

Table 1. Crystal data and structure refinement for kss-4.

Identification code	kss-4	
Empirical formula	C <sub>21</sub> H <sub>28</sub> N <sub>3</sub> O <sub>6</sub> Ru	
Formula weight	519.54	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5202(10) Å	α = 95.894(9)°.
	b = 11.2899(12) Å	β = 102.640(9)°.
	c = 12.7502(14) Å	γ = 109.373(9)°.
Volume	1108.3(2) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.557 g/cm <sup>3</sup>	
Absorption coefficient	0.749 mm <sup>-1</sup>	
F(000)	534	
Crystal size	0.2815 x 0.2134 x 0.1821 mm <sup>3</sup>	
Theta range for data collection	1.95 to 29.30°.	
Index ranges	-11 ≤ h ≤ 11, -15 ≤ k ≤ 15, -17 ≤ l ≤ 17	
Reflections collected	21097	
Independent reflections	5995 [R(int) = 0.1771]	
Completeness to theta = 29.30°	98.8 %	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5995 / 0 / 277	
Goodness-of-fit on F <sup>2</sup>	0.664	
Final R indices [I > 2σ(I)]	R1 = 0.0536, wR2 = 0.0653	
R indices (all data)	R1 = 0.1758, wR2 = 0.0850	
Extinction coefficient	0.0009(2)	
Largest diff. peak and hole	0.611 and -0.668 e. Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for kss-3.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Ru(1)	7539(1)	8360(1)	5807(1)	30(1)
N(32)	8372(6)	9987(4)	7047(4)	36(1)
N(33)	9401(7)	11122(5)	7007(5)	56(2)
O(37)	7853(6)	10328(5)	10088(4)	76(2)
N(31)	8019(7)	9885(5)	7983(5)	65(2)
O(36)	9271(9)	12395(5)	10287(5)	120(2)
C(34)	9691(8)	11854(6)	7987(6)	53(2)
C(35)	8791(9)	11066(6)	8611(6)	56(2)
C(11)	7279(5)	6507(4)	6214(5)	44(2)
C(12)	7048(6)	6412(3)	5091(5)	49(2)
C(13)	5830(7)	6819(4)	4479(3)	52(2)
C(14)	4843(5)	7321(4)	4990(5)	55(2)
C(15)	5075(5)	7415(4)	6113(5)	50(2)
C(16)	6293(6)	7008(4)	6725(3)	53(2)
C(36)	8667(10)	11327(8)	9745(7)	71(2)
C(26)	6486(9)	7050(7)	7960(7)	77(3)
C(39)	6454(11)	9289(8)	11309(7)	106(3)
C(22)	8169(9)	5889(6)	4553(7)	88(3)
C(38)	7677(11)	10522(8)	11201(7)	90(3)
C(23)	5589(10)	6774(7)	3253(6)	95(3)
C(24)	3639(8)	7916(6)	4366(7)	86(3)
C(21)	8737(8)	6171(6)	6886(7)	86(3)
O(46)	11652(13)	13742(8)	9051(7)	220(6)
C(25)	4043(8)	8003(7)	6720(7)	95(3)
C(45)	10717(18)	13238(8)	8277(10)	105(4)
O(45)	10328(12)	13914(8)	7658(10)	192(5)
C(48)	12823(17)	15571(9)	10327(10)	173(5)
C(47)	12291(19)	15179(10)	9237(11)	223(8)
O(1)	10213(4)	8918(3)	5868(3)	35(1)
O(2)	7773(4)	9666(3)	4712(3)	36(1)
C(01)	10688(7)	9785(5)	5318(5)	28(1)

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

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Ru(1)	29(1)	21(1)	37(1)	6(1)	11(1)	4(1)
N(32)	44(3)	35(3)	22(4)	-2(2)	19(3)	3(2)
N(33)	66(4)	50(3)	40(4)	-9(3)	12(3)	15(3)
O(37)	96(4)	66(3)	63(4)	14(3)	49(3)	8(3)
N(31)	62(4)	38(3)	71(5)	-14(3)	16(4)	0(3)
O(36)	209(7)	60(4)	77(5)	-3(3)	58(5)	23(4)
C(34)	51(4)	40(4)	59(6)	6(4)	15(4)	5(3)
C(35)	69(5)	43(4)	49(6)	5(4)	12(4)	15(4)
C(11)	39(4)	29(3)	74(6)	17(4)	25(4)	16(3)
C(12)	56(5)	20(3)	72(6)	5(4)	37(5)	2(3)
C(13)	56(5)	33(4)	43(5)	-3(3)	12(4)	-9(3)
C(14)	33(4)	31(4)	84(7)	7(4)	4(4)	-1(3)
C(15)	34(4)	36(4)	82(7)	13(4)	29(5)	4(3)
C(16)	66(5)	30(4)	47(6)	20(4)	6(5)	-1(4)
C(36)	80(6)	58(5)	68(7)	-7(5)	15(5)	23(5)
C(26)	91(6)	62(5)	88(7)	32(5)	41(5)	26(4)
C(39)	136(8)	120(7)	98(8)	70(6)	78(7)	50(6)
C(22)	81(5)	36(4)	136(9)	-11(5)	52(6)	2(4)
C(38)	114(7)	100(7)	51(6)	-4(5)	45(6)	24(6)
C(23)	111(7)	67(5)	60(7)	-6(5)	22(5)	-19(5)
C(24)	55(5)	67(5)	116(8)	15(5)	-7(5)	14(4)
C(21)	62(5)	53(4)	128(8)	31(5)	11(5)	8(4)
O(46)	259(11)	104(6)	113(8)	-4(6)	-46(7)	-99(6)
C(25)	61(5)	86(6)	151(9)	16(6)	49(6)	32(4)
C(45)	163(11)	37(5)	78(9)	9(5)	44(8)	-18(6)
O(45)	176(8)	70(5)	298(15)	31(7)	43(9)	17(5)
C(48)	259(15)	71(7)	165(14)	7(8)	59(12)	32(9)
C(47)	296(17)	77(8)	167(15)	-61(9)	76(14)	-81(9)
O(1)	32(2)	24(2)	53(3)	20(2)	13(2)	9(2)
O(2)	30(2)	31(2)	44(3)	9(2)	6(2)	9(2)
C(01)	30(4)	25(3)	24(4)	-4(3)	0(3)	10(3)

Table 4. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for kss-4.

	x	y	z	U(eq)
H(26A)	6756	7911	8319	115
H(26B)	7398	6762	8262	115
H(26C)	5422	6504	8068	115
H(39A)	5292	9254	11040	159
H(39B)	6663	9213	12066	159
H(39C)	6610	8600	10892	159
H(22A)	7520	5432	3826	132
H(22B)	8528	5322	4975	132
H(22C)	9168	6584	4520	132
H(38A)	7231	11198	11312	108
H(38B)	8785	10750	11734	108
H(23A)	5494	7557	3075	142
H(23B)	4557	6068	2857	142
H(23C)	6566	6667	3055	142
H(24A)	2470	7318	4173	130
H(24B)	3964	8122	3714	130
H(24C)	3729	8681	4822	130
H(21A)	9759	6522	6646	128
H(21B)	8400	5258	6787	128
H(21C)	8967	6522	7646	128
H(25A)	3347	8326	6216	142
H(25B)	4830	8689	7303	142
H(25C)	3310	7358	7017	142
H(48A)	11914	15147	10643	260
H(48B)	13114	16479	10500	260
H(48C)	13820	15368	10617	260
H(47A)	13237	15511	8912	268
H(47B)	11370	15466	8919	268

Table 1. Bond lengths [Å] and angles [°] for kss-4.

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Ru(1)-N(32)	2.104(5)
Ru(1)-O(2)	2.125(4)
Ru(1)-O(1)	2.134(3)
Ru(1)-C(13)	2.156(4)
Ru(1)-C(14)	2.156(4)
Ru(1)-C(12)	2.157(3)
Ru(1)-C(15)	2.158(4)
Ru(1)-C(11)	2.159(4)
Ru(1)-C(16)	2.159(4)
N(32)-N(31)	1.300(7)
N(32)-N(33)	1.305(6)
N(33)-C(34)	1.349(7)
O(37)-C(36)	1.289(8)
O(37)-C(38)	1.461(8)
N(31)-C(35)	1.349(7)
O(36)-C(36)	1.207(7)
C(34)-C(35)	1.405(8)
C(34)-C(45)	1.475(10)
C(35)-C(36)	1.479(9)
C(11)-C(12)	1.3900
C(11)-C(16)	1.3900
C(11)-C(21)	1.527(7)
C(12)-C(13)	1.3900
C(12)-C(22)	1.519(7)
C(13)-C(14)	1.3900
C(13)-C(23)	1.525(8)
C(14)-C(15)	1.3900
C(14)-C(24)	1.532(7)
C(15)-C(16)	1.3900
C(15)-C(25)	1.547(7)
C(16)-C(26)	1.541(8)
C(39)-C(38)	1.477(9)
O(46)-C(45)	1.082(13)
O(46)-C(47)	1.505(13)
C(45)-O(45)	1.222(14)
C(48)-C(47)	1.341(13)
O(1)-C(01)	1.271(6)

O(2)-C(01)#1	1.262(6)
C(01)-O(2)#1	1.262(6)
C(01)-C(01)#1	1.520(11)
N(32)-Ru(1)-O(2)	85.56(17)
N(32)-Ru(1)-O(1)	84.32(17)
O(2)-Ru(1)-O(1)	78.66(14)
N(32)-Ru(1)-C(13)	159.2(2)
O(2)-Ru(1)-C(13)	90.36(15)
O(1)-Ru(1)-C(13)	114.85(18)
N(32)-Ru(1)-C(14)	122.1(2)
O(2)-Ru(1)-C(14)	92.52(16)
O(1)-Ru(1)-C(14)	151.7(2)
C(13)-Ru(1)-C(14)	37.61(6)
N(32)-Ru(1)-C(12)	157.4(2)
O(2)-Ru(1)-C(12)	115.40(18)
O(1)-Ru(1)-C(12)	91.51(14)
C(13)-Ru(1)-C(12)	37.60(6)
C(14)-Ru(1)-C(12)	67.86(8)
N(32)-Ru(1)-C(15)	96.77(17)
O(2)-Ru(1)-C(15)	120.27(19)
O(1)-Ru(1)-C(15)	161.07(18)
C(13)-Ru(1)-C(15)	67.85(8)
C(14)-Ru(1)-C(15)	37.59(6)
C(12)-Ru(1)-C(15)	80.22(7)
N(32)-Ru(1)-C(11)	120.6(2)
O(2)-Ru(1)-C(11)	152.70(19)
O(1)-Ru(1)-C(11)	95.31(14)
C(13)-Ru(1)-C(11)	67.83(8)
C(14)-Ru(1)-C(11)	80.22(7)
C(12)-Ru(1)-C(11)	37.57(6)
C(15)-Ru(1)-C(11)	67.79(8)
N(32)-Ru(1)-C(16)	96.14(17)
O(2)-Ru(1)-C(16)	157.83(18)
O(1)-Ru(1)-C(16)	123.51(18)
C(13)-Ru(1)-C(16)	80.22(7)
C(14)-Ru(1)-C(16)	67.82(8)
C(12)-Ru(1)-C(16)	67.80(8)
C(15)-Ru(1)-C(16)	37.56(6)

C(11)-Ru(1)-C(16)	37.55(6)
N(31)-N(32)-N(33)	114.4(5)
N(31)-N(32)-Ru(1)	120.4(4)
N(33)-N(32)-Ru(1)	124.8(4)
N(32)-N(33)-C(34)	105.5(5)
C(36)-O(37)-C(38)	117.1(6)
N(32)-N(31)-C(35)	106.2(5)
N(33)-C(34)-C(35)	107.4(6)
N(33)-C(34)-C(45)	123.9(7)
C(35)-C(34)-C(45)	128.7(7)
N(31)-C(35)-C(34)	106.4(7)
N(31)-C(35)-C(36)	121.8(7)
C(34)-C(35)-C(36)	131.7(7)
C(12)-C(11)-C(16)	120.0
C(12)-C(11)-C(21)	119.1(5)
C(16)-C(11)-C(21)	120.7(5)
C(12)-C(11)-Ru(1)	71.14(13)
C(16)-C(11)-Ru(1)	71.24(13)
C(21)-C(11)-Ru(1)	125.2(3)
C(11)-C(12)-C(13)	120.0
C(11)-C(12)-C(22)	119.1(5)
C(13)-C(12)-C(22)	120.9(5)
C(11)-C(12)-Ru(1)	71.28(14)
C(13)-C(12)-Ru(1)	71.14(13)
C(22)-C(12)-Ru(1)	128.9(3)
C(14)-C(13)-C(12)	120.0
C(14)-C(13)-C(23)	118.6(5)
C(12)-C(13)-C(23)	121.3(5)
C(14)-C(13)-Ru(1)	71.21(13)
C(12)-C(13)-Ru(1)	71.25(13)
C(23)-C(13)-Ru(1)	128.1(3)
C(15)-C(14)-C(13)	120.0
C(15)-C(14)-C(24)	118.4(5)
C(13)-C(14)-C(24)	121.3(5)
C(15)-C(14)-Ru(1)	71.27(14)
C(13)-C(14)-Ru(1)	71.18(13)
C(24)-C(14)-Ru(1)	124.1(3)
C(16)-C(15)-C(14)	120.0
C(16)-C(15)-C(25)	118.3(5)

C(14)-C(15)-C(25)	121.7(5)
C(16)-C(15)-Ru(1)	71.27(13)
C(14)-C(15)-Ru(1)	71.14(14)
C(25)-C(15)-Ru(1)	128.6(3)
C(15)-C(16)-C(11)	120.0
C(15)-C(16)-C(26)	120.0(5)
C(11)-C(16)-C(26)	120.0(5)
C(15)-C(16)-Ru(1)	71.16(13)
C(11)-C(16)-Ru(1)	71.21(12)
C(26)-C(16)-Ru(1)	132.8(3)
O(36)-C(36)-O(37)	123.7(8)
O(36)-C(36)-C(35)	122.0(8)
O(37)-C(36)-C(35)	114.3(7)
O(37)-C(38)-C(39)	105.6(6)
C(45)-O(46)-C(47)	116.4(13)
O(46)-C(45)-O(45)	115.5(11)
O(46)-C(45)-C(34)	126.1(13)
O(45)-C(45)-C(34)	117.7(13)
C(48)-C(47)-O(46)	105.5(12)
C(01)-O(1)-Ru(1)	112.6(3)
C(01)#1-O(2)-Ru(1)	112.9(4)
O(2)#1-C(01)-O(1)	124.5(5)
O(2)#1-C(01)-C(01)#1	117.9(7)
O(1)-C(01)-C(01)#1	117.6(6)

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Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1



Table 1. Crystal data and structure refinement for mozs273.

Identification code	KSS-6	
Empirical formula	C <sub>27</sub> H <sub>33</sub> N <sub>3</sub> O <sub>6</sub> Ru	
Formula weight	596.63	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4032(4) Å	α = 111.292(3)°.
	b = 11.5596(5) Å	β = 92.407(4)°.
	c = 14.4230(6) Å	γ = 109.007(3)°.
Volume	1358.04(10) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.459 Mg/m <sup>3</sup>	
Absorption coefficient	0.622 mm <sup>-1</sup>	
F(000)	616	
Crystal size	0.25428 x 0.16292 x 0.15360 mm <sup>3</sup>	
Theta range for data collection	1.54 to 29.29°.	
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 15, -19 ≤ l ≤ 18	
Reflections collected	51183	
Independent reflections	7347 [R(int) = 0.0614]	
Completeness to theta = 29.29°	99.1 %	
Absorption correction	Numerical	
Max. and min. transmission	0.9096 and 0.7882	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	7347 / 0 / 331	
Goodness-of-fit on F <sup>2</sup>	0.919	
Final R indices [I > 2σ(I)]	R1 = 0.0442, wR2 = 0.0867	
R indices (all data)	R1 = 0.0759, wR2 = 0.0946	
Extinction coefficient	0.0040(6)	
Largest diff. peak and hole	0.818 and -0.744 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mozs273.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Ru(1)	7350(1)	9027(1)	1310(1)	37(1)
C(11)	7084(2)	10377(2)	638(2)	48(1)
C(12)	6203(2)	10409(2)	1390(1)	49(1)
C(13)	5151(2)	9228(2)	1371(2)	52(1)
C(14)	4981(2)	8017(2)	600(2)	52(1)
C(15)	5863(2)	7985(2)	-152(1)	52(1)
C(16)	6915(2)	9165(2)	-133(1)	51(1)
C(21)	8238(4)	11693(4)	655(3)	69(1)
C(22)	6428(5)	11768(4)	2250(3)	73(1)
C(24)	3867(4)	6697(4)	607(4)	80(1)
C(26)	7959(5)	9102(5)	-926(3)	76(1)
C(23)	4269(5)	9239(5)	2256(4)	79(1)
C(25)	5727(6)	6636(4)	-979(3)	82(1)
O(1)	8661(2)	7841(2)	862(2)	44(1)
O(2)	7053(2)	8042(2)	2280(2)	44(1)
C(31)	8733(3)	7170(3)	1396(2)	40(1)
C(32)	7853(3)	7302(3)	2208(2)	39(1)
C(33)	7794(4)	6693(3)	2900(3)	52(1)
C(34)	8483(4)	5842(4)	2983(3)	60(1)
C(35)	9439(4)	5333(4)	2404(3)	61(1)
C(36)	9932(4)	5584(4)	1592(3)	59(1)
C(37)	9626(4)	6376(3)	1147(3)	51(1)
N(3)	10103(3)	9945(3)	2879(2)	49(1)
N(2)	9329(3)	10387(3)	2385(2)	45(1)
N(1)	9930(3)	11711(3)	2674(2)	51(1)
C(41)	11261(4)	11034(3)	3521(2)	48(1)
C(42)	11154(4)	12128(3)	3388(3)	51(1)
C(51)	12381(4)	10939(4)	4210(3)	60(1)
O(51)	13642(4)	11703(4)	4546(3)	120(2)
O(52)	11817(3)	9874(3)	4403(3)	91(1)
C(53)	12773(7)	9661(6)	5086(5)	117(2)

C(54)	12009(8)	8445(7)	5140(5)	117(2)
C(61)	12118(5)	13555(4)	3957(3)	70(1)
O(61)	12620(6)	14021(4)	4860(3)	129(2)
O(62)	12562(4)	14205(3)	3420(2)	99(1)
C(63)	13622(7)	15604(4)	3956(4)	111(2)
C(64)	13761(5)	16200(5)	3217(4)	85(1)

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Table 3. Bond lengths [Å] and angles [°] for mozs273.

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Ru(1)-O(2)	2.077(2)
Ru(1)-O(1)	2.084(2)
Ru(1)-N(2)	2.102(3)
Ru(1)-C(14)	2.1494(19)
Ru(1)-C(13)	2.1567(19)
Ru(1)-C(15)	2.160(2)
Ru(1)-C(12)	2.1741(19)
Ru(1)-C(16)	2.1771(19)
Ru(1)-C(11)	2.1843(19)
C(11)-C(12)	1.3900
C(11)-C(16)	1.3900
C(11)-C(21)	1.545(4)
C(12)-C(13)	1.3900
C(12)-C(22)	1.549(4)
C(13)-C(14)	1.3900
C(13)-C(23)	1.550(4)
C(14)-C(15)	1.3900
C(14)-C(24)	1.547(4)
C(15)-C(16)	1.3900
C(15)-C(25)	1.542(4)
C(16)-C(26)	1.535(4)
O(1)-C(31)	1.290(4)
O(2)-C(32)	1.292(3)
C(31)-C(37)	1.402(4)
C(31)-C(32)	1.454(4)
C(32)-C(33)	1.407(4)
C(33)-C(34)	1.377(5)
C(34)-C(35)	1.379(5)
C(35)-C(36)	1.370(5)
C(36)-C(37)	1.385(5)
N(3)-N(2)	1.327(4)
N(3)-C(41)	1.343(4)
N(2)-N(1)	1.338(4)
N(1)-C(42)	1.340(4)

C(41)-C(42)	1.379(5)
C(41)-C(51)	1.475(5)
C(42)-C(61)	1.483(5)
C(51)-O(51)	1.175(4)
C(51)-O(52)	1.309(5)
O(52)-C(53)	1.443(5)
C(53)-C(54)	1.388(8)
C(61)-O(61)	1.218(5)
C(61)-O(62)	1.258(5)
O(62)-C(63)	1.478(5)
C(63)-C(64)	1.454(7)

O(2)-Ru(1)-O(1)	76.73(8)
O(2)-Ru(1)-N(2)	84.18(9)
O(1)-Ru(1)-N(2)	84.12(9)
O(2)-Ru(1)-C(14)	91.59(8)
O(1)-Ru(1)-C(14)	113.71(8)
N(2)-Ru(1)-C(14)	160.27(9)
O(2)-Ru(1)-C(13)	93.46(7)
O(1)-Ru(1)-C(13)	150.33(8)
N(2)-Ru(1)-C(13)	123.19(9)
C(14)-Ru(1)-C(13)	37.7
O(2)-Ru(1)-C(15)	116.74(8)
O(1)-Ru(1)-C(15)	91.42(8)
N(2)-Ru(1)-C(15)	157.06(9)
C(14)-Ru(1)-C(15)	37.6
C(13)-Ru(1)-C(15)	67.8
O(2)-Ru(1)-C(12)	120.78(8)
O(1)-Ru(1)-C(12)	162.45(7)
N(2)-Ru(1)-C(12)	98.03(9)
C(14)-Ru(1)-C(12)	67.7
C(13)-Ru(1)-C(12)	37.4
C(15)-Ru(1)-C(12)	79.8
O(2)-Ru(1)-C(16)	153.85(8)
O(1)-Ru(1)-C(16)	96.66(7)
N(2)-Ru(1)-C(16)	120.71(9)

C(14)-Ru(1)-C(16)	67.6
C(13)-Ru(1)-C(16)	79.8
C(15)-Ru(1)-C(16)	37.4
C(12)-Ru(1)-C(16)	67.2
O(2)-Ru(1)-C(11)	157.97(8)
O(1)-Ru(1)-C(11)	125.30(8)
N(2)-Ru(1)-C(11)	97.08(9)
C(14)-Ru(1)-C(11)	79.8
C(13)-Ru(1)-C(11)	67.4
C(15)-Ru(1)-C(11)	67.3
C(12)-Ru(1)-C(11)	37.2
C(16)-Ru(1)-C(11)	37.2
C(12)-C(11)-C(16)	120.0
C(12)-C(11)-C(21)	119.8(2)
C(16)-C(11)-C(21)	120.2(2)
C(12)-C(11)-Ru(1)	71.01(7)
C(16)-C(11)-Ru(1)	71.13(7)
C(21)-C(11)-Ru(1)	131.07(19)
C(13)-C(12)-C(11)	120.0
C(13)-C(12)-C(22)	120.9(2)
C(11)-C(12)-C(22)	119.1(2)
C(13)-C(12)-Ru(1)	70.60(7)
C(11)-C(12)-Ru(1)	71.80(7)
C(22)-C(12)-Ru(1)	129.3(2)
C(12)-C(13)-C(14)	120.0
C(12)-C(13)-C(23)	120.4(2)
C(14)-C(13)-C(23)	119.4(2)
C(12)-C(13)-Ru(1)	71.96(7)
C(14)-C(13)-Ru(1)	70.88(7)
C(23)-C(13)-Ru(1)	124.8(2)
C(13)-C(14)-C(15)	120.0
C(13)-C(14)-C(24)	120.0(2)
C(15)-C(14)-C(24)	119.9(2)
C(13)-C(14)-Ru(1)	71.45(7)
C(15)-C(14)-Ru(1)	71.58(7)
C(24)-C(14)-Ru(1)	126.8(2)

C(16)-C(15)-C(14)	120.0
C(16)-C(15)-C(25)	120.0(2)
C(14)-C(15)-C(25)	120.0(2)
C(16)-C(15)-Ru(1)	71.99(7)
C(14)-C(15)-Ru(1)	70.78(7)
C(25)-C(15)-Ru(1)	127.2(2)
C(15)-C(16)-C(11)	120.0
C(15)-C(16)-C(26)	119.2(2)
C(11)-C(16)-C(26)	120.7(2)
C(15)-C(16)-Ru(1)	70.63(7)
C(11)-C(16)-Ru(1)	71.70(7)
C(26)-C(16)-Ru(1)	126.4(2)
C(31)-O(1)-Ru(1)	115.40(18)
C(32)-O(2)-Ru(1)	115.78(18)
O(1)-C(31)-C(37)	118.2(3)
O(1)-C(31)-C(32)	116.2(3)
C(37)-C(31)-C(32)	125.6(3)
O(2)-C(32)-C(33)	118.4(3)
O(2)-C(32)-C(31)	115.6(3)
C(33)-C(32)-C(31)	126.0(3)
C(34)-C(33)-C(32)	130.8(3)
C(33)-C(34)-C(35)	130.0(3)
C(36)-C(35)-C(34)	126.6(3)
C(35)-C(36)-C(37)	130.4(3)
C(36)-C(37)-C(31)	130.7(3)
N(2)-N(3)-C(41)	105.5(3)
N(3)-N(2)-N(1)	112.9(2)
N(3)-N(2)-Ru(1)	119.45(19)
N(1)-N(2)-Ru(1)	127.7(2)
N(2)-N(1)-C(42)	105.0(3)
N(3)-C(41)-C(42)	108.0(3)
N(3)-C(41)-C(51)	121.4(3)
C(42)-C(41)-C(51)	130.6(3)
N(1)-C(42)-C(41)	108.6(3)
N(1)-C(42)-C(61)	123.0(3)
C(41)-C(42)-C(61)	128.3(3)

O(51)-C(51)-O(52)	122.6(4)
O(51)-C(51)-C(41)	125.4(4)
O(52)-C(51)-C(41)	112.0(3)
C(51)-O(52)-C(53)	118.3(4)
C(54)-C(53)-O(52)	109.5(5)
O(61)-C(61)-O(62)	121.8(4)
O(61)-C(61)-C(42)	122.3(4)
O(62)-C(61)-C(42)	115.1(3)
C(61)-O(62)-C(63)	116.6(4)
C(64)-C(63)-O(62)	106.3(4)

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Symmetry transformations used to generate equivalent atoms:



Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for mozs273. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Ru(1)	33(1)	39(1)	39(1)	20(1)	4(1)	9(1)
C(11)	44(2)	52(2)	53(2)	29(2)	1(2)	16(1)
C(12)	47(2)	54(2)	55(2)	28(2)	5(2)	21(2)
C(13)	40(2)	68(2)	61(2)	38(2)	11(2)	22(2)
C(14)	40(2)	51(2)	66(2)	32(2)	-5(2)	9(1)
C(15)	54(2)	54(2)	47(2)	19(2)	-8(2)	19(2)
C(16)	50(2)	64(2)	44(2)	29(2)	3(2)	20(2)
C(21)	63(2)	64(2)	85(3)	51(2)	2(2)	8(2)
C(22)	80(3)	68(3)	72(3)	17(2)	5(2)	41(2)
C(24)	50(2)	70(3)	116(4)	54(3)	-7(2)	-1(2)
C(26)	77(3)	107(3)	55(2)	39(2)	21(2)	39(3)
C(23)	64(2)	112(4)	88(3)	60(3)	36(2)	40(2)
C(25)	103(3)	63(2)	63(3)	9(2)	-16(2)	32(2)
O(1)	45(1)	52(1)	40(1)	24(1)	10(1)	16(1)
O(2)	39(1)	53(1)	48(1)	29(1)	13(1)	18(1)
C(31)	36(1)	35(2)	37(2)	11(1)	-2(1)	4(1)
C(32)	32(1)	38(2)	41(2)	17(1)	0(1)	6(1)
C(33)	49(2)	58(2)	56(2)	34(2)	13(2)	17(2)
C(34)	66(2)	61(2)	64(2)	41(2)	7(2)	18(2)
C(35)	65(2)	50(2)	71(3)	27(2)	-2(2)	22(2)
C(36)	59(2)	52(2)	64(2)	16(2)	4(2)	27(2)
C(37)	50(2)	52(2)	48(2)	16(2)	9(2)	19(2)
N(3)	44(1)	45(1)	49(2)	18(1)	-3(1)	8(1)
N(2)	43(1)	42(1)	45(2)	19(1)	2(1)	9(1)
N(1)	55(2)	43(1)	49(2)	20(1)	8(1)	10(1)
C(41)	43(2)	46(2)	41(2)	12(1)	1(1)	5(1)
C(42)	53(2)	44(2)	42(2)	14(1)	5(2)	3(1)
C(51)	48(2)	63(2)	49(2)	14(2)	-5(2)	6(2)
O(51)	74(2)	116(3)	126(3)	61(2)	-49(2)	-27(2)
O(52)	65(2)	91(2)	112(3)	56(2)	-27(2)	10(2)
C(53)	96(4)	122(5)	127(5)	65(4)	-44(4)	22(3)

C(54)	132(5)	149(6)	111(5)	78(4)	22(4)	74(5)
C(61)	84(3)	56(2)	46(2)	14(2)	8(2)	3(2)
O(61)	179(4)	77(2)	69(2)	15(2)	12(2)	-12(2)
O(62)	127(3)	60(2)	65(2)	22(2)	-1(2)	-17(2)
C(63)	133(5)	52(3)	90(4)	23(2)	-11(3)	-26(3)
C(64)	71(3)	69(3)	102(4)	37(3)	7(3)	5(2)

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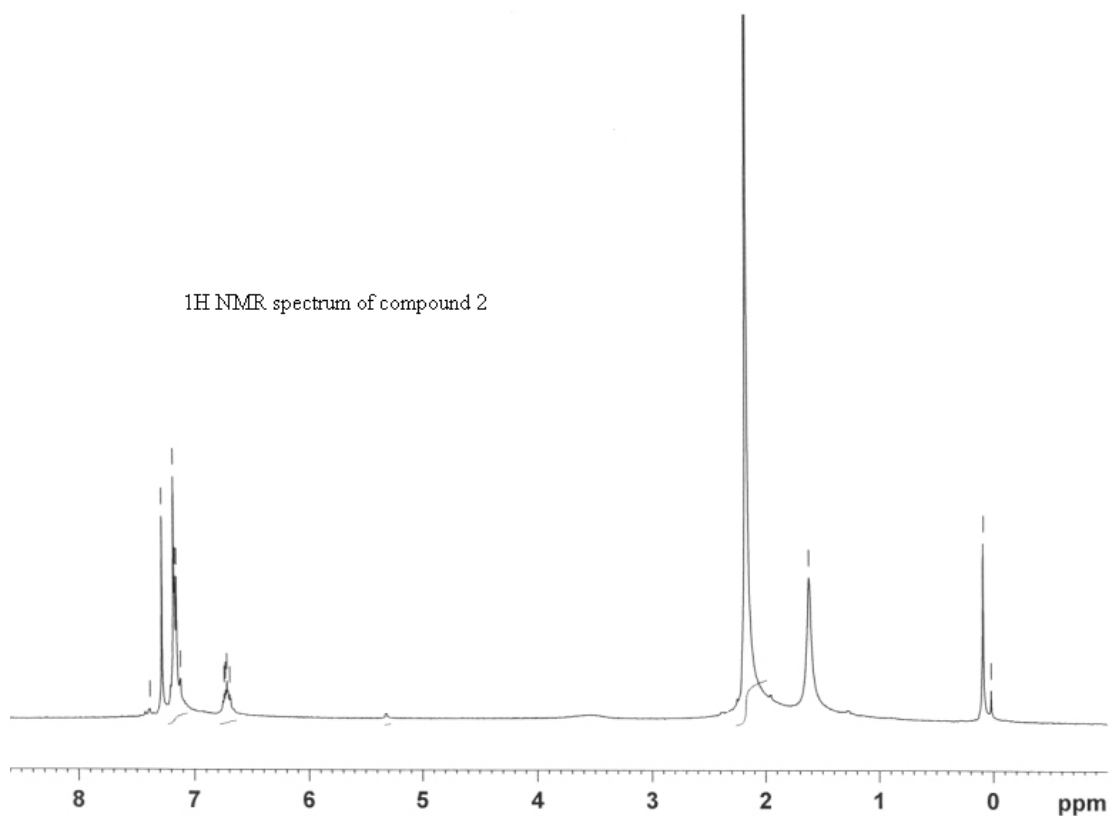
Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for mozs273.

	x	y	z	U(eq)
H(21A)	7705	12259	617	103
H(21B)	8749	11500	86	103
H(21C)	8979	12136	1270	103
H(22A)	5836	11621	2751	110
H(22B)	6098	12300	1976	110
H(22C)	7490	12224	2556	110
H(24A)	3100	6241	4	120
H(24B)	3386	6890	1189	120
H(24C)	4424	6142	632	120
H(26A)	8300	8374	-1029	115
H(26B)	8828	9923	-692	115
H(26C)	7402	8969	-1553	115
H(23A)	4694	10103	2803	119
H(23B)	4355	8577	2484	119
H(23C)	3210	9043	2028	119
H(25A)	5920	6745	-1596	123
H(25B)	4715	5995	-1090	123
H(25C)	6461	6327	-766	123
H(33)	7189	6901	3381	62
H(34)	8271	5569	3511	72
H(35)	9783	4761	2584	73
H(36)	10576	5153	1291	70
H(37)	10090	6383	591	62
H(53A)	13722	9665	4846	141
H(53B)	13017	10375	5753	141
H(54A)	11132	8480	5450	175
H(54B)	12683	8261	5538	175
H(54C)	11685	7752	4471	175
H(63A)	13217	16075	4519	133
H(63B)	14611	15639	4213	133

H(64A)	14103	15691	2645	128
H(64B)	14488	17100	3519	128
H(64C)	12784	16203	2998	128

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<sup>1</sup>H NMR spectrum of compound 2



<sup>1</sup>H NMR spectrum of compound 4

