680(3)	O(12)-C(12)-C(11)	114.6(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1A)-K(3)#1	2.854(3)	C(13)-C(12)-C(11)	119.5(4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1B)-S(1)	1.426(3)	C(12)-C(13)-C(14)	120.4(4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1B)-K(3)#2	2.920(3)	C(15)-C(14)-C(13)	120.7(4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1C)-S(1)	1.430(3)	C(14)-C(15)-C(16)	120.4(4)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1C)-K(1)#3	2.714(3)	C(11)-C(16)-C(15)	119.2(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1C)-K(3)#1	3.247(3)	C(11)-C(16)-C(17)	119.9(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(2A)-S(2)	1.439(2)	C(15)-C(16)-C(17)	120.9(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(2A)-K(3)	2.756(2)	N(1)-C(17)-C(16)	121.5(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(2A)-K(1)#1	3.049(3)	N(1)-C(18)-C(19)	109.4(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(2A)-K(1)#4	3.193(3)	C(18)-C(19)-S(1)	114.0(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(2B)-S(2)	1.443(2)	O(21)-C(21)-C(26)	123.3(3)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(2B)-K(2)	2.556(2)	O(21)-C(21)-C(22)	121.0(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(2B)-K(1)#1	2.845(3)	C(26)-C(21)-C(22)	115.7(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(2C)-S(2)	1.440(3)	O(22)-C(22)-C(23)	125.4(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(2C)-K(2)#5	2.576(3)	O(22)-C(22)-C(21)	113.7(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(2C)-K(1)#4	2.849(3)	C(23)-C(22)-C(21)	120.9(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O(21)-K(2)	2.805(2)	C(22)-C(23)-C(24)	121.6(4)
$\begin{array}{ccccccc} O(22)-K(1) & 2.806(2) & C(24)-C(25)-C(26) & 121.0(4) \\ S(1)-K(1) & 3.5718(15) & C(27)-C(26)-C(25) & 119.0(3) \\ S(1)-K(3)\#1 & 3.6064(10) & C(27)-C(26)-C(21) & 120.0(3) \\ S(2)-K(1)\#1 & 3.4842(11) & C(25)-C(26)-C(21) & 121.0(3) \\ S(2)-K(1)\#4 & 3.5298(12) & N(2)-C(27)-C(26) & 124.7(4) \\ \end{array}$	O(21)-K(1)	2.983(2)	C(25)-C(24)-C(23)	119.6(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 $3.5298(12)$ $N(2)$ - $C(27)$ - $C(26)$ $124.7(4)$	O(22)-K(1)	2.806(2)	C(24)-C(25)-C(26)	121.0(4)
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 $3.5298(12)$ $N(2)$ - $C(27)$ - $C(26)$ $124.7(4)$	S(1)-K(1)	3.5718(15)	C(27)-C(26)-C(25)	119.0(3)
S(2)-K(1)#13.4842(11)C(25)-C(26)-C(21)121.0(3)S(2)-K(1)#43.5298(12)N(2)-C(27)-C(26)124 7(4)	S(1)-K(3)#1	3.6064(10)	C(27)-C(26)-C(21)	120.0(3)
S(2)-K(1)#4 3.5298(12) N(2)-C(27)-C(26) 124 7(4)	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)

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

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) = K(1)	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)	1175(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)	133.2(2) 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(2)-O(21)-K(1)	118 2(3)	$O(12)$ $\pi 3^{-} K(1) - O(2A) \pi 2$ $O(22) - K(1) - O(2A) \pi 2$	7545(7)
C(22)-O(22)-C(210)	126.2(5)	$O(22)^{-}K(1)^{-}O(2K)^{+}Z$ $O(2B)^{+}L_{-}K(1)^{-}O(2A)^{+}Z$	115 82(7)
C(22) - O(22) - K(1)	120.50(19) 114.6(3)	O(2C)#2-K(1)-O(2A)#2	115.02(7)
O(1B)-S(1)-O(1C)	114.0(3) 114.08(18)	$O(2C)\pi 2 - K(1) - O(2K)\pi 2$ $O(21) - K(1) - O(2K)\pi 2$	11355(7)
O(1B) - S(1) - O(1C)	114.00(10) 113.08(18)	$O(2\Lambda) + 1 - K(1) - O(2\Lambda) + 2$ $O(2\Lambda) + 1 - K(1) - O(2\Lambda) + 2$	142.65(10)
O(1C) S(1) O(1A)	113.00(10) 111.80(10)	O(2A)#1- $K(1)$ - $O(2A)$ #2 O(1A) K(1) S(2)#1	94.64(7)
O(1C)-S(1)-O(1A) O(1B) S(1) C(10)	111.00(19) 107.38(18)	O(1A)- $K(1)$ - $S(2)$ #1 O(1C)#2 $K(1)$ $S(2)$ #1	94.04(7) 84.27(7)
O(1C) S(1) C(19)	107.38(18) 105.27(18)	O(1C)#3-K(1)-S(2)#1 O(22) V(1) S(2)#1	124.27(7)
O(10) - S(1) - O(19)	103.27(18) 104.21(17)	O(22)- $K(1)$ - $S(2)$ #1 O(22)#1 $V(1)$ $S(2)$ #1	134.01(0) 22.71(5)
O(1A) - S(1) - C(19) O(1B) S(1) K(1)	104.51(17) 72.50(12)	O(2D)#1-K(1)-S(2)#1 O(2C)#2 V(1) S(2)#1	23.71(3)
O(1D) - S(1) - K(1)	118 25(12)	O(2C)#2-K(1)-S(2)#1 O(21) K(1) S(2)#1	101.70(0)
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)	42.10(11) 121.02(12)	O(2A)#1-K(1)-S(2)#1 O(2A)#2 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 O(1A) K(1) S(2)#2	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	/5.42(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	11331(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)#7 $K(1) - K(2)S(2)$ #2- $K(1) - K(2)$	66 30(3)	O(1A)#1-K(3)-O(1C)#8	13456(7)
S(1)-K(1)-K(2)	17072(3)	O(1R)#9-K(3)-O(1C)#8	99.27(7)
O(2R) K(2) O(2R) #1	170.72(3) 00.38(13)	O(1B)#4 K(3) O(1C)#8	99.27(7) 80.73(7)
O(2B) K(2) O(2C) # 2	166.87(0)	O(1C)#1 K(3) $O(1C)$ #8	180.00(18)
O(2D)- $K(2)$ - $O(2C)$ #2	20.08(0)	O(1C)#1- $K(3)$ - $O(1C)$ #8 O(2A)#7 $V(2)$ $S(1)$ #1	86 52(6)
O(2D) K(2) O(2C) H(2)	89.06(9) 80.08(0)	O(2A) # 7 - K(3) - S(1) # 1	00.32(0)
O(2B)-K(2)-O(2C)#0	89.08(9)	O(2A)-K(3)-S(1)#1 O(1A)#9 K(2) S(1)#1	93.48(0) 157.75(6)
O(2B)#1- $K(2)$ - $O(2C)$ #6	100.8/(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)
$O(2\Lambda)$ #7-K(3)-O(1\Lambda)#1	107.18(8)	$O(1\Lambda) # 8 - K(3) - K(1) # 4$	83.01(6)
O(2A) - K(3) - O(1A) + 1	72 82(8)	$O(1\Lambda)#1-K(3)-K(1)#4$	06 00(6)
$O(1\Lambda) # 8 K(2) O(1\Lambda) # 1$	180.0	$O(1\pi)^{m} \Gamma K(3)^{-} K(1)^{m} \Phi$ $O(1R)^{\mu} O(2) V(1)^{\mu} \Phi$	125 02(7)
$O(1A)#0^{-}N(3)^{-}O(1A)#1$ O(2A)#7 V(2) O(1D)#0	02 12(0)	O(1D)#9- $K(3)$ - $K(1)$ #4 O(1P)#4 $V(2)$ $V(1)$ #4	123.92(7)
O(2A) # / - K(3) - O(1D) # 9 O(2A) W(2) O(1D) # 9	92.12(9) 07.00(0)	O(1D)#4- $N(3)$ - $N(1)$ #4 O(1C)#1 $V(2)$ $V(1)$ #4	34.00(7) 140.05(5)
U(2A) - K(3) - U(1B) = 0	87.88(9) 81.05(9)	O(1C) # 1 - K(3) - K(1) # 4	140.05(5)
O(1A)#8-K(3)- $O(1B)$ #9	81.05(8)	U(1U)#8-K(3)-K(1)#4	59.95(5)
O(1A)#1-K(3)-O(1B)#9	98.95(8)	S(1)#1-K(3)-K(1)#4	11/.669(19)
O(2A)#/-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;

Atom	U11	U22	U33	U23	U13	U12
$\overline{C(11)}$	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(12)	46(2)	67(3)	34(2)	-2(2)	13(2)	15(2)
C(14)	42(2)	75(3)	41(2)	-10(2)	13(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)	32(2) 38(2)	1(2)	25(2)	0(2)
C(18)	46(2)	40(2) 44(2)	43(2)	7(2)	17(2)	7(2)
C(10)	39(2)	48(2)	$\frac{13(2)}{38(2)}$	$\frac{7(2)}{8(2)}$	19(2)	11(2)
C(21)	36(2)	43(2)	25(2)	4(2)	11(1)	-2(2)
C(21)	37(2)	46(2)	30(2)	$\frac{1}{2}$	14(2)	-4(2)
C(22)	57(2) 53(2)	53(2)	41(2)	-10(2)	23(2)	-15(2)
C(23)	43(2)	77(3)	53(3)	-13(2)	23(2)	-21(2)
C(25)	41(2)	77(3)	48(2)	-2(2)	25(2)	0(2)
C(26)	36(2)	47(2)	33(2)	2(2) 2(2)	14(2)	0(2)
C(20)	39(2)	52(2)	37(2)	$\frac{2(2)}{4(2)}$	16(2)	6(2)
C(28)	$\frac{3}{44(2)}$	$\frac{32(2)}{46(2)}$	$\frac{37(2)}{49(2)}$	-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)	$\frac{37(2)}{38(2)}$	-4(2)	12(2)	7(2)
O(1A)	$\frac{40(2)}{80(2)}$	78(2)	34(2)	-2(1)	12(2) 13(1)	9(2)
O(1R)	67(2)	54(2)	$\frac{31(2)}{84(2)}$	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(2R)	72(2)	53(2)	$\frac{2}{42(2)}$	-8(1)	18(1)	19(1)
O(2C)	61(2)	68(2)	$\frac{12(2)}{48(2)}$	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 S3**. Anisotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for s97. The anisotropic displacement factor exponent takes the form:  $-2\pi^2$ [ h<sup>2</sup>a\*<sup>2</sup>U<sup>11</sup> + ... + 2 h k a\* b\* U<sup>12</sup> ]

Atom	Х	У	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 S4**. Hydrogen coordinates (x  $10^4$ ) and isotropic displacement parameters (Å<sup>2</sup> x  $10^3$ ) for s97.

**Table S5**. Torsion angles [°] for s97.

$\overline{O(11)}$ - $C(11)$ - $C(12)$ - $O(12)$	-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)	-1789(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- $O(1C)$ - $S(1)$ - $C(19)$	-10534(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(12) = C(14) = C(15) C(13) = C(14) = C(15) = C(16)	-2 7(6)	K(1) $K(1)$ $K(1)$ $K(1)$ $K(1)$ $K(1)$ $K(1)$ $K(1)$	5358(11)
O(11)-C(11)-C(16)-C(15)	-1763(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)	5.3(5)	K(1)=O(1A)=O(1A) K(2)=U(1A)=O(1B)	-21.9(2) 120.24(14)
C(12) C(11) C(16) C(17)	3.0(3)	K(1) O(1A) S(1) O(1C)	-139.24(14) 109.52(19)
C(12)- $C(11)$ - $C(10)$ - $C(17)$	-1/2.3(3) 1 5(5)	K(1)-O(1A)-S(1)-O(1C) K(2)#1 O(1A) S(1) O(1C)	108.33(18) 9.95(10)
C(14) - C(15) - C(16) - C(17)	-1.3(3) 176.2(4)	K(3)#1-O(1A)-S(1)-O(1C)	-0.03(19)
C(14)- $C(15)$ - $C(16)$ - $C(17)$	1/0.5(4)	K(1)-O(1A)-S(1)-O(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)	1/9.6(3)	K(3)#1- $O(1A)$ - $S(1)$ - $K(1)$	-11/.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(22) = C(21) = O(21) = C(210)	63(5)	$K(2)_{-}O(2B)_{-}S(2)_{-}O(2A)$	129.5(3) 119 6(4)
C(21)-C(22)-O(22)-C(210)	-172 6(3)	K(2) = O(2B) = S(2) = O(2A) K(1) # 1 = O(2B) = S(2) = O(2A)	6.63(19)
C(21) = C(22) = O(22) = C(210) 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(2) = O(2D) = O(2C) $K(1) = H_0(2R) = O(2C)$	-121 99(14)
K(3)#2-O(1B)-S(1)-O(1C)	-365(2)	K(1)#1-0(2B)-5(2)-0(2C) K(2) O(2B)- $S(2)$ -C(2Q)	-121.99(14) -123.2(4)
K(3)#2-O(1B)-S(1)-O(1C) K(3)#2-O(1B) S(1) O(1A)	-30.3(2)	K(2) = O(2D) = O(2) = O(20) $K(1) = H_0(2D) = O(20)$	$\frac{-123.2(4)}{123.83(16)}$
K(3)#2-O(1D)-O(1A) K(2)#2 O(1B) S(1) O(10)	$\frac{32.1(2)}{152.74(17)}$	K(1)#1- $O(2D)$ - $O(2)K(2)$ $O(2D)$ $S(2)$ $K(1)$ #1	123.03(10) 112.0(4)
K(3)#2-O(1D)-O(1)-O(19) K(2)#2 O(1D) S(1) V(1)	-132.74(17) 77.64(14)	K(2) - O(2D) - O(2) - K(1) + 1 K(2) - O(2D) - S(2) - K(1) + 4	112.9(4)
K(3)#2- $U(1D)$ - $S(1)$ - $K(1)V(2)$ #2 $O(1D)$ $S(1)$ $V(2)$ #1	//.04(14)	K(2)-O(2D)-O(2)-K(1)#4 K(1)#1 O(2D) S(2) K(1)#4	40.7(3)
к( <i>3)#2-</i> U(1В)-5(1)-К( <i>3)</i> #1	41.3(3)	<b>К</b> (1)#1-U(2B)-S(2)-K(1)#4	-72.0(3)

C(28)-C(29)-S(2)-O(2A)	-173.0(3)	C(21)-O(21)-K(1)-O(2C)#2
C(28)-C(29)-S(2)-O(2C)	-53.6(3)	K(2)-O(21)-K(1)-O(2C)#2
C(28)-C(29)-S(2)-O(2B)	66.5(3)	C(21)-O(21)-K(1)-O(2A)#1
C(28)-C(29)-S(2)-K(1)#1	120.9(3)	K(2)-O(21)-K(1)-O(2A)#1
C(28)-C(29)-S(2)-K(1)#4	-106.0(3)	C(21)-O(21)-K(1)-O(2A)#2
S(1)-O(1A)-K(1)-O(1C)#3	-70.65(19)	K(2)-O(21)-K(1)-O(2A)#2
K(3)#1-O(1A)-K(1)-O(1C)#3	49.82(10)	C(21)-O(21)-K(1)-S(2)#1
S(1)-O(1A)-K(1)-O(22)	68.90(19)	K(2)-O(21)-K(1)-S(2)#1
K(3)#1-O(1A)-K(1)-O(22)	-170.62(8)	C(21)-O(21)-K(1)-S(2)#2
S(1)-O(1A)-K(1)-O(2B)#1	-155.93(16)	K(2)-O(21)-K(1)-S(2)#2
K(3)#1-O(1A)-K(1)-O(2B)#1	-35.45(13)	C(21)-O(21)-K(1)-S(1)
S(1)-O(1A)-K(1)-O(2C)#2	5.4(4)	K(2)-O(21)-K(1)-S(1)
K(3)#1-O(1A)-K(1)-O(2C)#2	125.9(3)	C(21)-O(21)-K(1)-K(2)
S(1)-O(1A)-K(1)-O(21)	124.22(17)	O(1B)-S(1)-K(1)-O(1A)
K(3)#1-O(1A)-K(1)-O(21)	-115.30(9)	O(1C)-S(1)-K(1)-O(1A)
S(1)-O(1A)-K(1)-O(2A)#1	-149.7(2)	C(19)-S(1)-K(1)-O(1A)
K(3)#1-O(1A)-K(1)-O(2A)#1	-29.27(8)	K(3)#1- $S(1)$ - $K(1)$ - $O(1A)$
S(1)-O(1A)-K(1)-O(2A)#2	-9.6(2)	O(1B)-S(1)-K(1)-O(1C)#3
K(3)#1-O(1A)-K(1)-O(2A)#2	110.84(9)	O(1C)-S(1)-K(1)-O(1C)#3
S(1)-O(1A)-K(1)-S(2)#1	-154.32(17)	O(1A)-S(1)-K(1)-O(1C)#3
K(3)#1-O(1A)-K(1)-S(2)#1	-33.84(8)	C(19)-S(1)-K(1)-O(1C)#3
S(1)-O(1A)-K(1)-S(2)#2	-13.8(3)	K(3)#1- $S(1)$ - $K(1)$ - $O(1C)$ #3
K(3)#1-O(1A)-K(1)-S(2)#2	106.67(10)	O(1B)-S(1)-K(1)-O(22)
K(3)#1-O(1A)-K(1)-S(1)	120.5(2)	O(1C)-S(1)-K(1)-O(22)
S(1)-O(1A)-K(1)-K(2)	162.73(9)	O(1A)-S(1)-K(1)-O(22)
K(3)#1-O(1A)-K(1)-K(2)	-76.79(18)	C(19)-S(1)-K(1)-O(22)
C(22)-O(22)-K(1)-O(1A)	90.7(2)	K(3)#1- $S(1)$ - $K(1)$ - $O(22)$
C(210)-O(22)-K(1)-O(1A)	-78.4(3)	O(1B)-S(1)-K(1)-O(2B)#1
C(22)-O(22)-K(1)-O(1C)#3	-178.2(2)	O(1C)-S(1)-K(1)-O(2B)#1
C(210)-O(22)-K(1)-O(1C)#3	12.8(3)	O(1A)-S(1)-K(1)-O(2B)#1
C(22)-O(22)-K(1)-O(2B)#1	-42.0(3)	C(19)-S(1)-K(1)-O(2B)#1
C(210)-O(22)-K(1)-O(2B)#1	148.9(3)	K(3)#1-S(1)-K(1)-O(2B)#1
C(22)-O(22)-K(1)-O(2C)#2	-105.7(3)	O(1B)-S(1)-K(1)-O(2C)#2
C(210)-O(22)-K(1)-O(2C)#2	85.3(3)	O(1C)-S(1)-K(1)-O(2C)#2
C(22)-O(22)-K(1)-O(21)	-19.6(2)	O(1A)-S(1)-K(1)-O(2C)#2
C(210)-O(22)-K(1)-O(21)	171.3(3)	C(19)-S(1)-K(1)-O(2C)#2
C(22)-O(22)-K(1)-O(2A)#1	19.5(3)	K(3)#1-S(1)-K(1)-O(2C)#2
C(210)-O(22)-K(1)-O(2A)#1	-149.6(3)	O(1B)-S(1)-K(1)-O(21)
C(22)-O(22)-K(1)-O(2A)#2	-153.6(3)	O(1C)-S(1)-K(1)-O(21)
C(210)-O(22)-K(1)-O(2A)#2	37.3(3)	O(1A)-S(1)-K(1)-O(21)
C(22)-O(22)-K(1)-S(2)#1	-15.8(3)	C(19)-S(1)-K(1)-O(21)
C(210)-O(22)-K(1)-S(2)#1	175.1(2)	K(3)#1-S(1)-K(1)-O(21)
C(22)-O(22)-K(1)-S(2)#2	-129.0(2)	O(1B)-S(1)-K(1)-O(2A)#1
C(210)-O(22)-K(1)-S(2)#2	61.9(3)	O(1C)-S(1)-K(1)-O(2A)#1
C(22)-O(22)-K(1)-S(1)	110.5(2)	O(1A)-S(1)-K(1)-O(2A)#1
C(210)-O(22)-K(1)-S(1)	-58.6(3)	C(19)-S(1)-K(1)-O(2A)#1
C(22)-O(22)-K(1)-K(2)	-61.9(2)	K(3)#1-S(1)-K(1)-O(2A)#1
C(210)-O(22)-K(1)-K(2)	129.1(3)	O(1B)-S(1)-K(1)-O(2A)#2
C(21)-O(21)-K(1)-O(1A)	-66.4(2)	O(1C)-S(1)-K(1)-O(2A)#2
K(2)-O(21)-K(1)-O(1A)	157.43(8)	O(1A)-S(1)-K(1)-O(2A)#2
C(21)-O(21)-K(1)-O(1C)#3	158.7(3)	C(19)-S(1)-K(1)-O(2A)#2
K(2)-O(21)-K(1)-O(1C)#3	22.6(2)	K(3)#1-S(1)-K(1)-O(2A)#2
C(21)-O(21)-K(1)-O(22)	19.7(2)	O(1B)-S(1)-K(1)-S(2)#1
K(2)-O(21)-K(1)-O(22)	-116.44(9)	O(1C)-S(1)-K(1)-S(2)#1
C(21)-O(21)-K(1)-O(2B)#1	179.8(2)	O(1A)-S(1)-K(1)-S(2)#1
K(2)-O(21)-K(1)-O(2B)#1	43.72(6)	C(19)-S(1)-K(1)-S(2)#1

97.9(2)

-38.25(7)

-137.1(2) 86.74(7)

69.1(2) -66.99(7)-157.6(2)66.32(5) 88.4(2) -47.72(5)-45.6(2)178.31(4) 136.1(2) 159.1(2) -92.0(2) 60.2(3) -43.36(18) -95.17(14) 13.8(2) 105.8(2) 166.0(2) 62.40(7)

 $\begin{array}{r} 45.99(13)\\ 154.93(15)\\ -113.08(19)\\ -52.87(19)\\ -156.44(5)\\ -169.04(15)\\ -60.10(17)\\ 31.9(2)\\ 92.1(2)\\ -11.47(9)\\ -18.34(16)\\ 90.60(17)\\ -177.4(2)\\ -117.2(2)\\ 139.22(10) \end{array}$ 

93.56(14) -157.50(15) -65.51(19) -5.3(2) -108.87(6) -172.52(13) -63.58(16) 28.41(19) -88.61(19) -14.96(5) -29.54(13) 79.39(15) 171.39(19) -128.41(19)

128.02(5) -172.80(12) -63.86(15) 28.13(19) 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)	1/0.11(9)	
S(1)-K(1)-K(2)-O(2B)	34.4(2)	
O(1A) - K(1) - K(2) - O(2B) = 0	3/.30(1/)	
O(1C)#3-K(1)-K(2)-O(2B)#1 O(22) K(1) K(2) O(2D)#1	-03.12(11) 155 $42(10)$	
O(22)- $N(1)$ - $N(2)$ - $O(2B)$ #1 O(2C)#2 $V(1)$ $V(2)$ $O(2B)$ #1	133.43(10) 132.05(11)	
O(2C)#2- $N(1)$ - $N(2)$ - $O(2D)$ #1	-132.03(11) 108.31(10)	
O(21)- $N(1)$ - $N(2)$ - $O(2D)$ #1 $O(2A)$ #1_ $K(1)$ $K(2)$ $O(2D)$ #1	100.31(10) 13 $42(10)$	
O(2A)#1-K(1)-K(2)-O(2B)#1 O(2A)#2-K(1)-K(2)-O(2B)#1	13.42(10) -120.23(10)	
$S(2)#1_K(1)_K(2) \cap (2D)#1$	-129.23(10) 0 54(8)	
S(2)#1- $K(1)$ - $K(2)$ - $O(2D)$ #1	9.34(0)	

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	14159(8)
S(2)#7 $K(1) - K(2) - O(2C)$ #2 S(2)#2 - $K(1) - K(2) - O(2C)$ #2	7 23(8)
S(2)=K(1)-K(2)-O(2C)=2	-1285(0)
O(1A) - K(1) - K(2) - O(2C) + 6	-120.3(2)
O(1C) + 3 $V(1) V(2) O(2C)$ + 6	-137.57(17)
O(1C)#3-K(1)-K(2)-O(2C)#6	$\frac{33.73(11)}{41.71(10)}$
O(22)- $K(1)$ - $K(2)$ - $O(2C)$ #6	-41.71(10) 162.97(11)
O(2D)#1-K(1)-K(2)- $O(2C)$ #0	102.87(11)
O(2C)#2-K(1)-K(2)-O(2C)#0	30.82(10)
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(2R) # 1 - K(1) - K(2) - K(1) # 1	-29(100)
O(2D)#1-K(1)-K(2)-K(1)#1 O(2C)#2-K(1)-K(2)-K(1)#1	-161(100)
$O(2C)\pi 2^{-}K(1)^{-}K(2)^{-}K(1)\pi 1$ $O(21) V(1) V(2) V(1)\pi 1$	-101(100)
O(21)- $K(1)$ - $K(2)$ - $K(1)$ #1 O(24)#1 $K(1)$ $K(2)$ $K(1)$ #1	16(100)
O(2A)#1-N(1)-N(2)-N(1)#1	-10(100) 158(100)
U(2R)#2-K(1)-K(2)-K(1)#1	-130(100)
S(2)#1- $K(1)$ - $K(2)$ - $K(1)$ #1	-19(100)
S(2)#2-K(1)-K(2)-K(1)#1 S(1) V(1) V(2) V(1)#1	-134(100)
S(1)-K(1)-K(2)-K(1)#1 S(2) O(2A) K(2) O(2A) #7	/0(100)
S(2)-U(2A)-K(3)-U(2A)#/	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