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for

Alkali metal complexes based on bisheterocyclomethanide ligands

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1. ^{1}H, ^{13}C, ^{7}Li NMR spectroscopic data for compounds 1-3

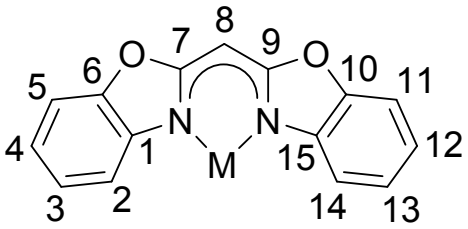

Figure 1. Ligand numbering for NMR spectroscopic data assignment.

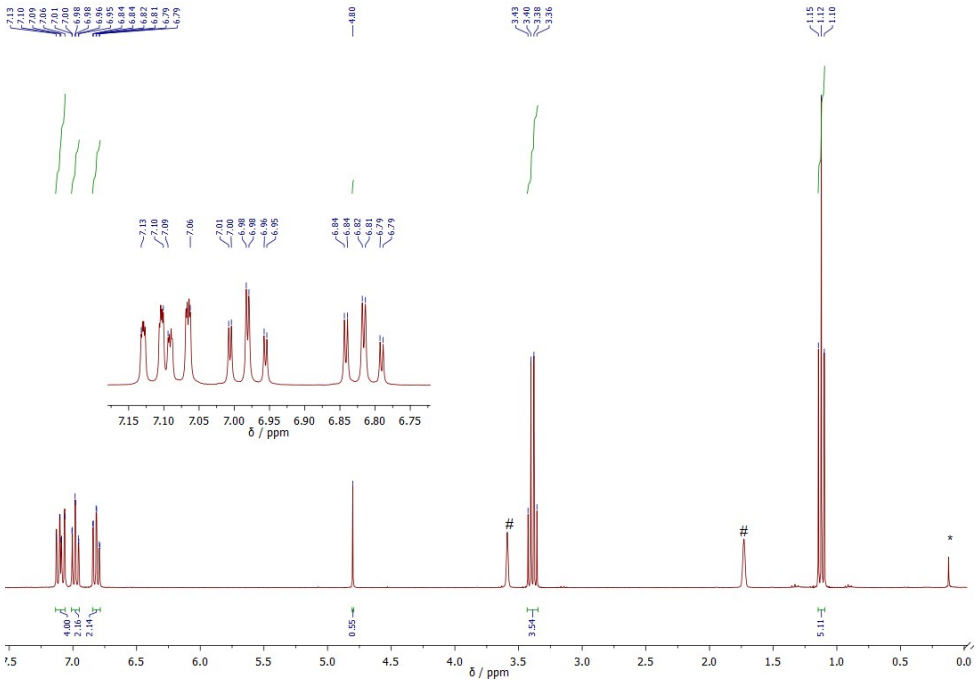

Figure 2. ^{1}H NMR spectrum of **1** in thf-d_8. The residual solvent signals are marked with #, grease is marked with *.

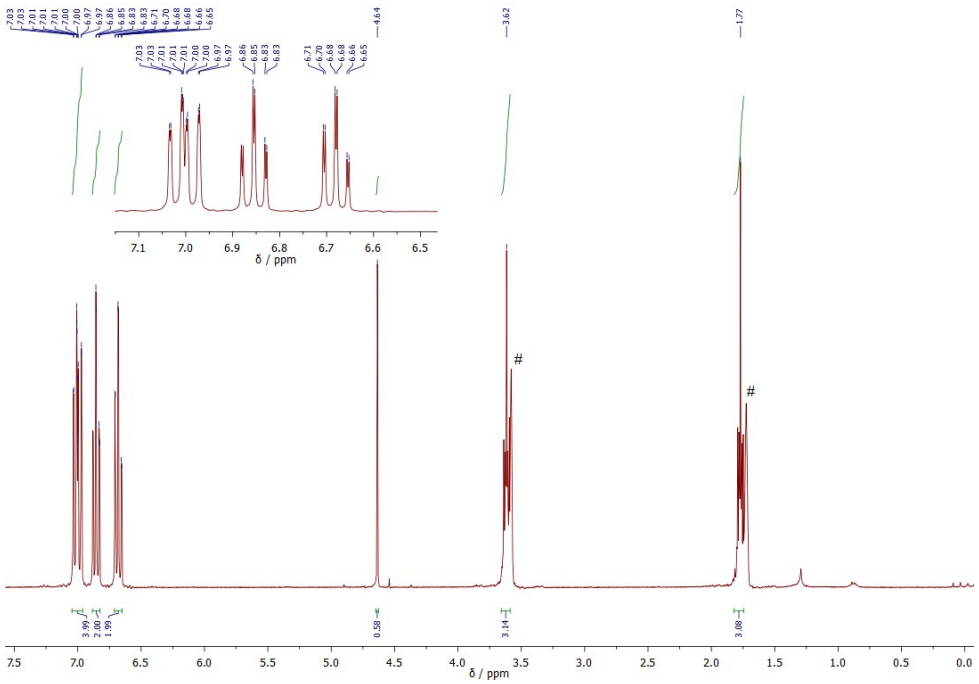

Figure 3. ^{1}H NMR spectrum of **2** in thf-d_8. The residual solvent signals are marked with #.

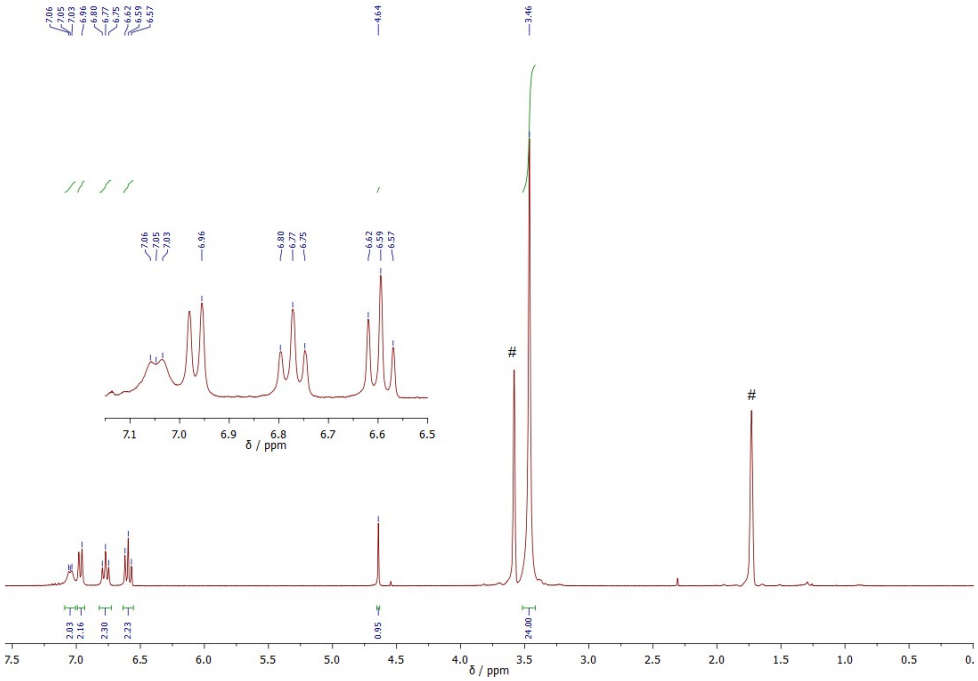

Figure 4. ^{1}H NMR spectrum of **3** in thf-d_8. The residual solvent signals are marked with #.

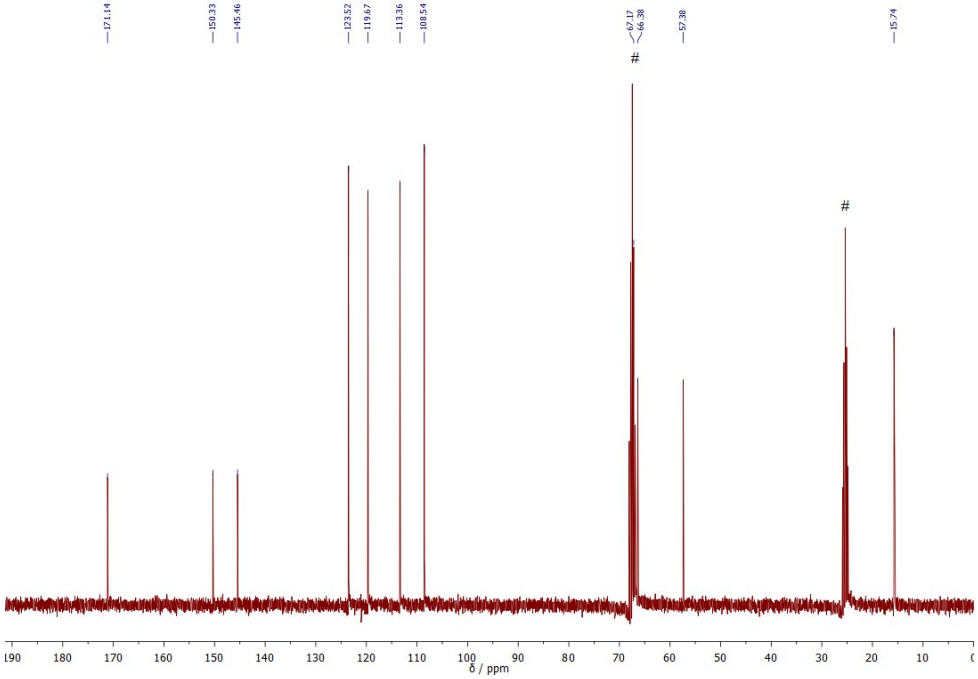

Figure 5. ^{13}C NMR spectrum of **1** in thf-d_8. The residual solvent signals are marked with #.

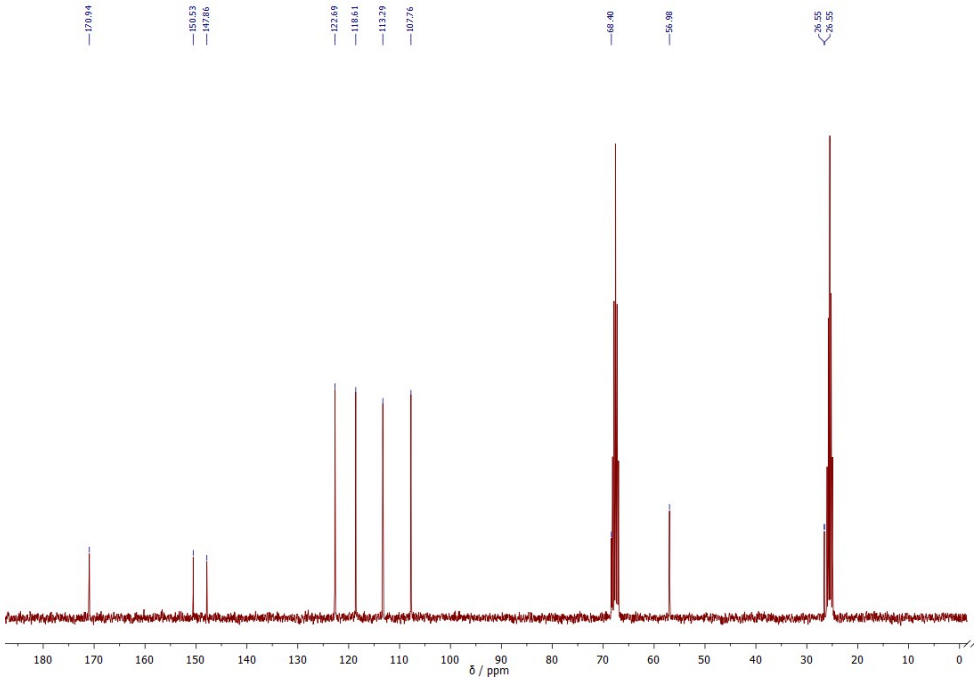

Figure 6. ^{13}C NMR spectrum of **2** in thf-d_8. The residual solvent signals are marked with #.

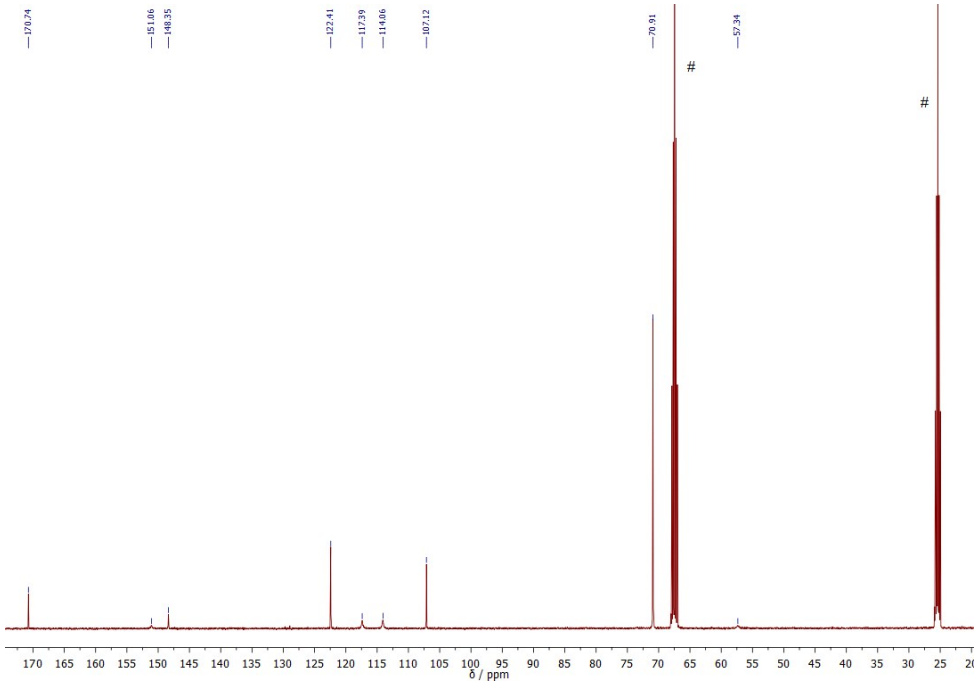

Figure 7. ^{13}C NMR spectrum of **3** in thf-d_8. The residual solvent signals are marked with #.

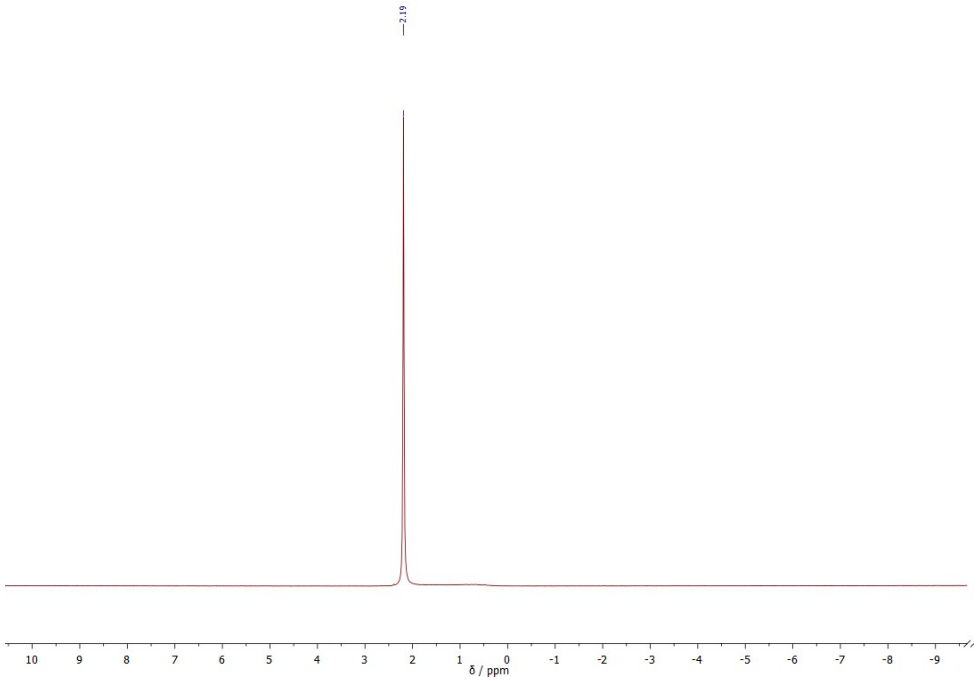

Figure 8. ^{7}Li NMR spectrum of **1** in thf-d_8.

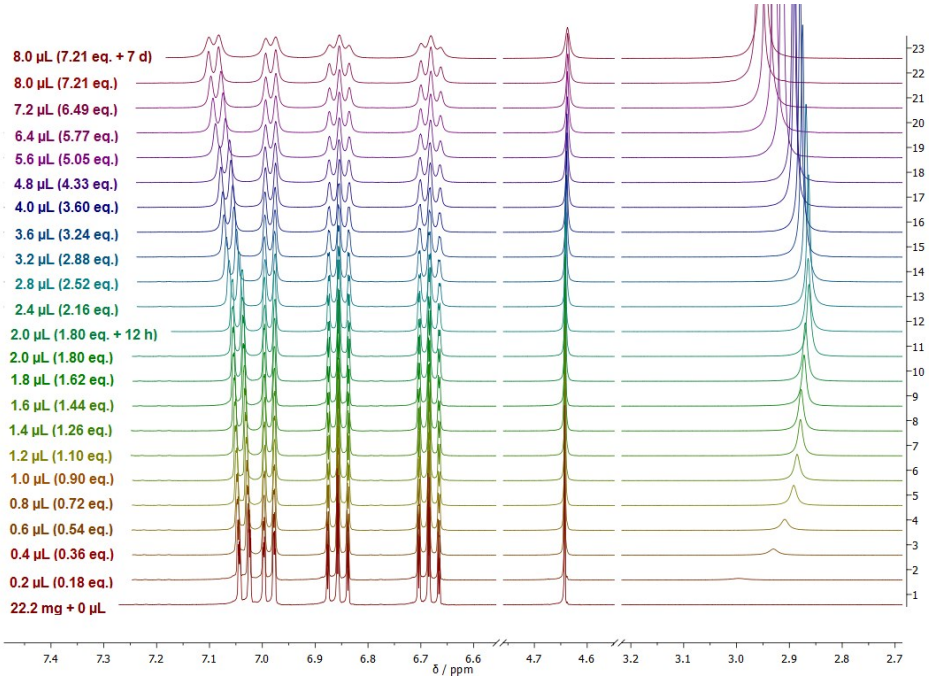

Figure 9. Stacked ^{1}H NMR spectra (thf-d_8) of a titration experiment of $[(\{NCOC_6H_4\}_2CH)K(thf)]_n$ (**2**) with water.

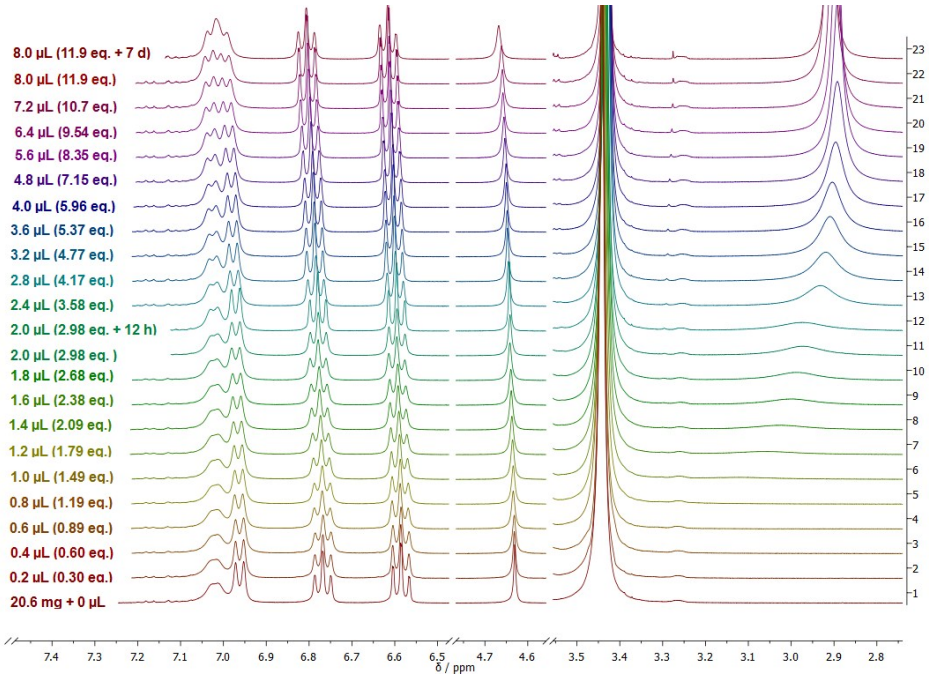

Figure 10. Stacked ^{1}H NMR spectra (thf-d_8) of a titration experiment of [({$NCOC_6H_4$}$_2$CH)K(18-crown-6)] (**3**) with water.

2. LIFDI spectrometry data of compound 1-3

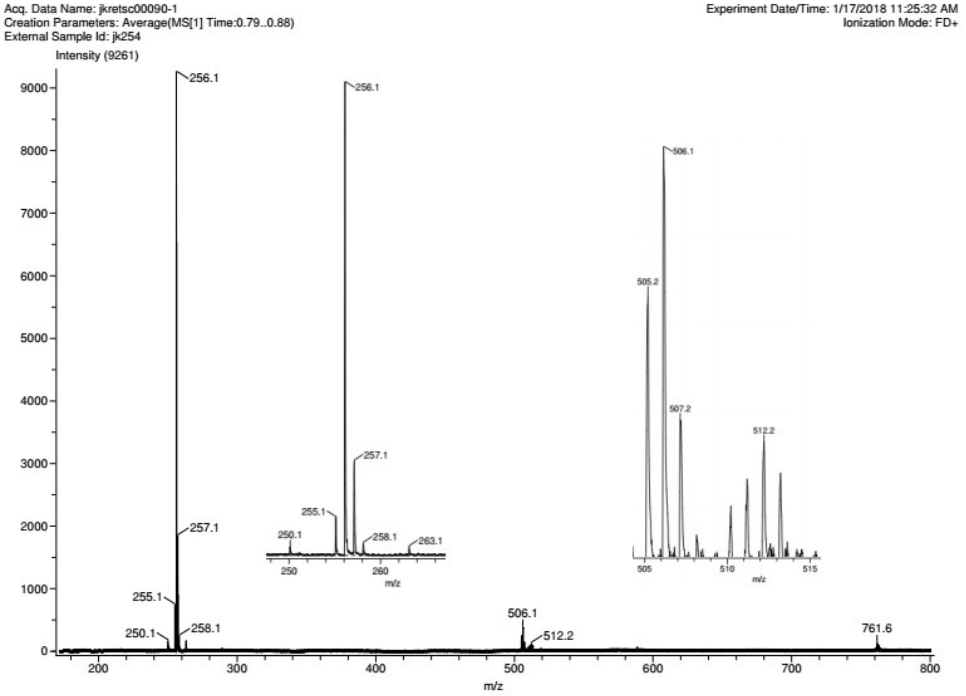

Figure 11. MS (LIFDI[+], toluene) of compound **1**: m/z = 256.08 (100) $[M-2Et_2O]^+$, 506.1 (4) $[M+(\{NCOC_6H_4\}_2CH_2)]^+$.

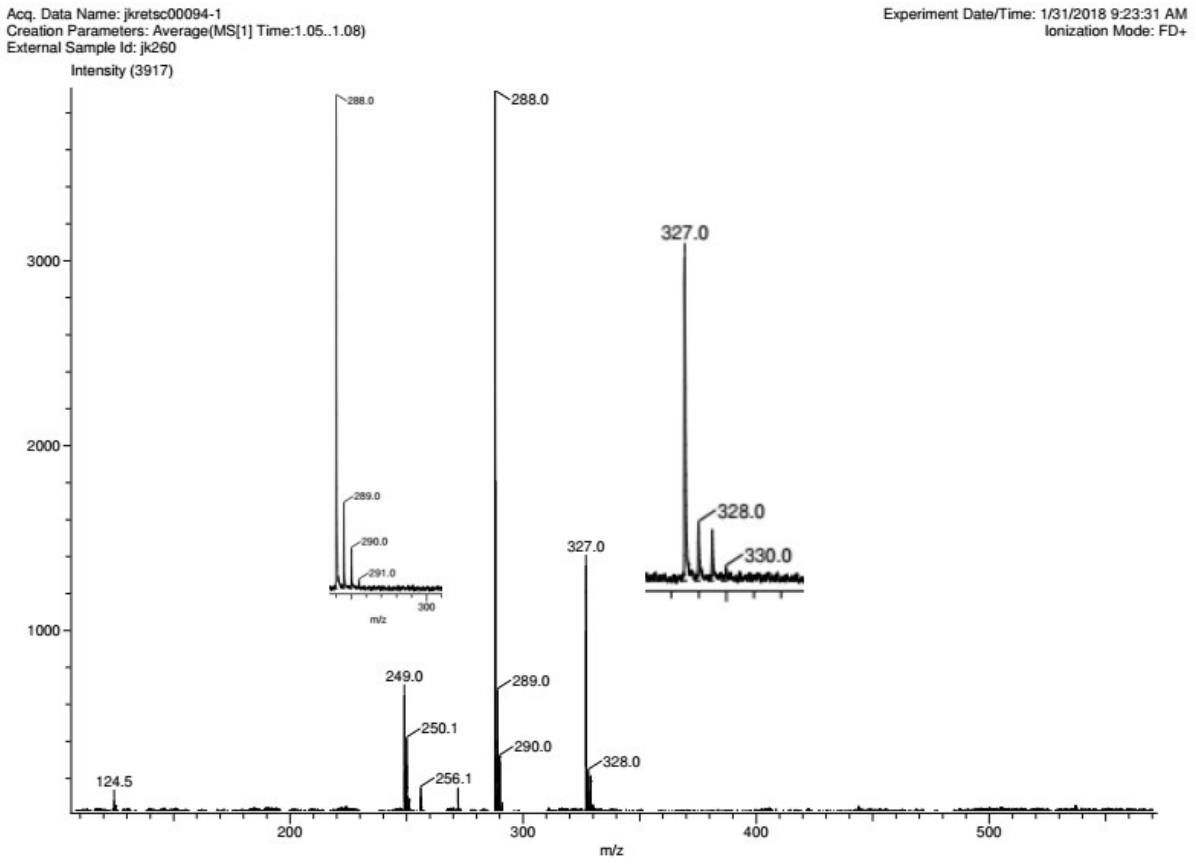

Figure 12. MS (LIFDI[+], toluene) of compound **2**: m/z = MS (LIFDI[+], toluene): m/z = 249.0 (11) $[M-K-thf]^+$, 288.0 (100) $[M-thf]^+$, 327.0 (28) $[M+K-thf]^+$.

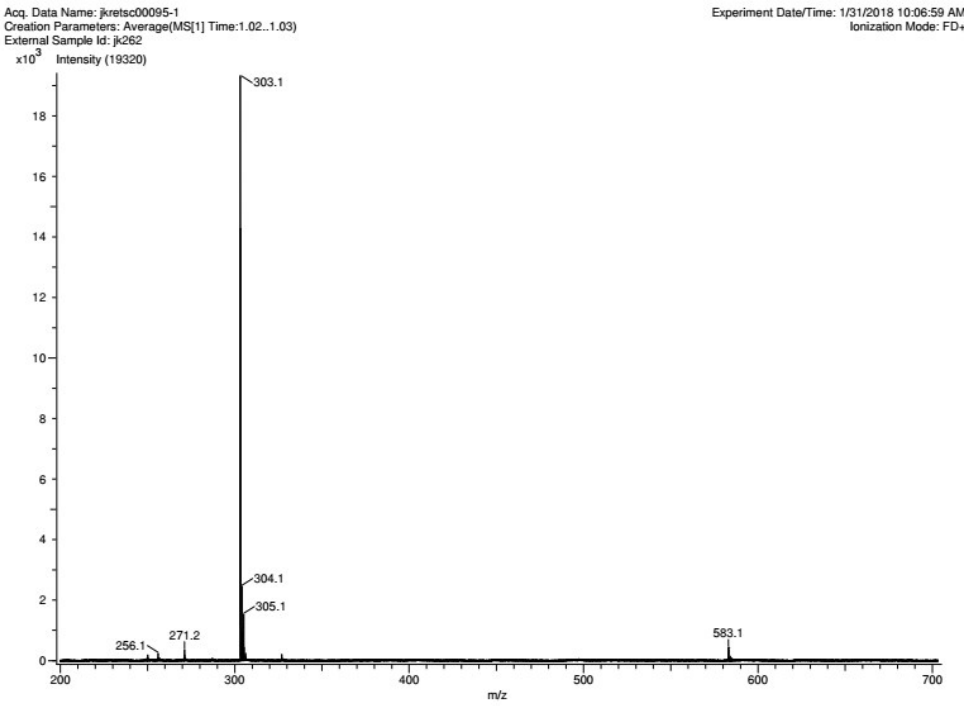

Figure 13. MS (LIFDI[+], toluene) of compound **2**: m/z = MS (LIFDI[+], toluene): m/z = 303.1 (100) $[M-(\{NCOC_6H_4\}_2CH)]^+$.

3. Crystallographic data for compounds 1-3

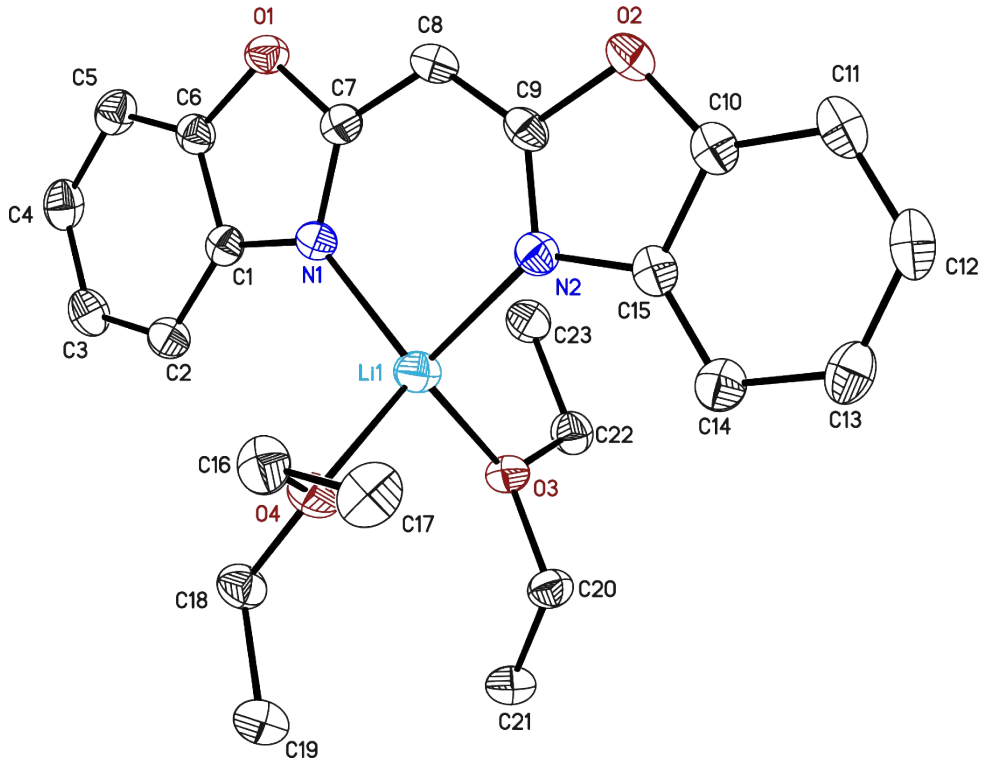

Figure 14. Asymmetric unit of **1**with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity.

Table 1. Crystal data and structure refinement for **1**.

Identification code	Compound **1**	
Empirical formula	$C_{23}H_{29}LiN_2O_4$	
Formula weight	404.42	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.284(3) Å	α = 90°
	b = 9.272(2) Å	β = 97.03(2)°
	c = 13.883(3) Å	γ = 90°
Volume	2208.1(8) $Å^3$	
Z	4	
Density (calculated)	1.217 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	864	
Crystal size	0.467 × 0.352 × 0.265 mm	
Theta range for data collection	2.375 to 25.547°	
Index ranges	−20<=h<=20, −11<=k<=11, −16<=l<=16	
Reflections collected	24547	
Independent reflections	4129 [R(int) = 0.0271]	
Completeness to theta = 25.242°	100.0%	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4129 / 1 / 279	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	$R1$ = 0.0334, $wR2$ = 0.0748	
R indices (all data)	$R1$ = 0.0440, $wR2$ = 0.0816	
Largest diff. peak and hole	0.210 and −0.155 $eÅ^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for compound **1**.

O(1)-C(6)	1.3882(15)
O(1)-C(7)	1.3962(15)
Li(1)-O(4)	1.978(2)
Li(1)-O(3)	1.980(2)
Li(1)-N(1)	1.995(2)
Li(1)-N(2)	2.004(2)
C(1)-N(1)	1.3913(16)
C(1)-C(2)	1.3938(18)
C(1)-C(6)	1.3941(17)
N(1)-C(7)	1.3297(16)
N(2)-C(9)	1.3334(16)
N(2)-C(15)	1.3942(16)
O(2)-C(10)	1.3822(16)
O(2)-C(9)	1.4027(15)
C(2)-C(3)	1.3906(19)
O(4)-C(18)	1.4383(15)
O(4)-C(16)	1.4420(16)
C(4)-C(3)	1.393(2)
C(4)-C(5)	1.3991(19)
O(3)-C(22)	1.4349(15)
O(3)-C(20)	1.4425(15)
C(7)-C(8)	1.3944(18)
C(6)-C(5)	1.3749(18)
C(8)-C(9)	1.3900(19)
C(8)-H(8)	0.951(12)
C(10)-C(11)	1.3759(19)
C(10)-C(15)	1.3950(18)
C(11)-C(12)	1.396(2)
C(12)-C(13)	1.396(2)
C(13)-C(14)	1.3954(19)
C(14)-C(15)	1.3904(19)
C(16)-C(17)	1.495(2)
C(18)-C(19)	1.5112(18)
C(20)-C(21)	1.5173(18)
C(22)-C(23)	1.5026(18)

C(6)-O(1)-C(7)	104.70(9)
O(4)-Li(1)-O(3)	102.96(10)
O(4)-Li(1)-N(1)	111.00(11)
O(3)-Li(1)-N(1)	120.06(12)
O(4)-Li(1)-N(2)	120.73(12)
O(3)-Li(1)-N(2)	109.09(11)
N(1)-Li(1)-N(2)	94.07(10)
N(1)-C(1)-C(2)	131.10(11)
N(1)-C(1)-C(6)	109.32(11)
C(2)-C(1)-C(6)	119.57(12)
C(7)-N(1)-C(1)	105.33(10)
C(7)-N(1)-Li(1)	122.48(10)
C(1)-N(1)-Li(1)	131.88(10)
C(9)-N(2)-C(15)	105.26(10)
C(9)-N(2)-Li(1)	121.73(11)
C(15)-N(2)-Li(1)	132.57(10)
C(10)-O(2)-C(9)	104.71(9)
C(3)-C(2)-C(1)	117.31(12)
C(18)-O(4)-C(16)	114.22(10)
C(18)-O(4)-Li(1)	122.56(10)
C(16)-O(4)-Li(1)	118.85(10)
C(3)-C(4)-C(5)	121.27(12)
C(22)-O(3)-C(20)	111.94(9)
C(22)-O(3)-Li(1)	125.86(10)
C(20)-O(3)-Li(1)	116.99(10)
C(2)-C(3)-C(4)	121.94(13)
N(1)-C(7)-C(8)	129.85(12)
N(1)-C(7)-O(1)	113.04(11)
C(8)-C(7)-O(1)	117.08(11)
C(5)-C(6)-O(1)	128.27(12)
C(5)-C(6)-C(1)	124.14(12)
O(1)-C(6)-C(1)	107.58(11)
C(6)-C(5)-C(4)	115.76(12)
C(9)-C(8)-C(7)	121.34(12)
N(2)-C(9)-C(8)	130.31(11)
N(2)-C(9)-O(2)	112.86(11)
C(8)-C(9)-O(2)	116.83(11)
C(11)-C(10)-O(2)	127.89(12)
C(11)-C(10)-C(15)	124.17(13)
O(2)-C(10)-C(15)	107.93(11)
C(10)-C(11)-C(12)	116.07(13)
C(13)-C(12)-C(11)	121.05(13)
C(14)-C(13)-C(12)	121.73(13)
C(15)-C(14)-C(13)	117.65(12)
C(14)-C(15)-N(2)	131.44(12)
C(14)-C(15)-C(10)	119.32(12)
N(2)-C(15)-C(10)	109.24(11)
O(4)-C(16)-C(17)	110.97(11)
O(4)-C(18)-C(19)	112.95(11)
O(3)-C(20)-C(21)	112.96(10)
O(3)-C(22)-C(23)	109.76(10)

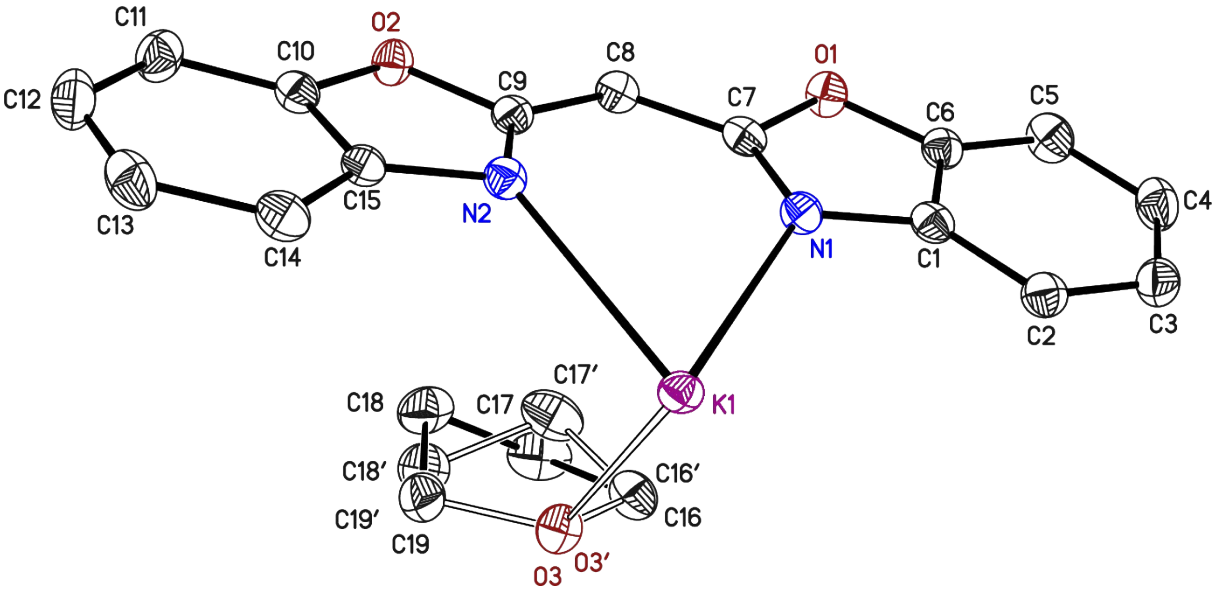

Figure 15. Molecular structure of **2** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. The disordered thf was refined with distance restraints and restraints for the anisotropic displacement parameters. The occupancy of the main position (O(3)-C(19)) refined to 0.744(13).

Table 3. Crystal data and structure refinement for **2**.

Identification code	Compound **2**	
Empirical formula	$C_{19}H_{17}KN_2O_3$	
Formula weight	360.44	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 11.200(2) Å	α = 90°
	b = 19.897(3) Å	β = 90°
	c = 7.745(2) Å	γ = 90°
Volume	1725.9(6) Å^3	
Z	4	
Density (calculated)	1.387 Mg/m^3	
Absorption coefficient	0.328 mm^{-1}	
F(000)	752	
Crystal size	0.364 × 0.177 × 0.126 mm	
Theta range for data collection	2.047 to 26.111°	
Index ranges	−13<=h<=13, −24<=k<=24, −9<=l<=9	
Reflections collected	26470	
Independent reflections	3432 [R(int) = 0.0238]	
Completeness to theta = 25.242°	100.0%	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3432 / 238 / 249	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	$R1$ = 0.0210, $wR2$ = 0.0556	
R indices (all data)	$R1$ = 0.0224, $wR2$ = 0.0566	
Absolute structure parameter	0.035(11)	
Largest diff. peak and hole	0.184 and −0.250 eÅ^{-3}	

Table 4. Bond lengths [Å] and angles [°] for compound **2**.

O(3)-C(16)	1.447(2)
O(3)-C(19)	1.451(2)
O(3)-K(1)	2.7573(15)
O(3)-K(1)#1	2.8265(16)
C(16)-C(17)	1.534(5)
C(16)-K(1)	3.474(2)
C(17)-C(18)	1.524(6)
C(18)-C(19)	1.515(4)
O(3')-C(16')	1.447(2)
O(3')-C(19')	1.451(2)
O(3')-K(1)	2.7573(15)
O(3')-K(1)#1	2.8265(16)
C(16')-C(17')	1.484(14)
C(16')-K(1)	3.474(2)
C(17')-C(18')	1.520(16)
C(18')-C(19')	1.506(11)
K(1)-N(2)	2.7542(17)
K(1)-N(1)	2.7621(16)
K(1)-N(2)#1	2.8936(17)
K(1)-N(1)#1	2.9901(17)
K(1)-C(7)#1	3.1037(18)
K(1)-C(9)#1	3.1038(19)
K(1)-C(8)#1	3.2101(19)
O(1)-C(6)	1.381(2)
O(1)-C(7)	1.396(2)
O(2)-C(10)	1.386(2)
O(2)-C(9)	1.398(2)
N(1)-C(7)	1.318(2)
N(1)-C(1)	1.404(2)
N(2)-C(9)	1.324(2)
N(2)-C(15)	1.401(2)
C(1)-C(6)	1.387(3)
C(1)-C(2)	1.397(3)
C(2)-C(3)	1.388(3)
C(3)-C(4)	1.396(3)
C(4)-C(5)	1.396(3)
C(5)-C(6)	1.385(3)
C(7)-C(8)	1.403(3)
C(8)-C(9)	1.403(3)
C(8)-H(8)	0.959(18)
C(10)-C(11)	1.376(3)
C(10)-C(15)	1.388(3)
C(11)-C(12)	1.394(3)
C(12)-C(13)	1.395(3)
C(13)-C(14)	1.393(3)
C(14)-C(15)	1.397(3)
C(16)-O(3)-C(19)	109.16(14)
C(16)-O(3)-K(1)	107.28(11)
C(19)-O(3)-K(1)	115.23(11)
C(16)-O(3)-K(1)#1	114.57(11)
C(19)-O(3)-K(1)#1	120.52(11)
K(1)-O(3)-K(1)#1	88.05(4)
O(3)-C(16)-C(17)	106.6(2)
O(3)-C(16)-K(1)	49.28(9)
C(17)-C(16)-K(1)	131.7(2)
C(18)-C(17)-C(16)	103.2(3)
C(19)-C(18)-C(17)	102.4(3)
O(3)-C(19)-C(18)	106.7(2)
C(16')-O(3')-C(19')	109.16(14)
C(16')-O(3')-K(1)	107.28(11)
C(19')-O(3')-K(1)	115.23(11)
K(1)-O(3')-K(1)#1	88.05(4)
O(3')-C(16')-C(17')	106.8(6)
O(3')-C(16')-K(1)	49.28(9)
C(17')-C(16')-K(1)	116.5(7)
C(16')-C(17')-C(18')	100.8(9)
C(19')-C(18')-C(17')	103.7(10)
O(3')-C(19')-C(18')	104.3(4)
N(2)-K(1)-O(3)	85.23(5)
N(2)-K(1)-O(3')	85.23(5)
N(2)-K(1)-N(1)	68.35(5)
O(3)-K(1)-N(1)	93.26(5)
O(3')-K(1)-N(1)	93.26(5)
N(2)-K(1)-O(3)#2	87.80(5)
O(3)-K(1)-O(3)#2	171.32(5)
N(1)-K(1)-O(3)#2	79.34(5)
N(2)-K(1)-N(2)#1	171.63(5)
O(3)-K(1)-N(2)#1	86.41(5)
N(1)-K(1)-N(2)#1	111.70(5)
O(3)#2-K(1)-N(2)#1	100.47(5)
N(2)-K(1)-N(1)#1	114.77(4)
O(3)-K(1)-N(1)#1	76.62(4)
N(1)-K(1)-N(1)#1	168.82(5)
O(3)#2-K(1)-N(1)#1	111.11(4)
N(2)#1-K(1)-N(1)#1	63.53(4)
N(2)-K(1)-C(7)#1	120.77(5)
O(3)-K(1)-C(7)#1	101.25(5)
N(1)-K(1)-C(7)#1	163.26(5)
O(3)#2-K(1)-C(7)#1	86.76(5)
N(2)#1-K(1)-C(7)#1	61.54(5)
N(1)#1-K(1)-C(7)#1	24.89(5)
N(2)-K(1)-C(9)#1	162.19(5)
O(3)-K(1)-C(9)#1	108.81(5)
O(3')-K(1)-C(9)#1	108.81(5)
N(1)-K(1)-C(9)#1	120.02(5)
O(3)#2-K(1)-C(9)#1	79.06(5)
N(2)#1-K(1)-C(9)#1	25.19(5)
N(1)#1-K(1)-C(9)#1	60.43(5)
C(7)#1-K(1)-C(9)#1	47.14(5)
N(2)-K(1)-C(8)#1	137.91(5)
O(3)-K(1)-C(8)#1	116.55(5)
N(1)-K(1)-C(8)#1	138.28(5)
O(3)#2-K(1)-C(8)#1	72.12(5)
N(2)#1-K(1)-C(8)#1	47.68(5)
N(1)#1-K(1)-C(8)#1	46.94(4)
C(7)#1-K(1)-C(8)#1	25.61(5)
C(9)#1-K(1)-C(8)#1	25.60(5)
N(2)-K(1)-C(16')	85.04(5)
O(3')-K(1)-C(16')	23.44(4)
N(1)-K(1)-C(16')	71.36(5)

N(2)#1-K(1)-C(16')	87.10(5)
N(1)#1-K(1)-C(16')	97.89(5)
C(7)#1-K(1)-C(16')	121.35(6)
C(9)#1-K(1)-C(16')	112.25(6)
C(8)#1-K(1)-C(16')	129.43(6)
N(2)-K(1)-C(16)	85.04(5)
O(3)-K(1)-C(16)	23.44(4)
N(1)-K(1)-C(16)	71.36(5)
O(3)#2-K(1)-C(16)	150.44(5)
N(2)#1-K(1)-C(16)	87.10(5)
N(1)#1-K(1)-C(16)	97.89(5)
C(7)#1-K(1)-C(16)	121.35(6)
C(9)#1-K(1)-C(16)	112.25(6)
C(8)#1-K(1)-C(16)	129.43(6)
C(6)-O(1)-C(7)	104.35(14)
C(10)-O(2)-C(9)	104.38(14)
C(7)-N(1)-C(1)	104.73(15)
C(7)-N(1)-K(1)	129.33(12)
C(1)-N(1)-K(1)	124.09(12)
C(7)-N(1)-K(1)#2	82.39(10)
C(1)-N(1)-K(1)#2	119.40(11)
K(1)-N(1)-K(1)#2	84.76(4)
C(9)-N(2)-C(15)	104.85(15)
C(9)-N(2)-K(1)	127.83(12)
C(15)-N(2)-K(1)	122.54(12)
C(9)-N(2)-K(1)#2	86.31(11)
C(15)-N(2)-K(1)#2	121.27(12)
K(1)-N(2)-K(1)#2	86.77(4)
C(6)-C(1)-C(2)	119.68(17)
C(6)-C(1)-N(1)	109.12(16)
C(2)-C(1)-N(1)	131.19(17)
C(3)-C(2)-C(1)	117.43(18)
C(2)-C(3)-C(4)	121.69(19)
C(5)-C(4)-C(3)	121.59(18)
C(6)-C(5)-C(4)	115.46(19)
O(1)-C(6)-C(5)	127.85(18)
O(1)-C(6)-C(1)	108.00(15)
C(5)-C(6)-C(1)	124.14(18)
N(1)-C(7)-O(1)	113.77(16)
N(1)-C(7)-C(8)	131.17(17)
O(1)-C(7)-C(8)	115.05(16)
N(1)-C(7)-K(1)#2	72.73(10)
O(1)-C(7)-K(1)#2	121.20(11)
C(8)-C(7)-K(1)#2	81.44(10)
C(9)-C(8)-C(7)	124.40(17)
C(9)-C(8)-K(1)#2	72.96(10)
C(7)-C(8)-K(1)#2	72.96(10)
C(9)-C(8)-H(8)	118.0(13)
C(7)-C(8)-H(8)	117.6(13)
K(1)#2-C(8)-H(8)	128.1(13)
N(2)-C(9)-O(2)	113.54(16)
N(2)-C(9)-C(8)	131.26(17)
O(2)-C(9)-C(8)	115.17(15)
N(2)-C(9)-K(1)#2	68.49(10)
O(2)-C(9)-K(1)#2	126.40(12)
C(8)-C(9)-K(1)#2	81.44(10)
C(11)-C(10)-O(2)	127.58(18)
C(11)-C(10)-C(15)	124.50(17)
O(2)-C(10)-C(15)	107.88(15)
C(10)-C(11)-C(12)	115.37(19)
C(11)-C(12)-C(13)	121.86(19)
C(14)-C(13)-C(12)	121.39(19)
C(13)-C(14)-C(15)	117.34(18)
C(10)-C(15)-C(14)	119.51(17)
C(10)-C(15)-N(2)	109.35(16)
C(14)-C(15)-N(2)	131.14(18)

Symmetry transformations used to generate equivalent atoms:

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

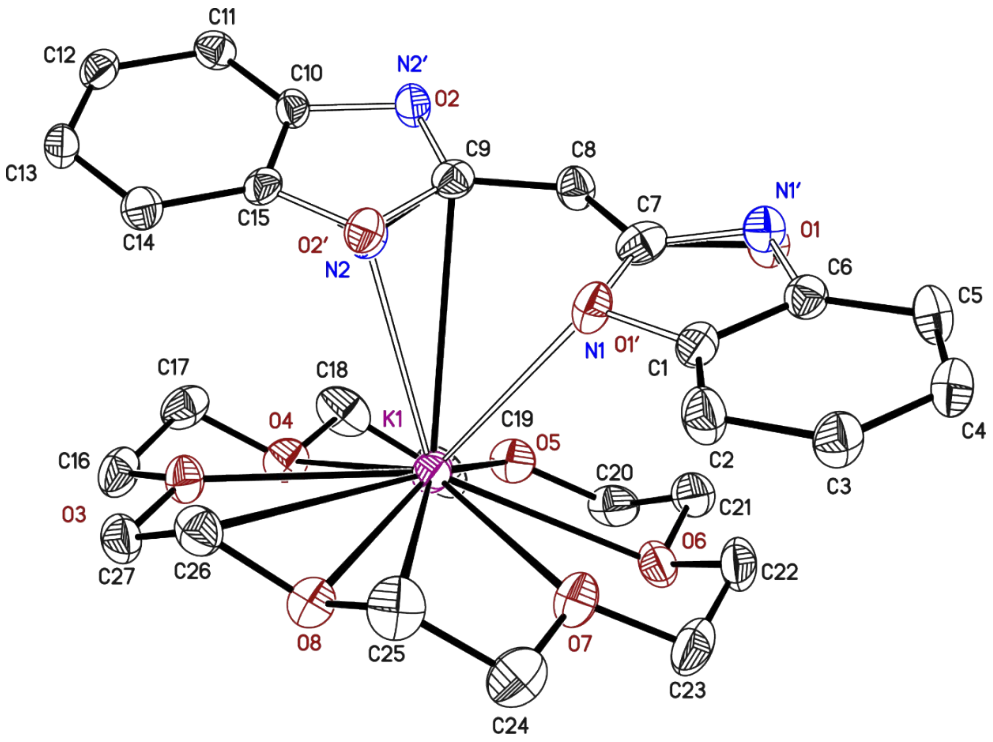

Figure 16. Molecular structure of **3** with thermal ellipsoids at 50% probability level. The hydrogen atoms are omitted for clarity. The disordered ligand was refined on two position. The occupancy of the main position refined to 0.61(3) for O(1)/N(1´) and 0.82(3) for O(2)/N(2).

Table 5. Crystal data and structure refinement for **3**.

Identification code	Compound **3**	
Empirical formula	$C_{27}H_{33}KN_2O_8$	
Formula weight	552.65	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pca2_1$	
Unit cell dimensions	a = 15.913(3) Å	α = 90°
	b = 10.981(2) Å	β = 90°
	c = 15.309(3) Å	γ = 90°
Volume	2675.1(9) Å^3	
Z	4	
Density (calculated)	1.372 Mg/m^3	
Absorption coefficient	0.251 mm^{-1}	
F(000)	1168	
Crystal size	0.226 × 0.172 × 0.098 mm	
Theta range for data collection	1.855 to 26.427°	
Index ranges	−19<=h<=19, −13<=k<=13, −19<=l<=19	
Reflections collected	33321	
Independent reflections	5489 [R(int) = 0.0478]	
Completeness to theta = 25.242°	100.0%	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5489 / 88 / 361	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0343, wR2 = 0.0693	
R indices (all data)	R1 = 0.0440, wR2 = 0.0727	
Absolute structure parameter	0.008(15)	
Largest diff. peak and hole	0.288 and −0.268 eÅ^{-3}	

Table 6. Bond lengths [Å] and angles [°] for compound **3**.

K(1)-O(7)	2.751(2)
K(1)-O(3)	2.814(3)
K(1)-O(8)	2.843(3)
K(1)-O(5)	2.848(3)
K(1)-N(2)	2.87(3)
K(1)-O(6)	2.941(3)
K(1)-O(2')	2.97(12)
K(1)-O(4)	2.995(3)
K(1)-C(9)	3.358(3)
K(1)-C(12)#1	3.362(3)
K(1)-N(1)	3.37(9)
K(1)-O(1')	3.42(5)
C(8)-H(8)	0.93(2)
C(8)-C(7)	1.384(4)
C(8)-C(9)	1.398(4)
C(7)-N(1)	1.33(2)
C(7)-N(1')	1.342(18)
C(7)-O(1')	1.371(14)
C(7)-O(1)	1.38(2)
N(1)-C(1)	1.40(2)
O(1)-C(6)	1.37(2)
C(5)-C(4)	1.382(4)
C(5)-C(6)	1.386(4)
C(2)-C(1)	1.370(4)
C(2)-C(3)	1.398(4)
C(1)-O(1')	1.377(13)
C(1)-C(6)	1.390(4)
C(6)-N(1')	1.390(17)
O(2)-C(10)	1.388(6)
O(2)-C(9)	1.398(7)
N(2)-C(9)	1.320(9)
N(2)-C(15)	1.404(8)
O(3)-C(16)	1.414(4)
O(3)-C(27)	1.422(4)
C(3)-C(4)	1.386(4)
O(5)-C(19)	1.416(4)
O(5)-C(20)	1.427(4)
O(4)-C(17)	1.420(4)
O(4)-C(18)	1.425(4)
O(6)-C(21)	1.422(4)
O(6)-C(22)	1.424(4)
O(7)-C(23)	1.421(4)
O(7)-C(24)	1.423(4)
C(9)-N(2')	1.35(3)
C(9)-O(2')	1.36(2)
O(8)-C(26)	1.426(3)
O(8)-C(25)	1.427(4)
C(10)-C(11)	1.372(4)
C(10)-C(15)	1.374(4)
C(10)-N(2')	1.40(2)
C(11)-C(12)	1.397(4)
C(12)-C(13)	1.380(5)
C(13)-C(14)	1.386(4)
C(14)-C(15)	1.392(4)
C(15)-O(2')	1.38(2)
C(16)-C(17)	1.498(5)
C(18)-C(19)	1.498(5)
C(20)-C(21)	1.484(5)
C(22)-C(23)	1.492(5)
C(24)-C(25)	1.495(4)
C(26)-C(27)	1.492(4)
O(7)-K(1)-O(3)	120.83(7)
O(7)-K(1)-O(8)	60.96(8)
O(3)-K(1)-O(8)	59.98(6)
O(7)-K(1)-O(5)	116.35(8)
O(3)-K(1)-O(5)	113.69(7)
O(8)-K(1)-O(5)	152.08(6)
O(7)-K(1)-N(2)	112.5(4)
O(3)-K(1)-N(2)	76.2(2)
O(8)-K(1)-N(2)	95.2(2)
O(5)-K(1)-N(2)	110.1(3)
O(7)-K(1)-O(6)	58.24(7)
O(3)-K(1)-O(6)	154.02(6)
O(8)-K(1)-O(6)	114.07(7)
O(5)-K(1)-O(6)	58.28(6)
N(2)-K(1)-O(6)	129.5(2)
O(7)-K(1)-O(2')	111.4(13)
O(3)-K(1)-O(2')	75.8(7)
O(8)-K(1)-O(2')	93.8(8)
O(5)-K(1)-O(2')	111.5(10)
O(6)-K(1)-O(2')	130.0(7)
O(7)-K(1)-O(4)	152.79(6)
O(3)-K(1)-O(4)	56.07(7)
O(8)-K(1)-O(4)	110.64(8)
O(5)-K(1)-O(4)	57.65(8)
N(2)-K(1)-O(4)	93.5(4)
O(6)-K(1)-O(4)	111.41(8)
O(2')-K(1)-O(4)	94.4(13)
O(7)-K(1)-C(9)	112.74(7)
O(3)-K(1)-C(9)	95.36(6)
O(8)-K(1)-C(9)	115.85(7)
O(5)-K(1)-C(9)	91.26(7)
N(2)-K(1)-C(9)	22.81(16)
O(6)-K(1)-C(9)	108.94(7)
O(2')-K(1)-C(9)	23.9(5)
O(4)-K(1)-C(9)	94.31(6)
O(7)-K(1)-C(12)#1	74.73(8)
O(3)-K(1)-C(12)#1	87.55(6)
O(8)-K(1)-C(12)#1	75.18(7)
O(5)-K(1)-C(12)#1	77.45(7)
N(2)-K(1)-C(12)#1	163.7(2)
O(6)-K(1)-C(12)#1	66.83(7)
O(2')-K(1)-C(12)#1	163.1(6)
O(4)-K(1)-C(12)#1	78.10(7)
C(9)-K(1)-C(12)#1	168.54(8)
O(7)-K(1)-N(1)	60.6(12)
O(3)-K(1)-N(1)	118.8(13)
O(8)-K(1)-N(1)	87.1(5)
O(5)-K(1)-N(1)	116.7(7)
N(2)-K(1)-N(1)	55.7(15)

O(6)-K(1)-N(1)	84.4(14)	C(18)-O(4)-K(1)	110.42(18)
O(4)-K(1)-N(1)	146.6(11)	C(21)-O(6)-C(22)	112.5(2)
C(9)-K(1)-N(1)	52.3(11)	C(21)-O(6)-K(1)	107.71(17)
C(12)#1-K(1)-N(1)	135.0(13)	C(22)-O(6)-K(1)	107.57(17)
O(7)-K(1)-O(1')	60.6(6)	C(23)-O(7)-C(24)	112.7(2)
O(3)-K(1)-O(1')	118.1(7)	C(23)-O(7)-K(1)	123.13(19)
O(8)-K(1)-O(1')	86.4(2)	C(24)-O(7)-K(1)	117.79(17)
O(5)-K(1)-O(1')	117.4(3)	N(2')-C(9)-O(2')	113.1(12)
O(6)-K(1)-O(1')	85.1(7)	N(2)-C(9)-O(2)	113.6(4)
O(2')-K(1)-O(1')	54.8(15)	N(2)-C(9)-C(8)	129.3(4)
O(4)-K(1)-O(1')	146.6(6)	N(2')-C(9)-C(8)	117.1(13)
C(9)-K(1)-O(1')	52.3(6)	O(2')-C(9)-C(8)	129.6(11)
C(12)#1-K(1)-O(1')	135.1(6)	O(2)-C(9)-C(8)	117.2(3)
H(8)-C(8)-C(7)	117.0(19)	N(2)-C(9)-K(1)	57.5(13)
H(8)-C(8)-C(9)	116.6(19)	N(2')-C(9)-K(1)	128(10)
C(7)-C(8)-C(9)	125.7(3)	O(2')-C(9)-K(1)	62(5)
N(1')-C(7)-O(1')	112.7(6)	O(2)-C(9)-K(1)	128.0(18)
N(1)-C(7)-O(1)	112.4(12)	C(8)-C(9)-K(1)	89.89(17)
N(1)-C(7)-C(8)	124.8(12)	C(26)-O(8)-C(25)	111.8(2)
N(1')-C(7)-C(8)	121.7(8)	C(26)-O(8)-K(1)	104.91(17)
O(1')-C(7)-C(8)	125.1(7)	C(25)-O(8)-K(1)	106.98(17)
O(1)-C(7)-C(8)	122.7(10)	C(11)-C(10)-C(15)	123.6(3)
C(7)-N(1)-C(1)	105.9(19)	C(11)-C(10)-O(2)	128.1(3)
C(7)-N(1)-K(1)	93(4)	C(15)-C(10)-O(2)	108.3(3)
C(1)-N(1)-K(1)	131(6)	C(11)-C(10)-N(2')	129.9(12)
C(6)-O(1)-C(7)	104.1(16)	C(15)-C(10)-N(2')	106.4(12)
C(4)-C(5)-C(6)	117.4(3)	C(10)-C(11)-C(12)	116.3(3)
C(1)-C(2)-C(3)	116.8(3)	C(10)-C(11)-K(1)#2	126.75(19)
C(2)-C(1)-O(1')	129.4(7)	C(12)-C(11)-K(1)#2	71.79(17)
C(2)-C(1)-C(6)	122.3(3)	C(13)-C(12)-C(11)	121.0(3)
O(1')-C(1)-C(6)	108.3(6)	C(13)-C(12)-K(1)#2	120.6(2)
C(2)-C(1)-N(1)	130.8(11)	C(11)-C(12)-K(1)#2	84.96(17)
C(6)-C(1)-N(1)	106.9(11)	C(12)-C(13)-C(14)	121.6(3)
O(1)-C(6)-C(5)	129.6(10)	C(13)-C(14)-C(15)	117.6(3)
C(5)-C(6)-N(1')	130.7(8)	C(10)-C(15)-O(2')	110.9(12)
O(1)-C(6)-C(1)	109.6(10)	C(10)-C(15)-C(14)	119.8(3)
C(5)-C(6)-C(1)	120.8(3)	O(2')-C(15)-C(14)	129.2(11)
N(1')-C(6)-C(1)	108.3(8)	C(10)-C(15)-N(2)	109.4(4)
C(7)-N(1')-C(6)	105.3(14)	C(14)-C(15)-N(2)	130.8(4)
C(7)-O(1')-C(1)	105.2(10)	C(9)-N(2')-C(10)	106(2)
C(7)-O(1')-K(1)	90(2)	C(9)-O(2')-C(15)	103.6(18)
C(1)-O(1')-K(1)	129(3)	C(9)-O(2')-K(1)	94(5)
C(10)-O(2)-C(9)	104.0(4)	C(15)-O(2')-K(1)	116(7)
C(9)-N(2)-C(15)	104.7(6)	O(3)-C(16)-C(17)	108.6(2)
C(9)-N(2)-K(1)	99.7(14)	O(4)-C(17)-C(16)	108.5(2)
C(15)-N(2)-K(1)	120.6(17)	O(4)-C(18)-C(19)	108.1(3)
C(16)-O(3)-C(27)	113.0(2)	O(5)-C(19)-C(18)	109.1(3)
C(16)-O(3)-K(1)	125.29(18)	O(5)-C(20)-C(21)	109.4(3)
C(27)-O(3)-K(1)	117.50(16)	O(6)-C(21)-C(20)	108.4(3)
C(4)-C(3)-C(2)	121.3(3)	O(6)-C(22)-C(23)	109.0(2)
C(19)-O(5)-C(20)	111.4(2)	O(7)-C(23)-C(22)	108.7(3)
C(19)-O(5)-K(1)	120.01(18)	O(7)-C(24)-C(25)	108.9(3)
C(20)-O(5)-K(1)	119.08(18)	O(8)-C(25)-C(24)	109.0(3)
C(5)-C(4)-C(3)	121.4(3)	O(8)-C(25)-K(1)	50.30(14)
C(17)-O(4)-C(18)	112.8(2)	C(24)-C(25)-K(1)	81.96(18)
C(17)-O(4)-K(1)	110.15(17)	O(8)-C(26)-C(27)	109.0(2)

O(8)-C(26)-K(1)	51.86(14)
C(27)-C(26)-K(1)	85.64(18)
O(3)-C(27)-C(26)	108.4(2)

Symmetry transformations used to generate equivalent atoms:

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