Supporting Information for

Heterobimetallic aluminate derivatives with bulky phenoxide ligands: catalyst for selective vinyl polymerization..

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1. **Diffusion-Ordered SpectroscopY (^{1}H-DOSY) NMR experiments**
2. **Glycidyl Methacrylate (GMA) polymerization studies: Experimental details, IR and DSC data.**
3. **Single-Crystal X-ray data for 2a·2C_7H_8, 2b·2C_7H_8, 3b·C_7H_8 and 3c·C_7H_8.**

1. Diffusion-Ordered NMR Spectroscopy (DOSY) experiments.

In Diffusion-Ordered Spectroscopy (DOSY) NMR experiments, a series of pulsed field gradient (PFG) stimulated echo experiments is performed and the results allow to generate a two dimensional spectrum where signals are dispersed depending on their diffusion coefficients.[1]

The diffusion coefficient (D) of a molecule is inversely proportional to its hydrodynamic radius as given in the Stokes-Einstein equation: $D = kT/(6\pi\eta r_H)$, where k is the Boltzman constant, T is the temperature, η is the viscosity, and r_H is the hydrodynamic radius, however this is only strictly valid for spherical molecules of a much bigger size than the solvent. From the Stokes-Einstein equation the relation between the diffusion coefficient of a molecule, D, and its volume, V, can be easily linearized by taking the logarithm of both sides: $\log D = A \cdot \log V + B$. In previous studies we could observed that, for our kind of molecules, the results were equivalents for D-V than for D-FW analysis, so considering the approximation that the FW is proportional to V, we used the next equation to calculate the FW: $\log D = A' \cdot \log FW + B'$.[2]

The DOSY experiments have shown to be very sensitive to experimental conditions such as temperature fluctuation, convention or viscosity, which changes produce variations on the diffusion coefficient value from one experiment to another for the same particle.[3,4] This problem can be overcome by using internal standards of known size, by measuring their diffusion coefficients in the same experiment as the compound we are interested in, that way, it will be possible to generate a calibration curve giving information on the size in solution of the molecule in study.[4,5]

If we get r^2 values higher than 0.97 in the calibration curve, the typical error between the experimental FW and the theorical one would be from -10% to +10%.[6]

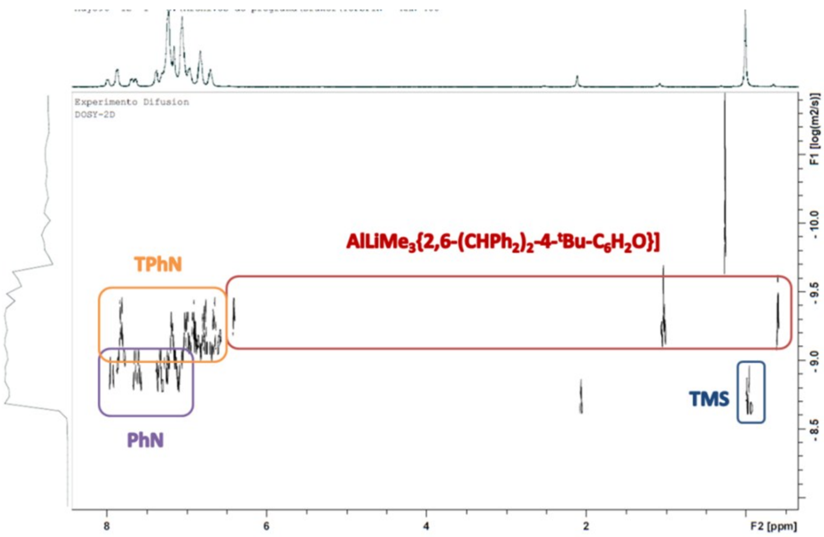
^{1}H DOSY of 1, 2a-c and 3a-c in the presence of internal standards:

In our case, the internal standards chosen were the compounds: 1,2,3,4-tetraphenylnaphthlene (TPhN, 432.55 g mol^{-1}); 1-phenylnaphthalene (PhN, 204.27 g mol^{-1}) and tetramethylsilane (TMS, 82.22 g mol^{-1}).

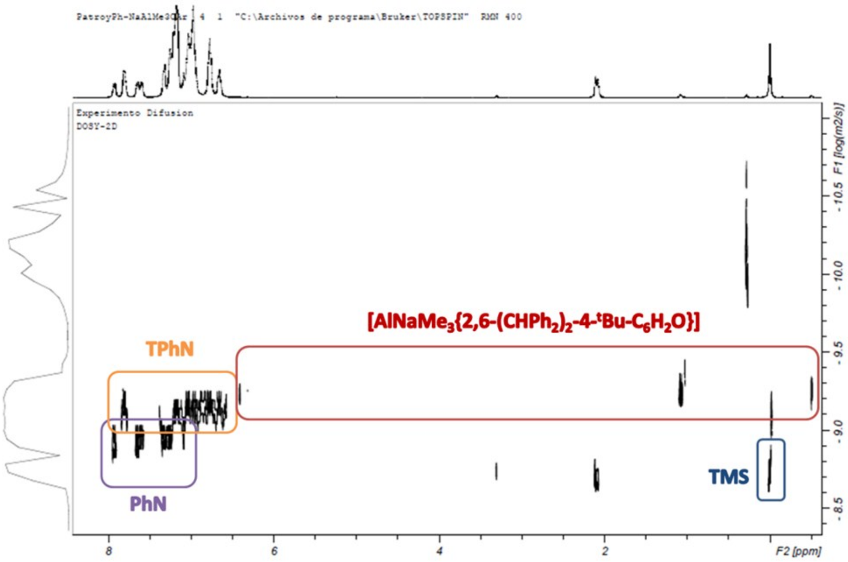
All NMR experiments were carried out on a Bruker AV400 spectrometer equipped with a probe PABBO BB-1H/D Z-GRD. 2D DOSY experiments were recorded under routine conditions at 298K with the bipolar-gradient LED (BPLED)[7] pulse sequence using a diffusion time of 100 ms and a LED delay of 5 ms. For each experiment, sine-shaped PFGs, with a duration of 1.5 ms followed by a recovery delay of 100 μs were incremented from 2% to 95% of the maximum strength in 16 equally spaced steps. The solvent used was C_6D_6.

Diffusion coefficients were calculated by fitting intensity data to the Stejskal-Tanner expression with estimates of errors taken from the variability in the calculated diffusion coefficients by consideration of different NMR responses for the same molecules of interest.

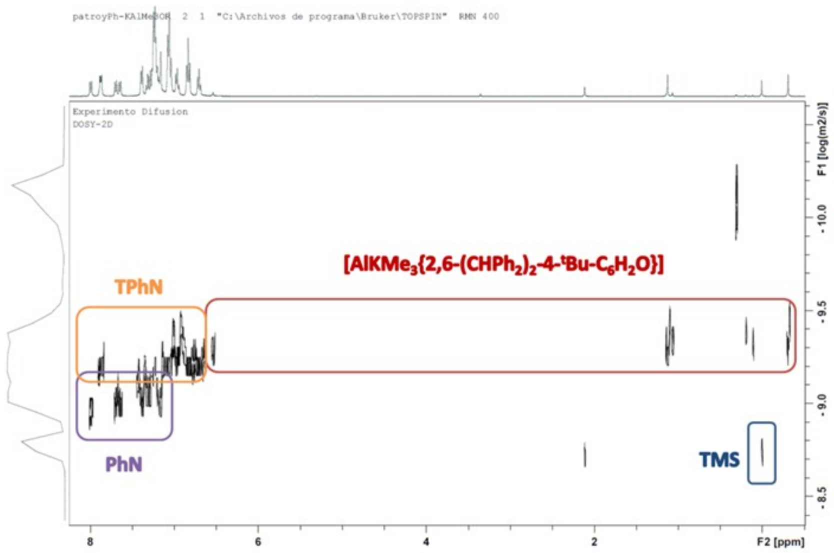
Figure S1 shows the DOSY experiment of the mixture of compounds **2a-c** or **3a-c** with TPhN, PhN and TMS that allow the determination of the translational self-diffusion coefficients (D) for all species in solution. Figure S2 shows the correlation diagrams between log D and log FW for the internal standard, and as we can observe, r^2 values are higher than 0.97, so we can apply these calibration curves in order to obtain the average size of each compound.



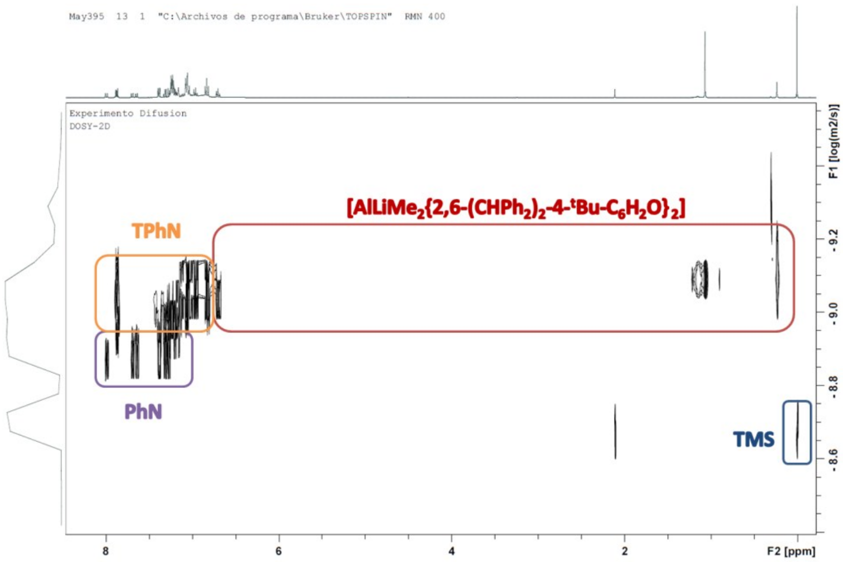
a)


Experimento Difusion
DOSY-2D
[AlNaMe$_3${2,6-(CHPh$_2$)$_2$-4-^{t}Bu-C$_6$H$_2$O}]
TPhN
PhN
TMS
F2 [ppm]
F1 [log(m2/s)]

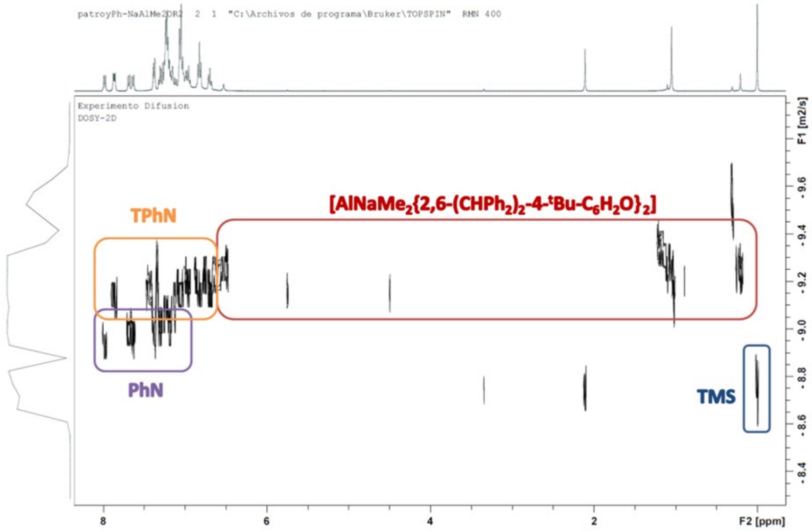
b)


Experimento Difusion
DOSY-2D
[AlKMe$_3${2,6-(CHPh$_2$)$_2$-4-^{t}Bu-C$_6$H$_2$O}]
TPhN
PhN
TMS
F2 [ppm]
F1 [log(m2/s)]

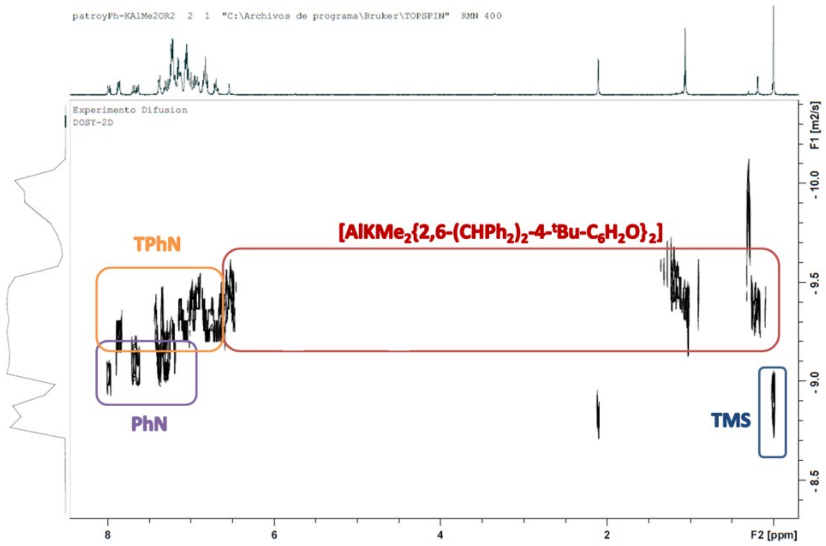
c)


Experimento Difusion
DOSY-2D
[AlLiMe$_2${2,6-(CHPh$_2$)$_2$-4-^{t}Bu-C$_6$H$_2$O}$_2$]
TPhN
PhN
TMS
F2 [ppm]
F1 [log(m2/s)]

d)

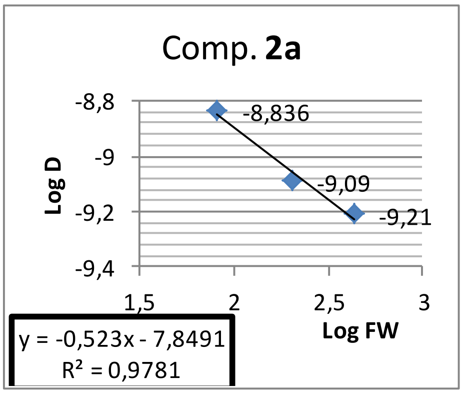


e)



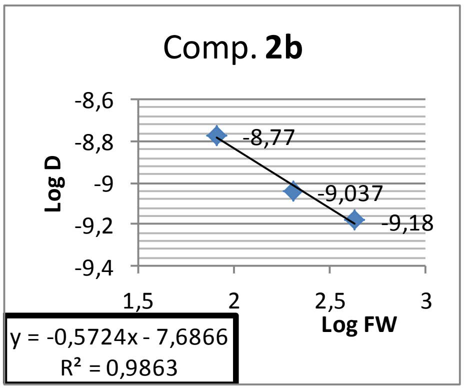
f)

Figure S1. 2D DOSY NMR experiments. The x- and y-axis represent the regular ^{1}H chemical shift and the relative diffusion rate, respectively. Mixture in C_6D_6 of TMS, PhN, TPhN and: a) **2a**. a) **2b**. c) **2c**. d) **3a**. e) **3b**. f) **3c**.



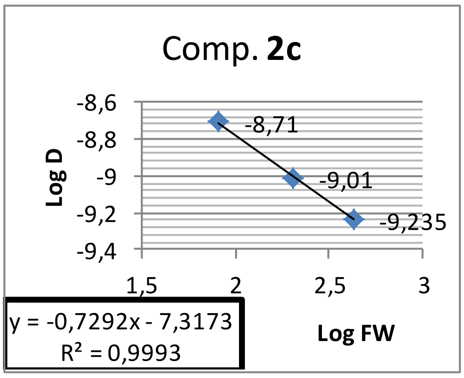
a)

	TMS	PhN	TPhN
log D	-8.770	-9.037	-9.180
log FW	1.91497747	2.31020459	2.63603632



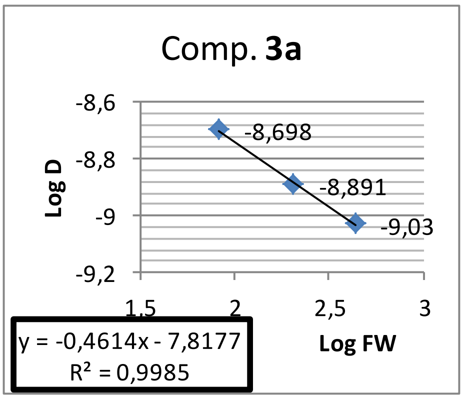
b)

	TMS	PhN	TPhN
log D	-8.836	-9.090	-9.210
log FW	1.91497747	2.31020459	2.63603632



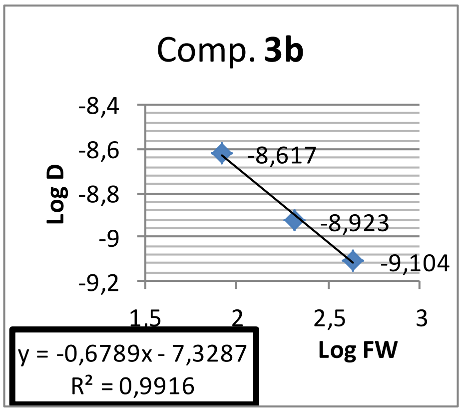
c)

	TMS	PhN	TPhN
log D	-8.710	-9.010	-9.235
log FW	1.91497747	2.31020459	2.63603632



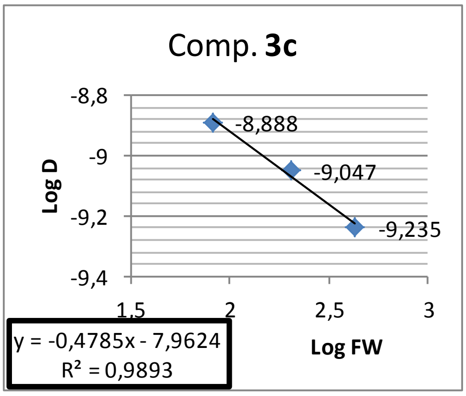
d)

	TMS	PhN	TPhN
log D	-8.698	-8.891	-9.030
log FW	1.91497747	2.31020459	2.63603632



e)

	TMS	PhN	TPhN
log D	-8.617	-8.923	-9.104
log FW	1.91497747	2.31020459	2.63603632



f)

	TMS	PhN	TPhN
log D	-8.888	-9.047	-9.235
log FW	1.91497747	2.31020459	2.63603632

Figure S2. Correlation between log D and log FW from the ^{1}H DOSY data for the mixture of TPhN, PhN, TMS and: a) **2a**. b) **2b**. b) **2c**. d) **3a**. e) **3b**. f) **3c**.

Table S1. D-FW analysis of ^{1}H DOSY data of **2a-c** and **3a-c**.

Compound	FW_{exp} (g mol^{-1})	log D	FW_t (g mol^{-1})	% error
2a	587	− 9.297	560.31	− 4.7%
2b	552	− 9.256	575.97	4.2%
2c	534	− 9.306	592.08	9.0%
3a	981	− 9.198	1026.66	4.4%
3b	985	− 9.361	1042.71	5.5%
3c	1107	− 9.419	1058.06	− 4.6%

As shown Table S1, complexes **2a-c** and **3a-c** are heterobimetallic in solution.

2. Glycidyl Methacrylate (GMA) polymerization studies

Polymerization of GMA with compounds 2a-c and 3a-c.

Monomer was purified by vacuum distillation using CaH_2 as dryer. Once it was purified, it was stored at −20 °C in the absence of light under Argon. Polymerization experiments were carried out in a range of different times. In one Teflon-valvulated flask of 50 mL the desired amount of catalyst was added and then 0.38 mL of GMA were added. The polymerization reactions were quenched by addition of 15 mL of Methanol. After 2 hours stirring, the polymer was filtered and then dried in a vacuum oven at 70 °C overnight. The PGMA obtained were characterized by IR. In Figure S3.b, the IR spectrum corresponding to the polymerization with 2a is shown, in it the signals corresponding to oxirane group are present (903 cm^{-1}), but the band for the acrylate group (1636 cm^{-1}) does not appear.

Combined Polymerization of Glycidyl Methacrylate.

Monomer was purified by vacuum distillation using CaH_2 as dryer. Once it was purified, it was stored at −20 °C in the absence of light under Argon. In one Teflon-valvulated flask of 50 mL inside of the glovebox 0.016 g (27.86 µmol) of [AlClMe{2,6-$(CHPh_2)_2$-4-^{t}Bu-C_6H_2O}] were added and then 0.38 mL (2.786 mmol) of GMA were added. After 30 minutes stirring at RT, 0.016 g (27.86 µmol) of **2** were added and the flask was heating at 100 °C for 7 h. The polymerization was quenched by addition of 15 mL of Methanol. After 2 hours stirring, the polymer was filtered and then dried in a vacuum oven at 70 °C overnight. The crosslinked Polyglycidyl Methacrylate obtained was characterized by IR (figure S3d). In the IR spectrum the signals corresponding to the acrylate group (1657 cm-1) has significantly reduced in comparison to the polymer obtained from ROP (figure S3c).

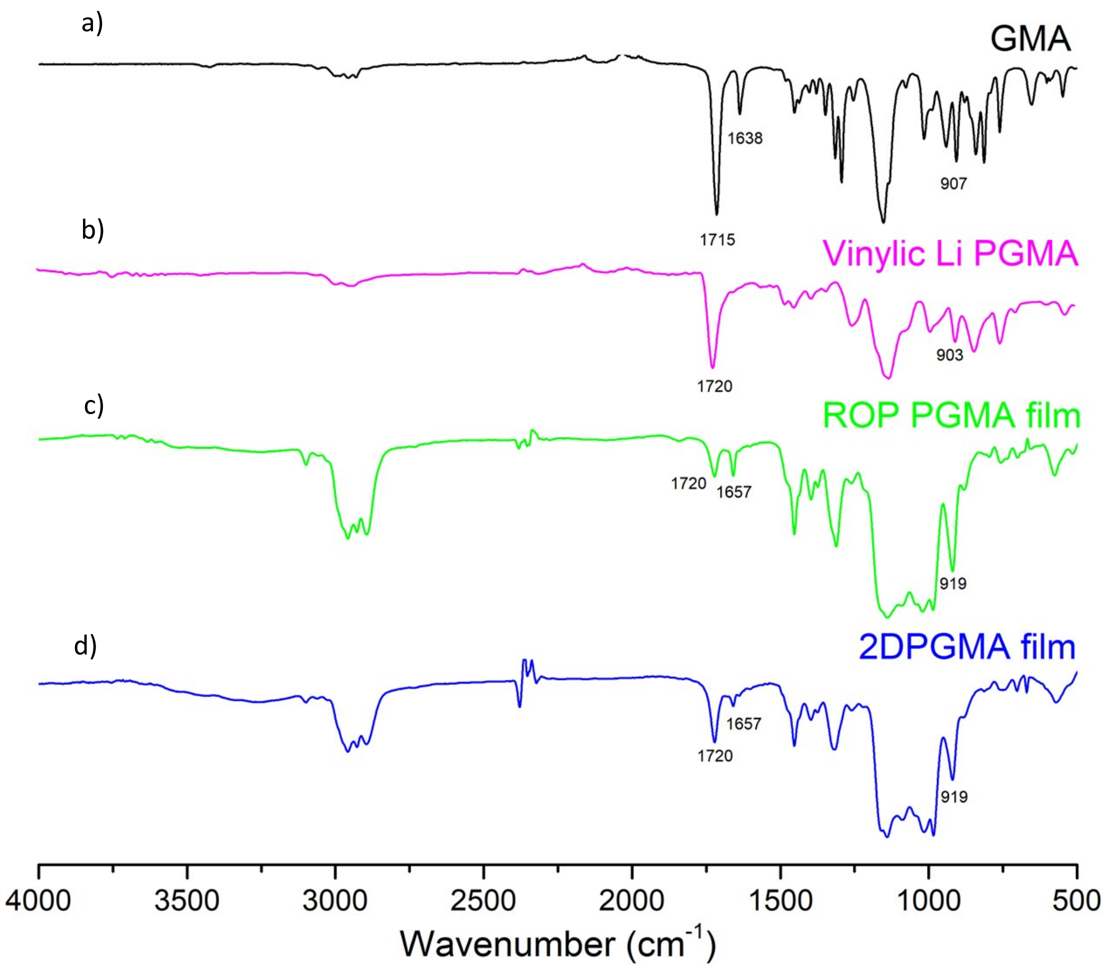


Figure S3. From top to bottom: a) IR spectra of: the monomer, GMA. b) The polymer obtained using as catalyst **2a** (vinylic Li PGMA): 1720 cm^{-1} corresponds to the tension for the ester, at 1130 cm^{-1} for the ether and at 903 cm−1 for the oxirane group, there is not any signal at 1638 cm^{-1} for the vinyl group. c) The polymer obtaining from ROP using the homometallic catalyst (ROP PGMA):[8] bands at 1720 cm^{-1} and 1638 cm^{-1} for the ester and the vinyl groups are present, but the signal for the oxirane group at 907 cm^{-1} is not observed. d) Polymer obtained from the combined polymerization of the homometallic and heterometallic catalyst (2DPGMA): the signal at 1720 cm^{-1} for the ester group is observed, while the one at 1657 cm^{-1} for the vinyl group has significantly reduced in comparison the initial polymer, ROP PGMA. Also, the band at 907 cm^{-1} for the oxirane group is not detected.

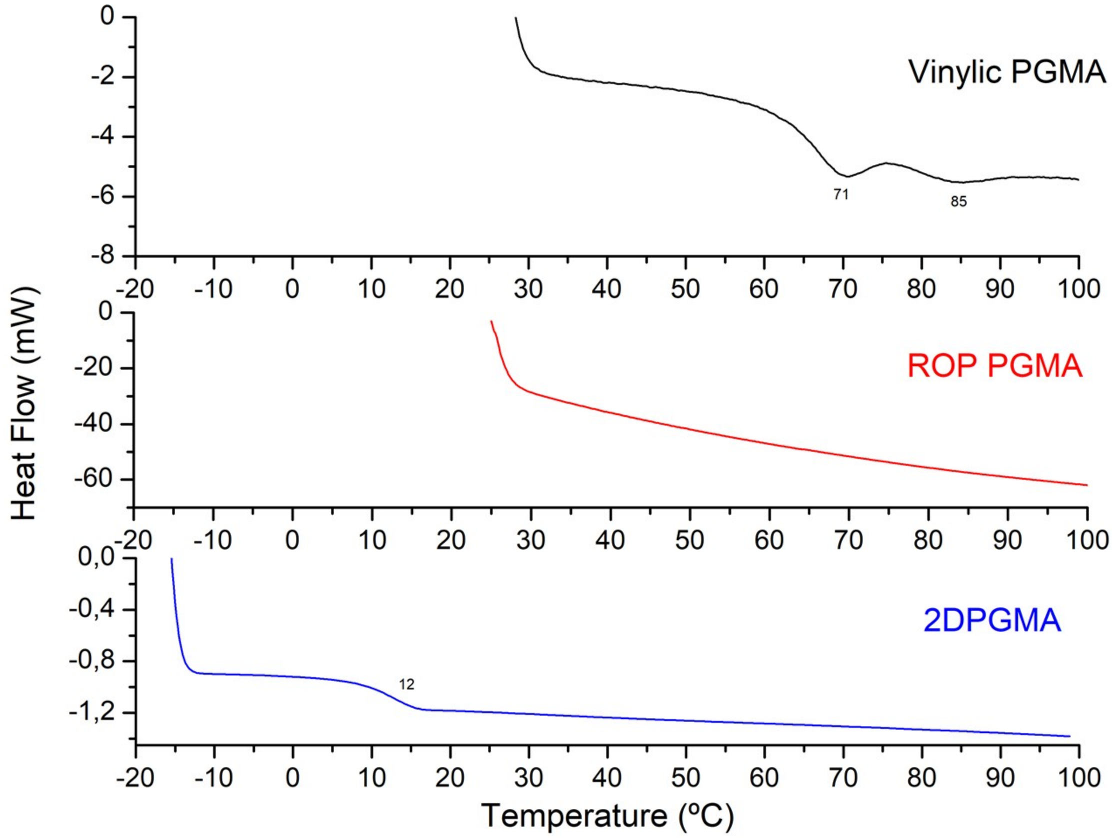


Figure S4. DSC-Profiles for the polymers obtained from vinyl polymerization (top, vinylic PGMA), ROP polymerization (middle, ROP PGMA)[8] and the combined polymerization using the homometallic and heterometallic catalysts (bottom, 2DPGMA).

3. Single-Crystal X-ray Data for $2a\cdot2C_7H_8$, $2b\cdot2C_7H_8$, $3b\cdot C_7H_8$ and $3c\cdot C_7H_8$.

Table S2 Crystallographic data for **$2a\cdot2C_7H_8$**, **$2b\cdot2C_7H_8$**, **$3b\cdot C_7H_8$** and **$3c\cdot C_7H_8$**.

	$2a\cdot2C_7H_8$	**$2b\cdot2C_7H_8$**	**$3b\cdot C_7H_8$**	**$3c\cdot C_7H_8$**
Empirical formula	$Li_2Al_2C_{78}H_{84}O\cdot 2C_7H_8$	$Na_2Al_2C_{78}H_{84}O\cdot 2C_7H_8$	$NaAlC_{74}H_{72}O_2\cdot C_7H_8$	$KAlC_{74}H_{72}O_2\cdot C_7H_8$
Formula weight	1305.55	1337.65	1135.42	1151.53
Color	Colorless	Colorless	Colorless	Colorless
Shape	Block	Prism	Prism	Block
Crystal size (mm)	0.49 x 0.42 x 0.40	0.49 x 0.33 x 0.32	0.30 x 0.25 x 0.13	0.43 x 0.41 x 0.37
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$	$P2_1/c$
a/b/c **(Å)**	15.5010(17)/ 10.2555(12)/ 30.557(4)	15.365(5)/ 9.989(3)/ 29.599(11)	10.356(5)/ 31.152(15)/ 21.128(10)	14.728(3)/ 24.467(4)/ 18.9575(16)
β (°)	98.606(8)	103.43(3)	102.94(4)	99.843(10)
V (Å^3)	4802.9(7)	4419(2)	6643(6)	6730.9(11)
Z	2	2	4	4
ρ_{calc} (g/cm^3)	0.903	0.867	1.135	1.138
μ (mm^{-1})/ F(000)	0.069/1400	0.083/1232	0.084/2424	0.138/2456
θ Range (°)	3.00-26.89	3.03-26.39	3.04-22.91	3.15-27.51
Reflns. Collected	69473	71329	17638	29613
R(int)	0.1994	0.2034	0.1841	0.0583
Data/restr/param	9454/0/387	9003/0/385	9097/0/766	15395/6/736
R_1/wR_2 (I > 2σ(I))^a	0.0993/0.2540	0.0871/0.2037	0.0757/0.1300	0.0717/0.1954
R_1/wR_2 (all data)^a	0.1501/ 0.2873	0.1356/ 0.2334	0.2300/ 0.1651	0.1327/ 0.2273
GOF	1.025	1032	0.925	1.024
Max/min Δρ (e.Å^{-3})	0.882/−0.417	0.382/−0.276	0.283/−0.233	0.853/−0.563

$R1 = \sum(||F_o|-|F_c||)/\sum|F_o|$; $wR2 = \{\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$; GOF = $\{\sum[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$

Figure S5. ORTEP plot of **2b** showing thermal ellipsoid plots (30% probability). Asymmetric unit (top). Packing (bottom).

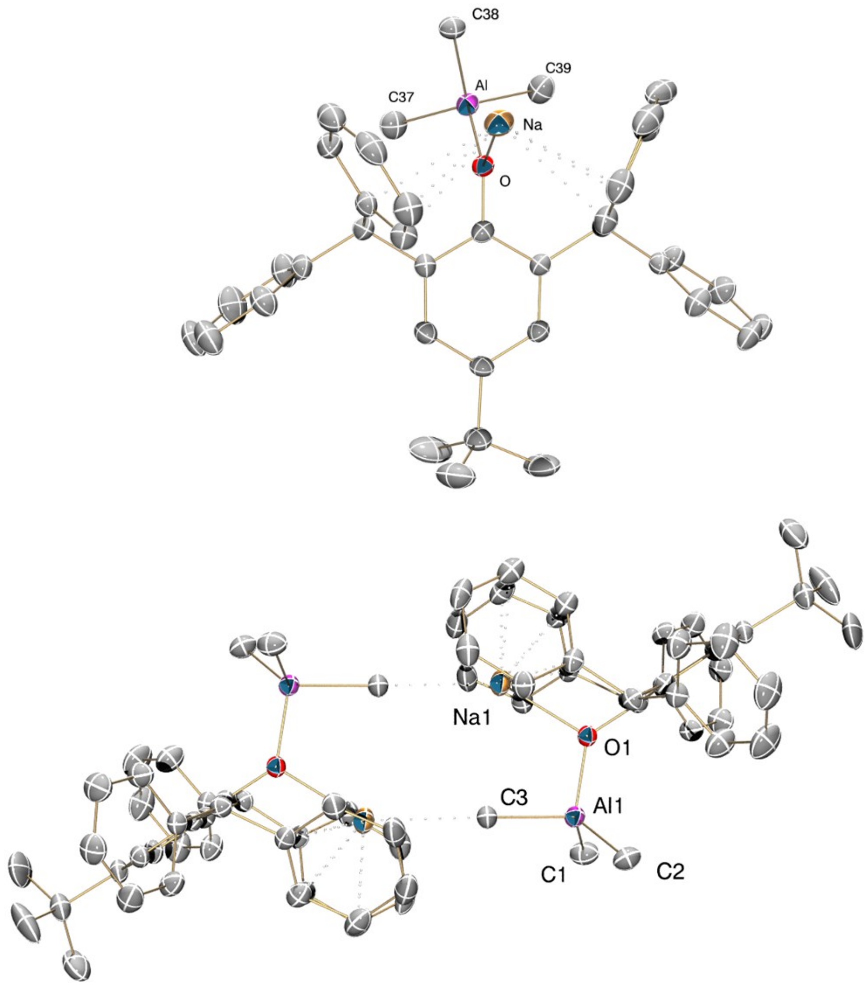


Table S3. Selected lengths (Å) for **2a**, **2b, 3b** and **3c**.

2a				**2b**			
Li1-O1	1.867(7)	**Al1-O1**	1.844(2)	**Na1-O1**	2.260(2)	**Al1-O1**	1.817(2)
Al1-C1	1.978(4)	**Al1-C3**	1.989(3)	**Al1-C1**	1.979(4)	**Al1-C3**	2.000(3)
Al1-C2	1.974(3)	**Li1···C3#1**	2.258(7)	**Al-C2**	1.987(4)	**Na1···C3#1**	2.731(3)
O1-C41	1.384(3)	**Li1···ct1**	2.742(7)	**O1-C4**	1.361(4)	**Na···ct1**	2.727(3)
		Li1···ct2	3.063(7)			**Na···ct2**	2.982(4)
3b				**3c**			
Na-O1	2.304(4)	**Na-O2**	2.316(4)	**K1-O1**	2.576(2)	**K1-O2**	2.9625(19)
Al1-C1	1.962(5)	**Al1-C2**	1.938(5)	**Al1-O1**	1.799(2)	**Al1-O2**	1.7934(19)
Al1-O1	1.801(3)	**Al1-O2**	1.806(3)	**Al1-C2**	1.962(3)	**Al1-C1**	1.981(3)
O1-C11	1.354(5)	**O2-C3**	1.365(5)	**O1-C3**	1.359(3)	**O2-C39**	1.368(3)
Na-C20	2.757(5)	**Na-C60**	2.711(5)	**K1···ct1**	2.909(3)	**K1···ct2**	2.8996(3)
Na-C21	2.814(6)	**Na-C61**	2.834(5)	**K1-C50**	3.102(3)	**K1-C20**	3.170(3)
Na-C25	3.041(6)	**Na-C65**	2.884(6)	**K1-C51**	3.334(4)	**K1-C21**	3.198(3)
Na···ct1	2.793(5)			**K1-C53**	3.344(3)	**K1-C22**	3.237(4)
Na···ct2	2.692(8)			**K1-C54**	3.112(3)	**K1-C23**	3.254(3)
				K1-C55	2.970(3)	**K1-C24**	3.216(3)
						K1-C25	3.170(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1. Ct = centroid.

Table S4. Bond lengths (Å) and angles (°) for compound **2a.**

Bond lengths (Å)			
C(1)-Al(1)	1.978(4)	C(19)-C(20)	1.392(6)
C(2)-Al(1)	1.974(4)	C(20)-C(22)	1.364(7)
C(3)-Al(1)	1.989(3)	C(22)-C(23)	1.372(7)
C(3)-Li(1)#1	2.258(7)	C(23)-C(24)	1.388(6)
C(4)-C(5)	1.371(6)	C(24)-Li(1)	2.568(8)
C(4)-C(43)	1.391(6)	C(25)-C(32)	1.518(6)
C(4)-C(7)	1.552(5)	C(25)-C(26)	1.519(5)
C(5)-C(6)	1.393(5)	C(26)-C(31)	1.380(6)
C(6)-C(41)	1.398(5)	C(26)-C(27)	1.392(7)
C(6)-C(25)	1.523(5)	C(27)-C(28)	1.394(7)
C(7)-C(10')	1.389(13)	C(28)-C(29)	1.372(9)
C(7)-C(8')	1.44(2)	C(29)-C(30)	1.364(9)
C(7)-C(8)	1.544(13)	C(30)-C(31)	1.393(7)
C(7)-C(9')	1.581(11)	C(32)-C(33)	1.377(6)
C(7)-C(9)	1.643(13)	C(32)-C(37)	1.399(5)
C(7)-C(10)	1.693(14)	C(33)-C(34)	1.384(6)
C(11)-C(42)	1.512(5)	C(34)-C(35)	1.403(8)
C(11)-C(18)	1.521(5)	C(35)-C(36)	1.339(8)
C(11)-C(12)	1.525(5)	C(36)-C(37)	1.360(7)
C(12)-C(17)	1.363(5)	C(41)-O(1)	1.383(4)
C(12)-C(13)	1.383(5)	C(41)-C(42)	1.395(5)
C(13)-C(14)	1.379(6)	C(41)-Li(1)	2.687(7)
C(14)-C(15)	1.352(7)	C(42)-C(43)	1.404(5)
C(15)-C(16)	1.372(7)	Al(1)-O(1)	1.844(2)
C(16)-C(17)	1.387(6)	Al(1)-Li(1)	3.267(7)
C(18)-C(24)	1.381(5)	Li(1)-O(1)	1.867(7)
C(18)-C(19)	1.389(5)	Li(1)-C(3)#1	2.258(7)
C(18)-Li(1)	2.741(8)		
Angles (°)			
Al(1)-C(3)-Li(1)#1	177.2(3)	C(29)-C(28)-C(27)	119.3(6)
C(5)-C(4)-C(43)	118.2(3)	C(30)-C(29)-C(28)	119.8(5)
C(5)-C(4)-C(7)	121.4(4)	C(29)-C(30)-C(31)	121.0(5)
C(43)-C(4)-C(7)	120.3(4)	C(26)-C(31)-C(30)	120.3(5)
C(4)-C(5)-C(6)	122.6(4)	C(33)-C(32)-C(37)	117.7(4)
C(5)-C(6)-C(41)	118.2(4)	C(33)-C(32)-C(25)	123.0(3)
C(5)-C(6)-C(25)	122.9(3)	C(37)-C(32)-C(25)	119.3(4)
C(41)-C(6)-C(25)	118.7(3)	C(32)-C(33)-C(34)	121.5(4)
C(10')-C(7)-C(8')	96.6(11)	C(33)-C(34)-C(35)	119.0(5)
C(10')-C(7)-C(4)	111.1(7)	C(36)-C(35)-C(34)	119.1(5)
C(8')-C(7)-C(4)	110.6(9)	C(35)-C(36)-C(37)	122.4(5)
C(8)-C(7)-C(4)	107.7(6)	C(36)-C(37)-C(32)	120.3(5)
C(10')-C(7)-C(9')	112.4(8)	O(1)-C(41)-C(42)	119.7(3)
C(8')-C(7)-C(9')	113.7(10)	O(1)-C(41)-C(6)	119.3(3)
C(4)-C(7)-C(9')	111.6(5)	C(42)-C(41)-C(6)	120.9(3)
C(8)-C(7)-C(9)	144.5(7)	O(1)-C(41)-Li(1)	40.53(19)
C(4)-C(7)-C(9)	107.5(6)	C(42)-C(41)-Li(1)	109.9(3)
C(8)-C(7)-C(10)	89.9(7)	C(6)-C(41)-Li(1)	111.2(3)
C(4)-C(7)-C(10)	106.9(6)	C(41)-C(42)-C(43)	118.3(3)
C(9)-C(7)-C(10)	83.9(7)	C(41)-C(42)-C(11)	118.7(3)
C(42)-C(11)-C(18)	112.5(3)	C(43)-C(42)-C(11)	123.0(3)
C(42)-C(11)-C(12)	113.4(3)	C(4)-C(43)-C(42)	121.6(4)
C(18)-C(11)-C(12)	111.4(3)	O(1)-Al(1)-C(2)	112.04(14)
C(17)-C(12)-C(13)	118.0(4)	O(1)-Al(1)-C(1)	111.48(15)
C(17)-C(12)-C(11)	120.3(3)	C(2)-Al(1)-C(1)	110.93(19)
C(13)-C(12)-C(11)	121.8(3)	O(1)-Al(1)-C(3)	100.10(13)
C(14)-C(13)-C(12)	120.5(4)	C(2)-Al(1)-C(3)	110.17(15)

C(15)-C(14)-C(13)	121.4(5)	C(1)-Al(1)-C(3)	111.70(18)
C(14)-C(15)-C(16)	118.6(4)	O(1)-Al(1)-Li(1)	28.49(12)
C(15)-C(16)-C(17)	120.4(5)	C(2)-Al(1)-Li(1)	117.45(18)
C(12)-C(17)-C(16)	121.1(4)	C(1)-Al(1)-Li(1)	126.4(2)
C(24)-C(18)-C(19)	118.1(3)	C(3)-Al(1)-Li(1)	72.00(14)
C(24)-C(18)-C(11)	122.6(3)	O(1)-Li(1)-C(3)#1	138.1(3)
C(19)-C(18)-C(11)	119.3(3)	O(1)-Li(1)-C(24)	97.4(3)
C(24)-C(18)-Li(1)	68.1(2)	C(3)#1-Li(1)-C(24)	117.2(3)
C(19)-C(18)-Li(1)	96.2(3)	O(1)-Li(1)-C(41)	28.78(13)
C(11)-C(18)-Li(1)	106.9(3)	C(3)#1-Li(1)-C(41)	164.7(3)
C(18)-C(19)-C(20)	120.4(4)	C(24)-Li(1)-C(41)	77.79(19)
C(22)-C(20)-C(19)	120.4(4)	O(1)-Li(1)-C(18)	77.0(2)
C(20)-C(22)-C(23)	120.1(4)	C(3)#1-Li(1)-C(18)	122.4(3)
C(22)-C(23)-C(24)	119.8(4)	C(24)-Li(1)-C(18)	29.92(13)
C(18)-C(24)-C(23)	121.3(4)	C(41)-Li(1)-C(18)	68.70(18)
C(18)-C(24)-Li(1)	82.0(3)	O(1)-Li(1)-Al(1)	28.11(12)
C(23)-C(24)-Li(1)	90.5(3)	C(3)#1-Li(1)-Al(1)	110.6(2)
C(32)-C(25)-C(26)	112.7(3)	C(24)-Li(1)-Al(1)	115.0(2)
C(32)-C(25)-C(6)	111.5(3)	C(41)-Li(1)-Al(1)	56.89(14)
C(26)-C(25)-C(6)	112.9(3)	C(18)-Li(1)-Al(1)	87.3(2)
C(31)-C(26)-C(27)	117.8(4)	C(41)-O(1)-Al(1)	125.9(2)
C(31)-C(26)-C(25)	122.3(4)	C(41)-O(1)-Li(1)	110.7(3)
C(27)-C(26)-C(25)	119.6(4)	Al(1)-O(1)-Li(1)	123.4(2)
C(26)-C(27)-C(28)	121.5(6)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1.

Table S5. Bond lengths (Å) and angles (°) for compound **2b.**

Al(1)-O(1)	1.817(2)	C(14)-C(15)	1.399(5)
Al(1)-C(1)	1.979(4)	C(14)-C(50)	1.519(4)
Al(1)-C(2)	1.987(4)	C(15)-C(16)	1.385(5)
Al(1)-C(3)	2.000(3)	C(16)-C(17)	1.371(6)
Al(1)-Na(1)	3.401(2)	C(17)-C(18)	1.382(6)
Na(1)-O(1)	2.260(2)	C(18)-C(19)	1.389(5)
Na(1)-C(3)#1	2.731(3)	C(21)-C(22)	1.379(5)
Na(1)-C(19)	2.853(4)	C(21)-C(26)	1.396(4)
Na(1)-C(18)	2.919(4)	C(21)-C(30)	1.518(4)
Na(1)-C(14)	3.003(3)	C(22)-C(23)	1.391(5)
Na(1)-C(22)	3.004(4)	C(23)-C(24)	1.372(6)
Na(1)-C(21)	3.078(3)	C(24)-C(25)	1.363(6)
Na(1)-C(4)	3.101(3)	C(25)-C(26)	1.388(5)
Na(1)-C(17)	3.109(4)	C(30)-C(31)	1.532(4)
O(1)-C(4)	1.361(4)	C(31)-C(32)	1.359(5)
C(4)-C(9)	1.393(4)	C(31)-C(36)	1.374(5)
C(4)-C(5)	1.398(4)	C(32)-C(33)	1.400(5)
C(5)-C(6)	1.389(4)	C(33)-C(34)	1.357(6)
C(5)-C(50)	1.531(4)	C(34)-C(35)	1.355(6)
C(6)-C(7)	1.388(4)	C(35)-C(36)	1.384(6)
C(7)-C(8)	1.386(4)	C(50)-C(51)	1.526(4)
C(7)-C(10)	1.536(5)	C(51)-C(56)	1.370(4)
C(8)-C(9)	1.389(4)	C(51)-C(52)	1.371(4)
C(9)-C(30)	1.519(4)	C(52)-C(53)	1.393(5)
C(10)-C(11)	1.506(6)	C(53)-C(54)	1.369(5)
C(10)-C(12)	1.515(6)	C(54)-C(55)	1.359(5)
C(10)-C(13)	1.523(6)	C(55)-C(56)	1.392(5)
C(14)-C(19)	1.375(5)		
Angles (°)			

O(1)-Al(1)-C(1)	112.48(14)	C(8)-C(9)-C(30)	121.9(3)
O(1)-Al(1)-C(2)	112.12(14)	C(4)-C(9)-C(30)	119.1(3)
C(1)-Al(1)-C(2)	110.87(17)	C(11)-C(10)-C(12)	109.1(4)
O(1)-Al(1)-C(3)	99.06(12)	C(11)-C(10)-C(13)	108.5(4)
C(1)-Al(1)-C(3)	109.75(17)	C(12)-C(10)-C(13)	109.9(4)
C(2)-Al(1)-C(3)	112.04(16)	C(11)-C(10)-C(7)	111.3(3)
O(1)-Al(1)-Na(1)	37.84(7)	C(12)-C(10)-C(7)	108.5(3)
C(1)-Al(1)-Na(1)	116.01(13)	C(13)-C(10)-C(7)	109.5(3)
C(2)-Al(1)-Na(1)	131.68(12)	C(19)-C(14)-C(15)	117.8(3)
C(3)-Al(1)-Na(1)	62.07(10)	C(19)-C(14)-C(50)	123.2(3)
O(1)-Na(1)-C(3)#1	146.34(10)	C(15)-C(14)-C(50)	119.0(3)
O(1)-Na(1)-C(19)	83.21(9)	C(19)-C(14)-Na(1)	70.41(18)
C(3)#1-Na(1)-C(19)	124.71(11)	C(15)-C(14)-Na(1)	85.04(19)
O(1)-Na(1)-C(18)	110.85(10)	C(50)-C(14)-Na(1)	114.00(18)
C(3)#1-Na(1)-C(18)	97.53(12)	C(16)-C(15)-C(14)	120.5(4)
C(19)-Na(1)-C(18)	27.82(10)	C(16)-C(15)-H(15)	119.7
O(1)-Na(1)-C(14)	66.21(8)	C(14)-C(15)-H(15)	119.7
C(3)#1-Na(1)-C(14)	129.86(11)	C(17)-C(16)-C(15)	120.4(4)
C(19)-Na(1)-C(14)	27.01(9)	C(17)-C(16)-H(16)	119.8
C(18)-Na(1)-C(14)	48.18(10)	C(15)-C(16)-H(16)	119.8
O(1)-Na(1)-C(22)	84.26(9)	C(16)-C(17)-C(18)	120.1(4)
C(3)#1-Na(1)-C(22)	112.62(11)	C(16)-C(17)-Na(1)	83.2(2)
C(19)-Na(1)-C(22)	87.36(11)	C(18)-C(17)-Na(1)	69.2(2)
C(18)-Na(1)-C(22)	93.22(12)	C(16)-C(17)-H(17)	119.9
C(14)-Na(1)-C(22)	105.62(10)	C(18)-C(17)-H(17)	119.9
O(1)-Na(1)-C(21)	69.69(9)	Na(1)-C(17)-H(17)	118.4
C(3)#1-Na(1)-C(21)	112.69(11)	C(17)-C(18)-C(19)	119.0(4)
C(19)-Na(1)-C(21)	106.48(11)	C(17)-C(18)-Na(1)	84.5(2)
C(18)-Na(1)-C(21)	118.38(12)	C(19)-C(18)-Na(1)	73.4(2)
C(14)-Na(1)-C(21)	115.93(10)	C(17)-C(18)-H(18)	120.5
C(22)-Na(1)-C(21)	26.18(9)	C(19)-C(18)-H(18)	120.5
O(1)-Na(1)-C(4)	23.33(8)	Na(1)-C(18)-H(18)	112.0
C(3)#1-Na(1)-C(4)	167.35(10)	C(14)-C(19)-C(18)	122.0(4)
C(19)-Na(1)-C(4)	67.79(10)	C(14)-C(19)-Na(1)	82.58(19)
C(18)-Na(1)-C(4)	95.10(10)	C(18)-C(19)-Na(1)	78.8(2)
C(14)-Na(1)-C(4)	59.83(9)	C(14)-C(19)-H(19)	119.0
C(22)-Na(1)-C(4)	67.17(9)	C(18)-C(19)-H(19)	119.0
C(21)-Na(1)-C(4)	61.08(9)	Na(1)-C(19)-H(19)	109.5
O(1)-Na(1)-C(17)	119.84(10)	C(22)-C(21)-C(26)	117.9(3)
C(3)#1-Na(1)-C(17)	79.22(11)	C(22)-C(21)-C(30)	123.3(3)
C(19)-Na(1)-C(17)	46.99(11)	C(26)-C(21)-C(30)	118.8(3)
C(18)-Na(1)-C(17)	26.27(11)	C(22)-C(21)-Na(1)	73.9(2)
C(14)-Na(1)-C(17)	54.29(10)	C(26)-C(21)-Na(1)	89.1(2)
C(22)-Na(1)-C(17)	117.64(13)	C(30)-C(21)-Na(1)	106.58(18)
C(21)-Na(1)-C(17)	143.66(12)	C(21)-C(22)-C(23)	121.2(3)
C(4)-Na(1)-C(17)	112.46(10)	C(21)-C(22)-Na(1)	79.9(2)
O(1)-Na(1)-Al(1)	29.56(6)	C(23)-C(22)-Na(1)	85.4(2)
C(3)#1-Na(1)-Al(1)	117.12(8)	C(21)-C(22)-H(22)	119.4
C(19)-Na(1)-Al(1)	105.02(8)	C(24)-C(23)-C(22)	120.3(4)
C(18)-Na(1)-Al(1)	129.20(9)	C(25)-C(24)-C(23)	119.3(3)
C(14)-Na(1)-Al(1)	81.10(7)	C(24)-C(25)-C(26)	121.1(4)
C(22)-Na(1)-Al(1)	104.85(8)	C(25)-C(26)-C(21)	120.3(3)
C(21)-Na(1)-Al(1)	82.59(7)	C(21)-C(30)-C(9)	110.5(3)
C(4)-Na(1)-Al(1)	52.86(6)	C(21)-C(30)-C(31)	113.7(3)
C(17)-Na(1)-Al(1)	123.90(10)	C(9)-C(30)-C(31)	112.3(2)
C(4)-O(1)-Al(1)	131.66(18)	C(32)-C(31)-C(36)	118.4(3)
C(4)-O(1)-Na(1)	115.56(17)	C(32)-C(31)-C(30)	123.5(3)
Al(1)-O(1)-Na(1)	112.59(10)	C(36)-C(31)-C(30)	118.1(3)
O(1)-C(4)-C(9)	119.5(3)	C(31)-C(32)-C(33)	120.8(4)
O(1)-C(4)-C(5)	120.0(3)	C(34)-C(33)-C(32)	120.1(4)

C(9)-C(4)-C(5)	120.3(3)	C(35)-C(34)-C(33)	119.2(4)
O(1)-C(4)-Na(1)	41.10(12)	C(34)-C(35)-C(36)	120.9(4)
C(9)-C(4)-Na(1)	109.07(19)	C(31)-C(36)-C(35)	120.5(4)
C(5)-C(4)-Na(1)	111.8(2)	C(14)-C(50)-C(51)	112.3(2)
C(6)-C(5)-C(4)	118.6(3)	C(14)-C(50)-C(5)	110.3(2)
C(6)-C(5)-C(50)	123.5(3)	C(51)-C(50)-C(5)	113.8(2)
C(4)-C(5)-C(50)	117.9(3)	C(56)-C(51)-C(52)	118.5(3)
C(7)-C(6)-C(5)	122.4(3)	C(56)-C(51)-C(50)	119.1(3)
C(8)-C(7)-C(6)	117.4(3)	C(52)-C(51)-C(50)	122.3(3)
C(8)-C(7)-C(10)	119.2(3)	C(51)-C(52)-C(53)	120.8(3)
C(6)-C(7)-C(10)	123.4(3)	C(54)-C(53)-C(52)	119.6(3)
C(7)-C(8)-C(9)	122.3(3)	C(55)-C(54)-C(53)	120.2(3)
C(8)-C(9)-C(4)	118.9(3)	C(54)-C(55)-C(56)	119.9(4)
		C(51)-C(56)-C(55)	120.9(3)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z.

Table S6. Bond lengths (Å) and angles (°) for compound **3b.**

Bond lengths (Å)			
Na(1)-O(1)	2.304(4)	C(26)-C(29)	1.508(7)
Na(1)-O(2)	2.316(4)	C(26)-C(27)	1.526(7)
Na(1)-C(60)	2.711(5)	C(26)-C(28)	1.513(7)
Na(1)-C(20)	2.757(5)	C(30)-C(31)	1.378(6)
Na(1)-C(21)	2.814(6)	C(30)-C(35)	1.384(7)
Na(1)-C(61)	2.834(5)	C(31)-C(32)	1.376(7)
Na(1)-C(65)	2.884(6)	C(32)-C(33)	1.381(7)
Na(1)-C(25)	3.041(6)	C(33)-C(34)	1.368(7)
Na(1)-Al(1)	3.148(3)	C(34)-C(35)	1.380(7)
Al(1)-O(2)	1.806(3)	C(40)-C(41)	1.362(7)
Al(1)-O(1)	1.801(3)	C(40)-C(45)	1.368(7)
Al(1)-C(2)	1.938(5)	C(41)-C(42)	1.400(7)
Al(1)-C(1)	1.962(5)	C(42)-C(43)	1.350(7)
O(1)-C(11)	1.354(5)	C(43)-C(44)	1.368(7)
O(2)-C(3)	1.365(5)	C(44)-C(45)	1.386(7)
C(3)-C(4)	1.402(6)	C(50)-C(55)	1.381(7)
C(3)-C(8)	1.409(6)	C(50)-C(51)	1.362(7)
C(4)-C(5)	1.397(6)	C(51)-C(52)	1.398(8)
C(4)-C(9)	1.516(6)	C(52)-C(53)	1.352(8)
C(5)-C(6)	1.392(6)	C(53)-C(54)	1.367(9)
C(6)-C(7)	1.391(6)	C(54)-C(55)	1.379(8)
C(6)-C(66)	1.518(7)	C(60)-C(65)	1.384(6)
C(7)-C(8)	1.376(6)	C(60)-C(61)	1.371(6)
C(8)-C(10)	1.498(6)	C(61)-C(62)	1.399(7)
C(9)-C(80)	1.508(7)	C(62)-C(63)	1.367(7)
C(9)-C(90)	1.511(7)	C(63)-C(64)	1.365(8)
C(10)-C(60)	1.518(7)	C(64)-C(65)	1.391(7)
C(10)-C(70)	1.515(6)	C(66)-C(68)	1.499(7)
C(11)-C(16)	1.397(6)	C(66)-C(67)	1.504(7)
C(11)-C(12)	1.424(6)	C(66)-C(69)	1.569(7)
C(12)-C(13)	1.394(6)	C(70)-C(71)	1.359(7)
C(12)-C(18)	1.518(6)	C(70)-C(75)	1.388(6)
C(13)-C(14)	1.365(6)	C(71)-C(72)	1.386(7)
C(14)-C(15)	1.400(6)	C(72)-C(73)	1.377(7)
C(14)-C(26)	1.519(6)	C(73)-C(74)	1.352(7)
C(15)-C(16)	1.391(6)	C(74)-C(75)	1.368(7)
C(16)-C(17)	1.520(6)	C(80)-C(85)	1.385(7)
C(17)-C(40)	1.527(7)	C(80)-C(81)	1.401(7)

C(17)-C(50)	1.529(7)	C(81)-C(82)	1.374(7)
C(18)-C(30)	1.517(6)	C(82)-C(83)	1.367(7)
C(18)-C(20)	1.542(6)	C(83)-C(84)	1.371(7)
C(20)-C(25)	1.374(6)	C(84)-C(85)	1.384(7)
C(20)-C(21)	1.375(6)	C(90)-C(91)	1.380(7)
C(21)-C(22)	1.390(7)	C(90)-C(95)	1.401(7)
C(22)-C(23)	1.364(7)	C(91)-C(92)	1.372(8)
C(23)-C(24)	1.350(7)	C(92)-C(93)	1.384(9)
C(24)-C(25)	1.401(7)	C(93)-C(94)	1.356(8)
		C(94)-C(95)	1.365(7)
Angles (°)			
O(1)-Na(1)-O(2)	68.85(12)	C(30)-C(18)-C(20)	111.6(4)
O(1)-Na(1)-C(60)	117.08(17)	C(12)-C(18)-C(20)	111.5(4)
O(2)-Na(1)-C(60)	75.39(14)	C(25)-C(20)-C(21)	118.7(5)
O(1)-Na(1)-C(20)	77.25(15)	C(25)-C(20)-C(18)	122.2(5)
O(2)-Na(1)-C(20)	115.82(16)	C(21)-C(20)-C(18)	119.1(5)
C(60)-Na(1)-C(20)	165.09(18)	C(25)-C(20)-Na(1)	88.2(3)
O(1)-Na(1)-C(21)	100.15(16)	C(21)-C(20)-Na(1)	78.0(3)
O(2)-Na(1)-C(21)	109.68(15)	C(18)-C(20)-Na(1)	102.7(3)
C(60)-Na(1)-C(21)	140.76(19)	C(20)-C(21)-C(22)	121.4(5)
C(20)-Na(1)-C(21)	28.55(13)	C(20)-C(21)-Na(1)	73.4(3)
O(1)-Na(1)-C(61)	140.67(17)	C(22)-C(21)-Na(1)	92.0(3)
O(2)-Na(1)-C(61)	79.53(15)	C(23)-C(22)-C(21)	118.5(6)
C(60)-Na(1)-C(61)	28.52(14)	C(22)-C(23)-C(24)	121.8(6)
C(20)-Na(1)-C(61)	139.71(19)	C(23)-C(24)-C(25)	119.4(6)
C(21)-Na(1)-C(61)	112.44(19)	C(20)-C(25)-C(24)	120.2(5)
O(1)-Na(1)-C(65)	112.95(16)	C(20)-C(25)-Na(1)	65.0(3)
O(2)-Na(1)-C(65)	98.97(17)	C(24)-C(25)-Na(1)	91.8(3)
C(60)-Na(1)-C(65)	28.43(13)	C(29)-C(26)-C(14)	113.6(5)
C(20)-Na(1)-C(65)	144.80(19)	C(29)-C(26)-C(27)	108.0(4)
C(21)-Na(1)-C(65)	142.35(19)	C(14)-C(26)-C(27)	108.4(4)
C(61)-Na(1)-C(65)	48.76(16)	C(29)-C(26)-C(28)	107.4(5)
O(1)-Na(1)-C(25)	82.04(14)	C(14)-C(26)-C(28)	110.5(4)
O(2)-Na(1)-C(25)	139.53(15)	C(27)-C(26)-C(28)	108.8(5)
C(60)-Na(1)-C(25)	144.76(17)	C(31)-C(30)-C(35)	116.6(5)
C(20)-Na(1)-C(25)	26.85(13)	C(31)-C(30)-C(18)	124.2(5)
C(21)-Na(1)-C(25)	47.45(15)	C(35)-C(30)-C(18)	119.2(5)
C(61)-Na(1)-C(25)	136.47(17)	C(30)-C(31)-C(32)	121.8(5)
C(65)-Na(1)-C(25)	118.47(19)	C(31)-C(32)-C(33)	120.0(6)
O(1)-Na(1)-Al(1)	34.38(9)	C(34)-C(33)-C(32)	119.9(6)
O(2)-Na(1)-Al(1)	34.55(8)	C(33)-C(34)-C(35)	118.9(6)
C(60)-Na(1)-Al(1)	95.82(14)	C(34)-C(35)-C(30)	122.8(6)
C(20)-Na(1)-Al(1)	98.79(13)	C(41)-C(40)-C(45)	118.3(5)
C(21)-Na(1)-Al(1)	109.76(14)	C(41)-C(40)-C(17)	123.6(5)
C(61)-Na(1)-Al(1)	110.38(14)	C(45)-C(40)-C(17)	118.0(5)
C(65)-Na(1)-Al(1)	107.70(15)	C(40)-C(41)-C(42)	120.1(6)
C(25)-Na(1)-Al(1)	112.94(13)	C(43)-C(42)-C(41)	120.3(6)
O(2)-Al(1)-O(1)	92.75(15)	C(42)-C(43)-C(44)	120.6(6)
O(2)-Al(1)-C(2)	117.40(19)	C(45)-C(44)-C(43)	118.3(6)
O(1)-Al(1)-C(2)	108.9(2)	C(44)-C(45)-C(40)	122.2(6)
O(2)-Al(1)-C(1)	107.77(19)	C(55)-C(50)-C(51)	118.7(6)
O(1)-Al(1)-C(1)	118.01(19)	C(55)-C(50)-C(17)	118.9(6)
C(2)-Al(1)-C(1)	111.2(2)	C(51)-C(50)-C(17)	122.4(5)
O(2)-Al(1)-Na(1)	46.63(11)	C(50)-C(51)-C(52)	119.0(6)
O(1)-Al(1)-Na(1)	46.23(11)	C(53)-C(52)-C(51)	121.6(7)
C(2)-Al(1)-Na(1)	127.16(19)	C(52)-C(53)-C(54)	120.0(7)
C(1)-Al(1)-Na(1)	121.64(17)	C(53)-C(54)-C(55)	118.7(7)
C(11)-O(1)-Al(1)	128.4(3)	C(50)-C(55)-C(54)	122.0(6)
C(11)-O(1)-Na(1)	129.6(3)	C(65)-C(60)-C(61)	117.9(5)

Al(1)-O(1)-Na(1)	99.40(15)	C(65)-C(60)-C(10)	118.2(5)
C(3)-O(2)-Al(1)	124.9(3)	C(61)-C(60)-C(10)	123.8(5)
C(3)-O(2)-Na(1)	131.6(3)	C(65)-C(60)-Na(1)	82.7(3)
Al(1)-O(2)-Na(1)	98.82(15)	C(61)-C(60)-Na(1)	80.7(3)
O(2)-C(3)-C(4)	119.9(5)	C(10)-C(60)-Na(1)	106.6(3)
O(2)-C(3)-C(8)	119.8(5)	C(60)-C(61)-C(62)	121.4(5)
C(4)-C(3)-C(8)	120.3(5)	C(60)-C(61)-Na(1)	70.8(3)
C(3)-C(4)-C(5)	118.1(5)	C(62)-C(61)-Na(1)	89.4(3)
C(3)-C(4)-C(9)	120.2(5)	C(63)-C(62)-C(61)	119.4(5)
C(5)-C(4)-C(9)	121.7(5)	C(62)-C(63)-C(64)	120.5(6)
C(6)-C(5)-C(4)	123.2(5)	C(65)-C(64)-C(63)	119.7(6)
C(5)-C(6)-C(7)	115.9(4)	C(64)-C(65)-C(60)	121.2(6)
C(5)-C(6)-C(66)	122.3(5)	C(64)-C(65)-Na(1)	90.4(4)
C(7)-C(6)-C(66)	121.8(5)	C(60)-C(65)-Na(1)	68.8(3)
C(6)-C(7)-C(8)	124.0(5)	C(68)-C(66)-C(67)	108.8(5)
C(7)-C(8)-C(3)	118.2(5)	C(68)-C(66)-C(6)	110.0(5)
C(7)-C(8)-C(10)	122.8(5)	C(67)-C(66)-C(6)	113.8(5)
C(3)-C(8)-C(10)	118.9(5)	C(68)-C(66)-C(69)	107.7(5)
C(80)-C(9)-C(4)	113.1(4)	C(67)-C(66)-C(69)	107.8(5)
C(80)-C(9)-C(90)	110.9(4)	C(6)-C(66)-C(69)	108.6(5)
C(4)-C(9)-C(90)	113.3(4)	C(71)-C(70)-C(75)	117.1(5)
C(60)-C(10)-C(8)	111.9(4)	C(71)-C(70)-C(10)	119.8(5)
C(60)-C(10)-C(70)	110.1(4)	C(75)-C(70)-C(10)	123.1(5)
C(8)-C(10)-C(70)	115.3(4)	C(70)-C(71)-C(72)	122.5(5)
O(1)-C(11)-C(16)	122.2(5)	C(73)-C(72)-C(71)	118.8(6)
O(1)-C(11)-C(12)	119.7(5)	C(74)-C(73)-C(72)	119.7(6)
C(16)-C(11)-C(12)	117.9(5)	C(73)-C(74)-C(75)	120.9(5)
C(13)-C(12)-C(11)	119.3(5)	C(74)-C(75)-C(70)	121.1(5)
C(13)-C(12)-C(18)	122.9(5)	C(85)-C(80)-C(81)	115.9(5)
C(11)-C(12)-C(18)	117.8(5)	C(85)-C(80)-C(9)	123.4(5)
C(14)-C(13)-C(12)	123.5(5)	C(81)-C(80)-C(9)	120.5(5)
C(15)-C(14)-C(13)	116.5(4)	C(82)-C(81)-C(80)	123.2(5)
C(15)-C(14)-C(26)	121.7(5)	C(81)-C(82)-C(83)	119.0(6)
C(13)-C(14)-C(26)	121.7(5)	C(82)-C(83)-C(84)	119.8(6)
C(14)-C(15)-C(16)	122.6(5)	C(85)-C(84)-C(83)	120.9(6)
C(15)-C(16)-C(11)	120.1(5)	C(84)-C(85)-C(80)	121.2(5)
C(15)-C(16)-C(17)	122.0(5)	C(91)-C(90)-C(95)	117.6(5)
C(11)-C(16)-C(17)	117.8(5)	C(91)-C(90)-C(9)	123.6(6)
C(40)-C(17)-C(16)	110.5(4)	C(95)-C(90)-C(9)	118.6(6)
C(40)-C(17)-C(50)	114.1(4)	C(90)-C(91)-C(92)	121.4(6)
C(16)-C(17)-C(50)	112.8(4)	C(91)-C(92)-C(93)	120.4(7)
C(30)-C(18)-C(12)	112.4(4)	C(94)-C(93)-C(92)	118.4(7)
		C(95)-C(94)-C(93)	122.3(6)
		C(94)-C(95)-C(90)	120.0(6)

Table S7. Bond lengths (Å) and angles (°) for compound **3c.**

Bond lengths (Å)			
Al(1)-O(2)	1.7934(19)	C(64)-C(65)	1.389(4)
Al(1)-O(1)	1.7988(18)	C(66)-C(65)	1.373(5)
Al(1)-C(2)	1.962(3)	C(66)-C(67)	1.381(5)
Al(1)-C(1)	1.981(3)	C(68)-C(67)	1.389(5)
Al(1)-K(1)	3.6014(11)	C(69)-C(74)	1.378(5)
K(1)-O(1)	2.5761(19)	C(69)-C(70)	1.392(5)
K(1)-O(2)	2.9625(19)	C(70)-C(71)	1.376(6)

K(1)-C(55)	2.970(3)	C(71)-C(72)	1.331(7)
K(1)-C(50)	3.102(3)	C(74)-C(73)	1.417(6)
K(1)-C(54)	3.112(3)	C(73)-C(72)	1.380(7)
K(1)-C(25)	3.170(3)	C(4)-C(5)	1.385(4)
K(1)-C(20)	3.170(3)	C(4)-C(3)	1.407(3)
K(1)-C(21)	3.198(3)	C(4)-C(13)	1.523(4)
K(1)-C(24)	3.216(3)	C(5)-C(6)	1.386(4)
K(1)-C(22)	3.237(4)	C(26)-C(27)	1.518(4)
K(1)-C(23)	3.254(3)	C(26)-C(8)	1.522(3)
K(1)-C(51)	3.334(4)	C(26)-C(33)	1.528(4)
O(2)-C(39)	1.368(3)	C(7)-C(6)	1.384(3)
O(1)-C(3)	1.359(3)	C(7)-C(8)	1.389(4)
C(42)-C(41)	1.390(3)	C(8)-C(3)	1.395(4)
C(42)-C(43)	1.394(4)	C(9)-C(12)	1.511(5)
C(42)-C(45)	1.533(4)	C(9)-C(10)	1.517(5)
C(41)-C(40)	1.387(3)	C(9)-C(11)	1.528(4)
C(43)-C(44)	1.385(4)	C(9)-C(6)	1.538(4)
C(40)-C(39)	1.402(3)	C(20)-C(25)	1.382(4)
C(40)-C(49)	1.525(3)	C(20)-C(21)	1.388(4)
C(39)-C(44)	1.405(3)	C(20)-C(13)	1.524(4)
C(55)-C(54)	1.386(4)	C(33)-C(34)	1.380(4)
C(55)-C(50)	1.393(4)	C(33)-C(38)	1.394(4)
C(55)-C(49)	1.538(4)	C(13)-C(14)	1.522(4)
C(45)-C(46)	1.505(5)	C(38)-C(37)	1.379(4)
C(45)-C(48)	1.513(4)	C(27)-C(28)	1.380(4)
C(45)-C(47)	1.554(5)	C(27)-C(32)	1.396(4)
C(44)-C(62)	1.522(3)	C(14)-C(15)	1.374(5)
C(49)-C(56)	1.524(3)	C(14)-C(19)	1.384(5)
C(53)-C(52)	1.381(5)	C(37)-C(36)	1.365(4)
C(53)-C(54)	1.396(4)	C(34)-C(35)	1.380(4)
C(57)-C(58)	1.387(4)	C(35)-C(36)	1.385(5)
C(57)-C(56)	1.396(4)	C(28)-C(29)	1.394(5)
C(50)-C(51)	1.381(5)	C(32)-C(31)	1.372(5)
C(56)-C(61)	1.373(4)	C(30)-C(29)	1.367(5)
C(52)-C(51)	1.371(5)	C(30)-C(31)	1.380(5)
C(61)-C(60)	1.385(5)	C(23)-C(22)	1.356(5)
C(58)-C(59)	1.359(5)	C(23)-C(24)	1.365(5)
C(60)-C(59)	1.363(6)	C(25)-C(24)	1.399(5)
C(63)-C(68)	1.377(4)	C(21)-C(22)	1.390(5)
C(63)-C(64)	1.387(4)	C(15)-C(16)	1.394(5)
C(63)-C(62)	1.525(4)	C(16)-C(17)	1.340(7)
C(62)-C(69)	1.527(4)	C(19)-C(18)	1.416(6)
		C(17)-C(18)	1.374(8)

Angles (°)

O(2)-Al(1)-O(1)	97.00(9)	C(58)-C(57)-C(56)	120.2(3)
O(2)-Al(1)-C(2)	107.53(12)	C(55)-C(54)-C(53)	120.8(3)
O(1)-Al(1)-C(2)	116.30(12)	C(55)-C(54)-K(1)	71.16(16)
O(2)-Al(1)-C(1)	117.52(13)	C(53)-C(54)-K(1)	87.0(2)
O(1)-Al(1)-C(1)	107.44(11)	C(51)-C(50)-C(55)	121.4(3)
C(2)-Al(1)-C(1)	110.74(15)	C(51)-C(50)-K(1)	87.24(19)
O(2)-Al(1)-K(1)	55.00(6)	C(55)-C(50)-K(1)	71.52(16)
O(1)-Al(1)-K(1)	42.39(6)	C(61)-C(56)-C(57)	118.3(3)
C(2)-Al(1)-K(1)	119.71(10)	C(61)-C(56)-C(49)	120.7(3)
C(1)-Al(1)-K(1)	128.84(11)	C(57)-C(56)-C(49)	121.0(3)
O(1)-K(1)-O(2)	57.62(5)	C(51)-C(52)-C(53)	119.3(3)
O(1)-K(1)-C(55)	114.07(7)	C(51)-C(52)-K(1)	73.9(2)
O(2)-K(1)-C(55)	66.97(6)	C(53)-C(52)-K(1)	74.28(19)
O(1)-K(1)-C(50)	127.55(8)	C(52)-C(51)-C(50)	120.5(3)
O(2)-K(1)-C(50)	92.11(6)	C(52)-C(51)-K(1)	82.8(2)
C(55)-K(1)-C(50)	26.41(7)	C(50)-C(51)-K(1)	68.32(18)

O(1)-K(1)-C(54)	121.87(7)	C(56)-C(61)-C(60)	120.7(3)
O(2)-K(1)-C(54)	64.85(7)	C(59)-C(58)-C(57)	120.3(3)
C(55)-K(1)-C(54)	26.21(8)	C(59)-C(60)-C(61)	120.3(4)
C(50)-K(1)-C(54)	44.99(8)	C(58)-C(59)-C(60)	120.2(3)
O(1)-K(1)-C(25)	77.98(7)	C(68)-C(63)-C(64)	117.8(3)
O(2)-K(1)-C(25)	117.25(7)	C(68)-C(63)-C(62)	119.8(3)
C(55)-K(1)-C(25)	165.42(9)	C(64)-C(63)-C(62)	122.4(3)
C(50)-K(1)-C(25)	149.83(8)	C(44)-C(62)-C(69)	110.6(2)
C(54)-K(1)-C(25)	140.57(9)	C(44)-C(62)-C(63)	113.3(2)
O(1)-K(1)-C(20)	64.64(6)	C(69)-C(62)-C(63)	114.0(2)
O(2)-K(1)-C(20)	92.49(6)	C(63)-C(64)-C(65)	120.6(3)
C(55)-K(1)-C(20)	151.60(8)	C(65)-C(66)-C(67)	119.2(3)
C(50)-K(1)-C(20)	167.18(9)	C(63)-C(68)-C(67)	122.0(3)
C(54)-K(1)-C(20)	127.79(8)	C(66)-C(65)-C(64)	120.8(3)
C(25)-K(1)-C(20)	25.19(7)	C(66)-C(67)-C(68)	119.5(3)
O(1)-K(1)-C(21)	78.67(7)	C(74)-C(69)-C(70)	117.0(4)
O(2)-K(1)-C(21)	83.00(7)	C(74)-C(69)-C(62)	120.1(3)
C(55)-K(1)-C(21)	127.86(8)	C(70)-C(69)-C(62)	122.8(3)
C(50)-K(1)-C(21)	144.46(9)	C(71)-C(70)-C(69)	122.2(4)
C(54)-K(1)-C(21)	102.81(8)	C(72)-C(71)-C(70)	120.3(5)
C(25)-K(1)-C(21)	43.77(8)	C(69)-C(74)-C(73)	120.6(5)
C(20)-K(1)-C(21)	25.17(7)	C(72)-C(73)-C(74)	119.1(4)
O(1)-K(1)-C(24)	103.27(8)	C(71)-C(72)-C(73)	120.9(5)
O(2)-K(1)-C(24)	133.36(8)	C(5)-C(4)-C(3)	118.9(2)
C(55)-K(1)-C(24)	141.64(9)	C(5)-C(4)-C(13)	122.0(2)
C(50)-K(1)-C(24)	126.53(9)	C(3)-C(4)-C(13)	119.0(2)
C(54)-K(1)-C(24)	122.37(9)	C(4)-C(5)-C(6)	123.0(2)
C(25)-K(1)-C(24)	25.30(8)	C(27)-C(26)-C(8)	110.8(2)
C(20)-K(1)-C(24)	44.35(8)	C(27)-C(26)-C(33)	112.4(2)
C(21)-K(1)-C(24)	50.49(9)	C(8)-C(26)-C(33)	113.8(2)
O(1)-K(1)-C(22)	103.61(8)	C(6)-C(7)-C(8)	122.4(2)
O(2)-K(1)-C(22)	96.69(8)	C(7)-C(8)-C(3)	119.6(2)
C(55)-K(1)-C(22)	116.04(9)	C(7)-C(8)-C(26)	122.4(2)
C(50)-K(1)-C(22)	123.19(9)	C(3)-C(8)-C(26)	117.6(2)
C(54)-K(1)-C(22)	89.98(9)	C(12)-C(9)-C(10)	109.7(3)
C(25)-K(1)-C(22)	50.82(9)	C(12)-C(9)-C(11)	107.2(3)
C(20)-K(1)-C(22)	44.30(8)	C(10)-C(9)-C(11)	109.8(3)
C(21)-K(1)-C(22)	24.95(8)	C(12)-C(9)-C(6)	112.6(2)
C(24)-K(1)-C(22)	42.70(10)	C(10)-C(9)-C(6)	107.8(2)
O(1)-K(1)-C(23)	116.19(8)	C(11)-C(9)-C(6)	109.8(2)
O(2)-K(1)-C(23)	120.77(9)	O(1)-C(3)-C(8)	120.7(2)
C(55)-K(1)-C(23)	121.50(9)	O(1)-C(3)-C(4)	120.0(2)
C(50)-K(1)-C(23)	116.12(9)	C(8)-C(3)-C(4)	119.2(2)
C(54)-K(1)-C(23)	98.91(9)	O(1)-C(3)-K(1)	40.34(11)
C(25)-K(1)-C(23)	43.94(9)	C(8)-C(3)-K(1)	114.38(16)
C(20)-K(1)-C(23)	51.56(8)	C(4)-C(3)-K(1)	108.34(16)
C(21)-K(1)-C(23)	43.41(9)	C(25)-C(20)-C(21)	117.9(3)
C(24)-K(1)-C(23)	24.34(9)	C(25)-C(20)-C(13)	122.9(3)
C(22)-K(1)-C(23)	24.12(9)	C(21)-C(20)-C(13)	119.1(3)
O(1)-K(1)-C(51)	151.20(8)	C(25)-C(20)-K(1)	77.37(16)
O(2)-K(1)-C(51)	111.02(7)	C(21)-C(20)-K(1)	78.52(18)
C(55)-K(1)-C(51)	44.67(7)	C(13)-C(20)-K(1)	113.39(15)
C(50)-K(1)-C(51)	24.44(8)	C(34)-C(33)-C(38)	117.9(3)
C(54)-K(1)-C(51)	50.50(8)	C(34)-C(33)-C(26)	123.3(2)
C(25)-K(1)-C(51)	126.82(8)	C(38)-C(33)-C(26)	118.8(2)
C(20)-K(1)-C(51)	143.98(8)	C(7)-C(6)-C(5)	116.9(2)
C(21)-K(1)-C(51)	128.61(9)	C(7)-C(6)-C(9)	123.5(2)
C(24)-K(1)-C(51)	102.40(9)	C(5)-C(6)-C(9)	119.6(2)
C(22)-K(1)-C(51)	104.05(9)	C(14)-C(13)-C(4)	112.5(2)
C(23)-K(1)-C(51)	92.49(9)	C(14)-C(13)-C(20)	111.6(2)

C(39)-O(2)-Al(1)	124.31(16)	C(4)-C(13)-C(20)	111.9(2)
C(39)-O(2)-K(1)	131.81(14)	C(37)-C(38)-C(33)	120.9(3)
Al(1)-O(2)-K(1)	95.28(7)	C(28)-C(27)-C(32)	116.6(3)
C(3)-O(1)-Al(1)	130.70(16)	C(28)-C(27)-C(26)	123.7(2)
C(3)-O(1)-K(1)	119.70(14)	C(32)-C(27)-C(26)	119.7(3)
Al(1)-O(1)-K(1)	109.53(8)	C(15)-C(14)-C(19)	119.0(3)
C(41)-C(42)-C(43)	116.5(2)	C(15)-C(14)-C(13)	122.7(3)
C(41)-C(42)-C(45)	122.4(2)	C(19)-C(14)-C(13)	118.2(3)
C(43)-C(42)-C(45)	121.0(2)	C(36)-C(37)-C(38)	120.3(3)
C(40)-C(41)-C(42)	122.7(2)	C(35)-C(34)-C(33)	121.2(3)
C(44)-C(43)-C(42)	122.8(2)	C(34)-C(35)-C(36)	119.9(3)
C(41)-C(40)-C(39)	119.6(2)	C(27)-C(28)-C(29)	122.3(3)
C(41)-C(40)-C(49)	120.5(2)	C(27)-C(28)-K(1)	83.78(18)
C(39)-C(40)-C(49)	119.8(2)	C(29)-C(28)-K(1)	89.5(2)
O(2)-C(39)-C(40)	120.5(2)	C(31)-C(32)-C(27)	121.4(3)
O(2)-C(39)-C(44)	120.7(2)	C(29)-C(30)-C(31)	119.1(3)
C(40)-C(39)-C(44)	118.8(2)	C(22)-C(23)-C(24)	119.4(3)
C(54)-C(55)-C(50)	117.6(3)	C(22)-C(23)-K(1)	77.3(2)
C(54)-C(55)-C(49)	123.1(2)	C(24)-C(23)-K(1)	76.3(2)
C(50)-C(55)-C(49)	119.1(2)	C(20)-C(25)-C(24)	120.2(3)
C(54)-C(55)-K(1)	82.63(17)	C(20)-C(25)-K(1)	77.44(16)
C(50)-C(55)-K(1)	82.07(16)	C(24)-C(25)-K(1)	79.19(18)
C(49)-C(55)-K(1)	101.55(15)	C(37)-C(36)-C(35)	119.7(3)
C(46)-C(45)-C(48)	111.2(3)	C(32)-C(31)-C(30)	120.9(3)
C(46)-C(45)-C(42)	110.4(3)	C(23)-C(24)-C(25)	120.9(3)
C(48)-C(45)-C(42)	112.7(2)	C(23)-C(24)-K(1)	79.4(2)
C(46)-C(45)-C(47)	108.2(3)	C(25)-C(24)-K(1)	75.51(17)
C(48)-C(45)-C(47)	106.4(3)	C(30)-C(29)-C(28)	119.7(3)
C(42)-C(45)-C(47)	107.7(3)	C(20)-C(21)-C(22)	120.9(3)
C(43)-C(44)-C(39)	119.5(2)	C(20)-C(21)-K(1)	76.31(17)
C(43)-C(44)-C(62)	120.3(2)	C(22)-C(21)-K(1)	79.1(2)
C(39)-C(44)-C(62)	119.9(2)	C(14)-C(15)-C(16)	120.8(4)
C(56)-C(49)-C(40)	112.5(2)	C(17)-C(16)-C(15)	119.8(5)
C(56)-C(49)-C(55)	111.8(2)	C(14)-C(19)-C(18)	119.9(5)
C(40)-C(49)-C(55)	112.1(2)	C(23)-C(22)-C(21)	120.7(3)
C(52)-C(53)-C(54)	120.3(3)	C(23)-C(22)-K(1)	78.6(2)
C(52)-C(53)-K(1)	82.3(2)	C(21)-C(22)-K(1)	75.9(2)
C(54)-C(53)-K(1)	68.36(18)	C(16)-C(17)-C(18)	121.7(5)
		C(17)-C(18)-C(19)	118.7(5)

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