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SUPPORTING INFORMATION

Title: Synthesis and Characterization of New Pentacoordinate Iron-Based Aryloxide Complexes
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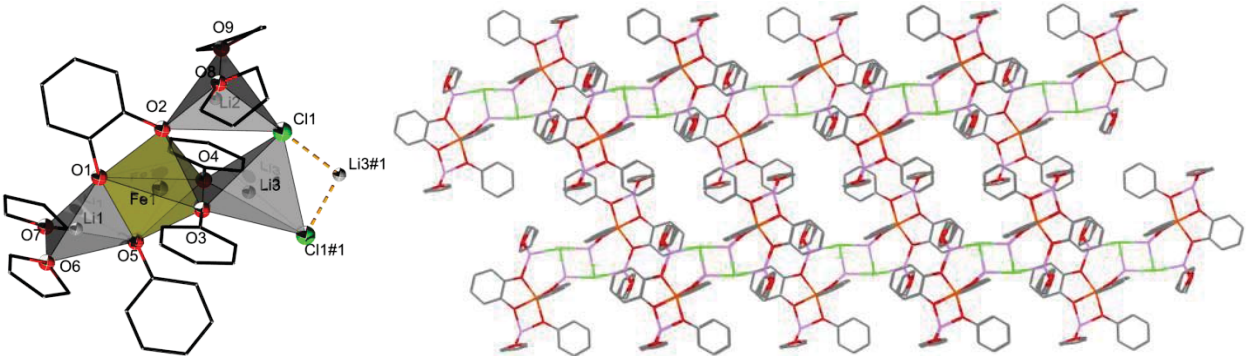

Figure S1. View of both Li and Fe nuclear polyhedral arrangement and the view of the packing in through b-axis of the compound **1**

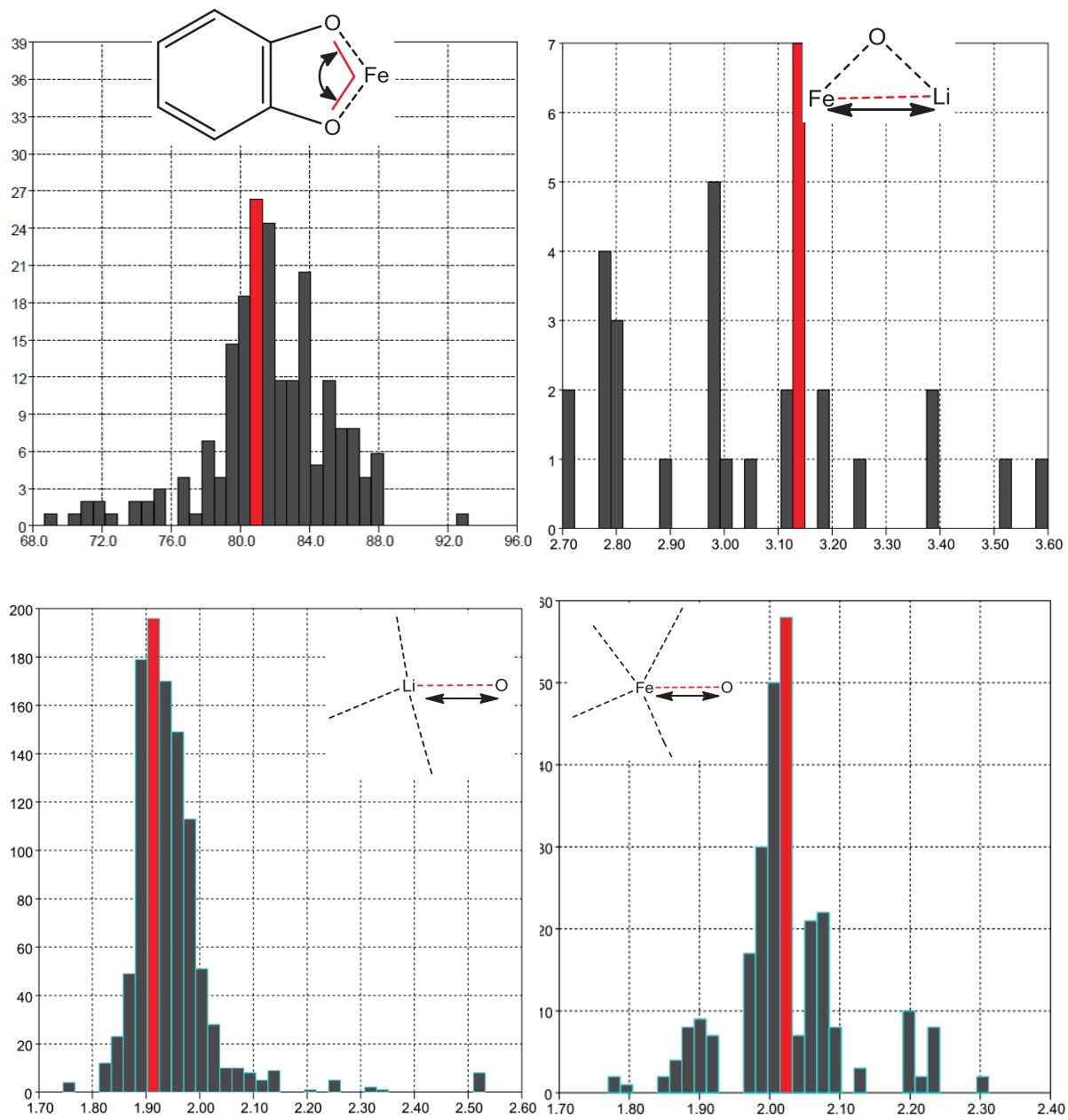

Figure S2: The top histograms show the list of values of well-defined bite O-Fe-O angle of the catecholate(left) and distance Fe─Li with the oxo-bridg (right). The buttom histograms show the bond lenghts values of Li-O and Fe-O in a O-tetra- and penta-coordinated sphere respectively. Datas have been colected from CSD.version 5.32 (August 2011). (Number of publication in y-axis (vertical) and the angles or bond length in degre or Angström in x –axis (hotizontal)).

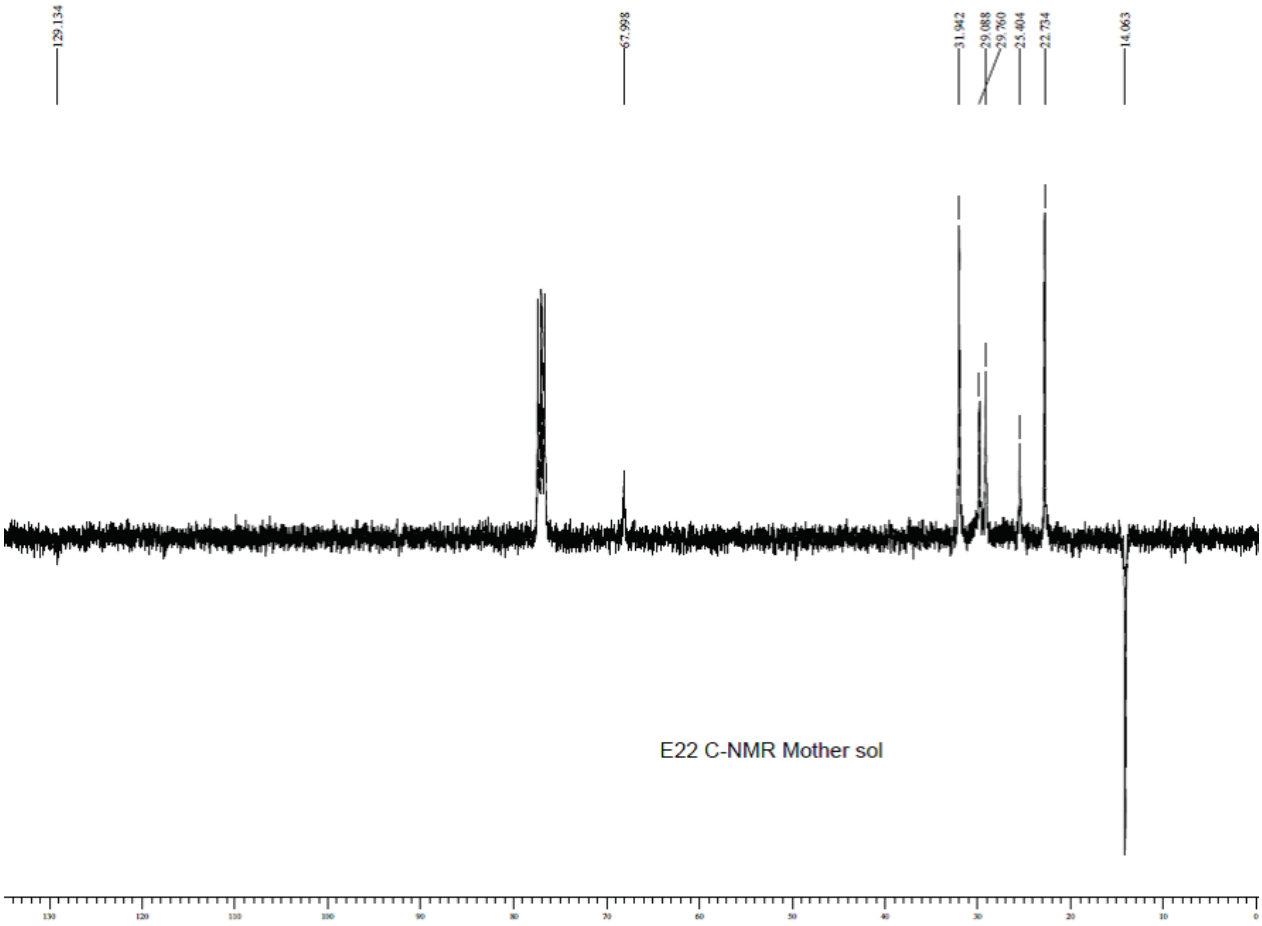

Figure S3: C-NMR of the mother solution of compound **1** in $CDCl_3$ solvent.

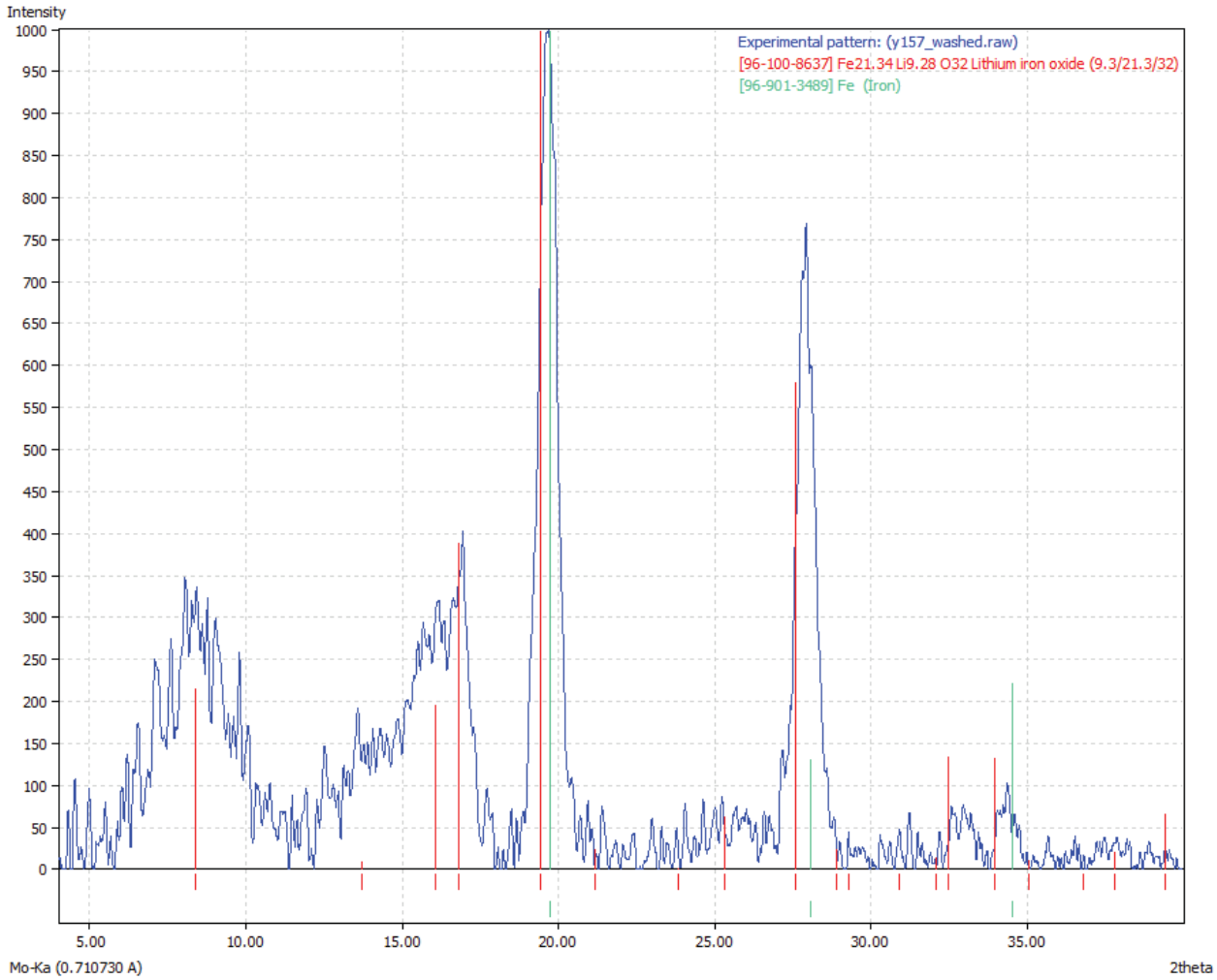

Figure S4: XRPD of the compound **1** heated up at 600°C at 5°C/min.

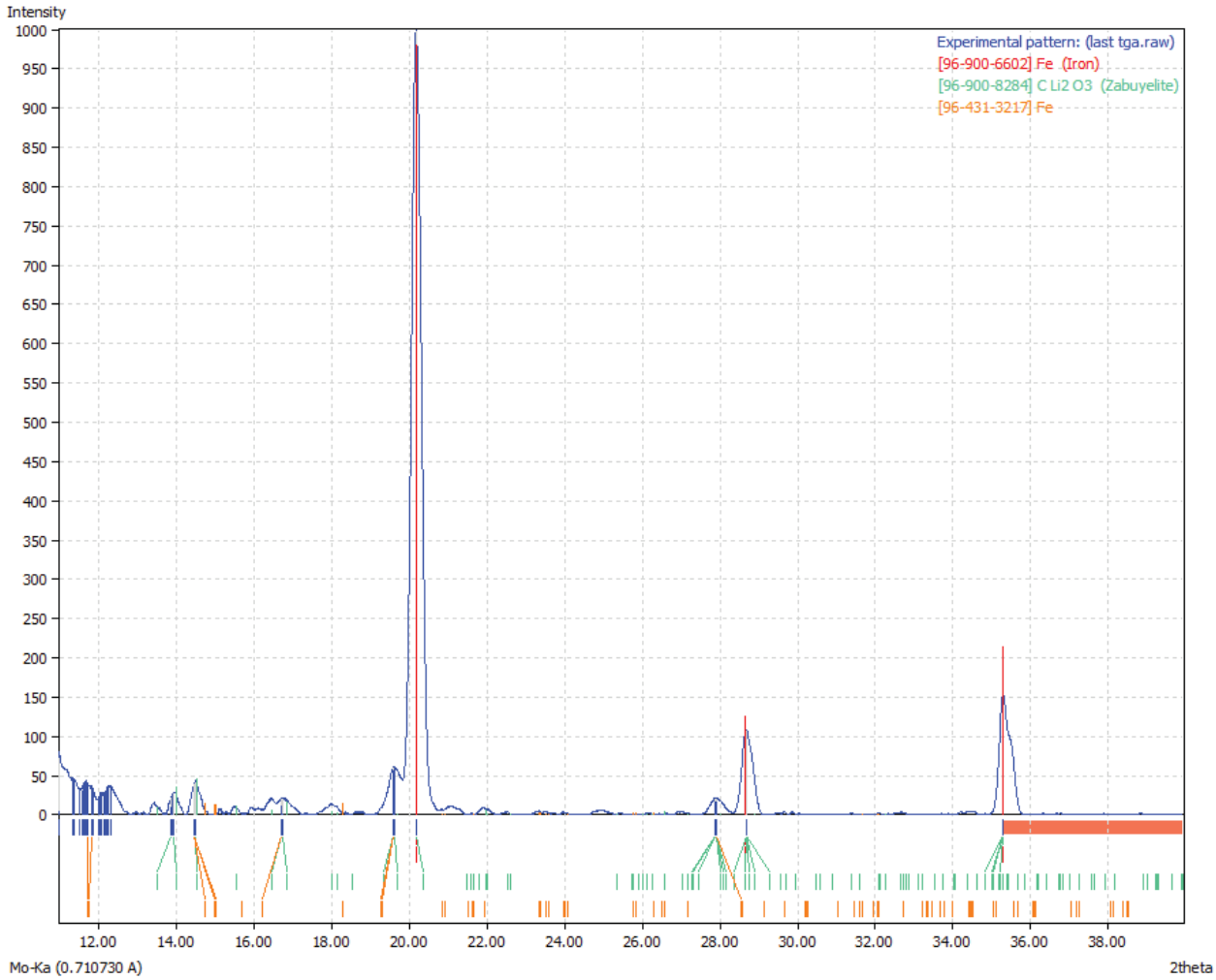

Figure S5: XRPD of the TGA residue of compound **1** heated util 600°C at 10°C/min.

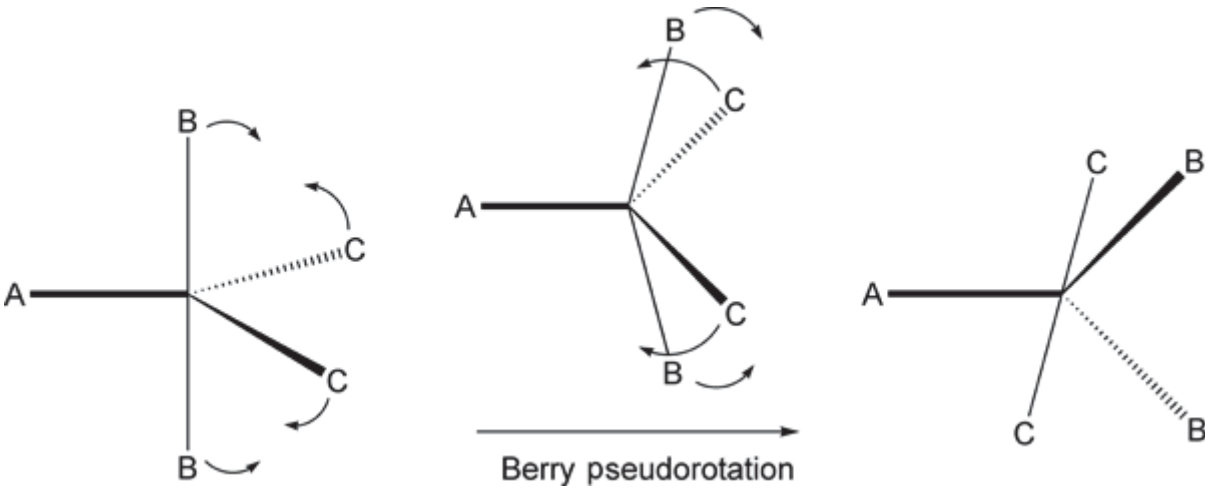

Figure S6: The Berry pseudorotation in the trigonal bipyramidal complex of Iron.

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There pentahedral complexes are less common than four and six coordinated complexes. They can be square bipyramidal (C_{4v}) or trigonal bipyramidal (D_{3h}), in our case. The trigonal bipyramidal minimizes ligand-ligand repulsion in contrary to the steric constraint on ligand that can bond to more than one site to a metal atom. By the Berry pseudorotation we can easily observe transposition from the axial position of a pair of ligands to the equatorial position (R. S. Berry, *J Chem Phys* **1960**, *32*, 933–938)

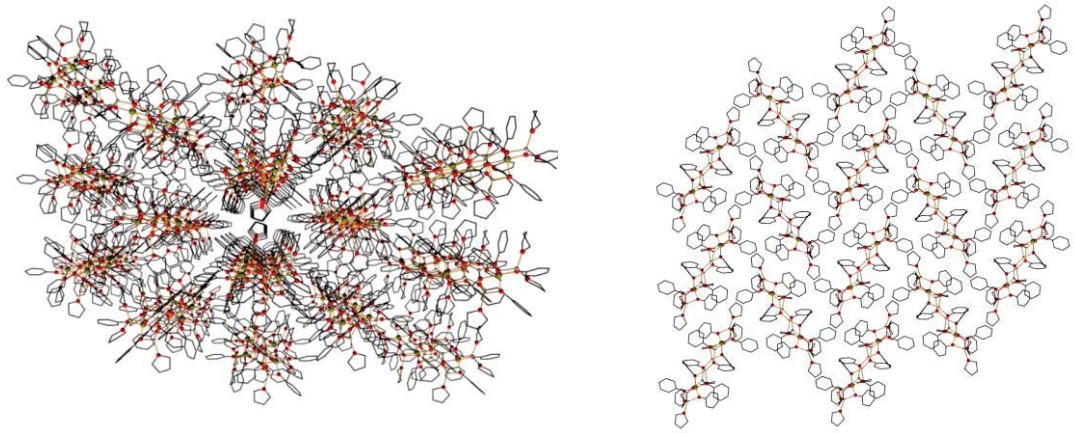

Figure S7: Viewing of the central projection packing of the compound **3** through the *c*-axis (left) and in the a-axis (right) which shown the it's zigzag fashion arrangement.

Table S1 : Bond lengths [Å] for Compound **1**

Fe(1)-O(3)	1.8977(19)	O(6)-C(25)	1.311(6)
Fe(1)-O(4)	1.9036(19)	O(6)-C(28)	1.437(5)
Fe(1)-O(1)	1.958(2)	O(6)-Li(1)	1.909(6)
Fe(1)-O(5)	1.967(2)	O(7)-C(29)	1.341(5)
Fe(1)-O(2)	2.014(2)	O(7)-C(32)	1.447(5)
Fe(1)-Li(3)	2.807(5)	O(7)-Li(1)	1.908(6)
Fe(1)-Li(1)	2.969(6)	O(8)-C(33)	1.361(4)
Cl(1)-Li(3)#1	2.308(5)	O(8)-C(36)	1.428(5)
Cl(1)-Li(3)	2.310(6)	O(8)-Li(2)	1.956(6)
Cl(1)-Li(2)	2.376(5)	O(9)-C(37)	1.377(4)
O(1)-C(1)	1.345(4)	O(9)-C(40)	1.446(5)
O(1)-Li(1)	1.902(7)	O(9)-Li(2)	1.947(7)
O(2)-C(6)	1.353(4)	C(1)-C(2)	1.388(4)
O(2)-Li(2)	1.966(7)	C(1)-C(6)	1.409(5)
O(3)-C(7)	1.341(3)	C(2)-C(3)	1.398(5)
O(3)-Li(3)	1.955(5)	C(2)-H(1)	0.9300
O(4)-C(13)	1.346(3)	C(3)-C(4)	1.347(6)
O(4)-Li(3)	1.956(5)	C(3)-H(2)	0.9300
O(5)-C(19)	1.347(4)	C(4)-C(5)	1.399(5)
O(5)-Li(1)	1.935(6)	C(4)-H(3)	0.9300

C(5)-C(6)	1.360(5)	C(18)-H(14)	0.9300
C(5)-H(4)	0.9300	C(19)-C(20)	1.389(5)
C(7)-C(12)	1.382(5)	C(19)-C(24)	1.396(5)
C(7)-C(8)	1.391(5)	C(20)-C(21)	1.378(5)
C(8)-C(9)	1.374(6)	C(20)-H(15)	0.9300
C(8)-H(5)	0.9300	C(21)-C(22)	1.383(5)
C(9)-C(10)	1.349(7)	C(21)-H(16)	0.9300
C(9)-H(6)	0.9300	C(22)-C(23)	1.365(5)
C(10)-C(11)	1.372(7)	C(22)-H(17)	0.9300
C(10)-H(7)	0.9300	C(23)-C(24)	1.363(5)
C(11)-C(12)	1.398(6)	C(23)-H(18)	0.9300
C(11)-H(8)	0.9300	C(24)-H(19)	0.9300
C(12)-H(9)	0.9300	C(25)-C(26)	1.455(9)
C(13)-C(14)	1.384(5)	C(25)-H(21)	0.9700
C(13)-C(18)	1.400(5)	C(25)-H(20)	0.9700
C(14)-C(15)	1.391(6)	C(26)-C(27)	1.317(8)
C(14)-H(10)	0.9300	C(26)-H(22)	0.9700
C(15)-C(16)	1.357(8)	C(26)-H(23)	0.9700
C(15)-H(11)	0.9300	C(27)-C(28)	1.445(7)
C(16)-C(17)	1.366(8)	C(27)-H(25)	0.9700
C(16)-H(12)	0.9300	C(27)-H(24)	0.9700
C(17)-C(18)	1.376(5)	C(28)-H(26)	0.9700
C(17)-H(13)	0.9300	C(28)-H(27)	0.9700

C(29)-C(30)	1.519(7)
C(29)-H(28)	0.9700
C(29)-H(29)	0.9700
C(30)-C(31)	1.347(7)
C(30)-H(31)	0.9700
C(30)-H(30)	0.9700
C(31)-C(32)	1.402(7)
C(31)-H(32)	0.9700
C(31)-H(33)	0.9700
C(32)-H(34)	0.9700
C(32)-H(35)	0.9700
C(33)-C(34)	1.423(6)
C(33)-H(36)	0.9700
C(33)-H(37)	0.9700
C(34)-C(35)	1.394(7)
C(34)-H(38)	0.9700
C(34)-H(39)	0.9700
C(35)-C(36)	1.501(7)
C(35)-H(41)	0.9700
C(35)-H(40)	0.9700
C(36)-H(42)	0.9700
C(36)-H(43)	0.9700
C(37)-C(38)	1.459(6)
C(37)-H(45)	0.9700
C(37)-H(44)	0.9700
C(38)-C(39)	1.371(7)
C(38)-H(46)	0.9700
C(38)-H(47)	0.9700
C(39)-C(40)	1.477(7)
C(39)-H(49)	0.9700
C(39)-H(48)	0.9700
C(40)-H(51)	0.9700
C(40)-H(50)	0.9700
Li(2)-Li(3)	3.310(8)
Li(3)-Cl(1)#1	2.308(5)
Li(3)-Li(3)#1	2.918(10)

Symmetry transformations used to generate equivalent atoms:

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

Table S2: Bond lengths [Å] for compound **2**.

C(1)-O(1)	1.372(8)	C(12)-H(12)	0.9300
C(1)-C(6)	1.385(11)	C(13)-O(3)	1.355(8)
C(1)-C(2)	1.394(11)	C(13)-C(18)	1.388(10)
C(2)-C(3)	1.383(12)	C(13)-C(14)	1.402(10)
C(2)-H(2)	0.9300	C(14)-C(15)	1.382(12)
C(3)-C(4)	1.342(15)	C(14)-H(14)	0.9300
C(3)-H(3)	0.9300	C(15)-C(16)	1.368(14)
C(4)-C(5)	1.385(14)	C(15)-H(15)	0.9300
C(4)-H(4)	0.9300	C(16)-C(17)	1.358(13)
C(5)-C(6)	1.386(11)	C(16)-H(16)	0.9300
C(5)-H(5)	0.9300	C(17)-C(18)	1.393(11)
C(6)-H(6)	0.9300	C(17)-H(17)	0.9300
C(7)-O(2)	1.368(8)	C(18)-H(18)	0.9300
C(7)-C(12)	1.372(11)	C(19)-C(24)	1.374(10)
C(7)-C(8)	1.391(11)	C(19)-O(4)	1.380(8)
C(7)-Li(1)	2.748(15)	C(19)-C(20)	1.399(10)
C(8)-C(9)	1.396(12)	C(20)-C(21)	1.402(10)
C(8)-H(8)	0.9300	C(20)-H(20)	0.9300
C(9)-C(10)	1.337(16)	C(21)-C(22)	1.370(12)
C(9)-H(9)	0.9300	C(21)-H(21)	0.9300
C(10)-C(11)	1.351(16)	C(22)-C(23)	1.378(12)
C(10)-H(10)	0.9300	C(22)-H(22)	0.9300
C(11)-C(12)	1.401(12)	C(23)-C(24)	1.374(10)
C(11)-H(11)	0.9300	C(23)-H(23)	0.9300

C(24)-H(24)	0.9300	C(37)-C(42)	1.363(10)
C(25)-C(26)	1.362(11)	C(37)-C(38)	1.406(10)
C(25)-O(5)	1.390(8)	C(38)-C(39)	1.408(12)
C(25)-C(30)	1.398(11)	C(38)-H(38)	0.9300
C(26)-C(27)	1.386(12)	C(39)-C(40)	1.358(13)
C(26)-H(26)	0.9300	C(39)-H(39)	0.9300
C(27)-C(28)	1.389(17)	C(40)-C(41)	1.373(13)
C(27)-H(27)	0.9300	C(40)-H(40)	0.9300
C(28)-C(29)	1.334(17)	C(41)-C(42)	1.387(11)
C(28)-H(28)	0.9300	C(41)-H(41)	0.9300
C(29)-C(30)	1.386(13)	C(42)-H(42)	0.9300
C(29)-H(29)	0.9300	C(43)-O(8)	1.366(6)
C(30)-H(30)	0.9300	C(43)-C(44)	1.3900
C(31)-C(36)	1.366(11)	C(43)-C(48)	1.3900
C(31)-C(32)	1.390(11)	C(44)-C(45)	1.3900
C(31)-O(6)	1.390(9)	C(44)-H(44)	0.9300
C(32)-C(33)	1.398(14)	C(45)-C(46)	1.3900
C(32)-H(32)	0.9300	C(45)-H(45)	0.9300
C(33)-C(34)	1.377(17)	C(46)-C(47)	1.3900
C(33)-H(33)	0.9300	C(46)-H(46)	0.9300
C(34)-C(35)	1.330(17)	C(47)-C(48)	1.3900
C(34)-H(34)	0.9300	C(47)-H(47)	0.9300
C(35)-C(36)	1.377(13)	C(48)-H(48)	0.9300
C(35)-H(35)	0.9300	C(49)-O(9)	1.371(8)
C(36)-H(36)	0.9300	C(49)-C(50)	1.394(10)
C(37)-O(7)	1.350(8)	C(49)-C(54)	1.406(10)

C(50)-C(51)	1.372(12)	C(63)-C(64)	1.360(15)
C(50)-H(50)	0.9300	C(63)-H(63)	0.9300
C(51)-C(52)	1.359(14)	C(64)-C(65)	1.362(15)
C(51)-H(51)	0.9300	C(64)-H(64)	0.9300
C(52)-C(53)	1.369(14)	C(65)-C(66)	1.386(11)
C(52)-H(52)	0.9300	C(65)-H(65)	0.9300
C(53)-C(54)	1.367(12)	C(66)-H(66)	0.9300
C(53)-H(53)	0.9300	C(67)-C(72)	1.364(10)
C(54)-H(54)	0.9300	C(67)-O(12)	1.367(8)
C(55)-O(10)	1.361(8)	C(67)-C(68)	1.368(10)
C(55)-C(56)	1.363(9)	C(67)-Li(7)	2.721(16)
C(55)-C(60)	1.402(10)	C(68)-C(69)	1.401(13)
C(56)-C(57)	1.387(10)	C(68)-H(68)	0.9300
C(56)-H(56)	0.9300	C(69)-C(70)	1.373(16)
C(57)-C(58)	1.343(12)	C(69)-H(69)	0.9300
C(57)-H(57)	0.9300	C(70)-C(71)	1.372(15)
C(58)-C(59)	1.369(13)	C(70)-H(70)	0.9300
C(58)-H(58)	0.9300	C(71)-C(72)	1.405(12)
C(59)-C(60)	1.385(12)	C(71)-H(71)	0.9300
C(59)-H(59)	0.9300	C(72)-H(72)	0.9300
C(60)-H(60)	0.9300	C(73)-O(13)	1.366(8)
C(61)-O(11)	1.372(8)	C(73)-C(78)	1.379(12)
C(61)-C(66)	1.382(10)	C(73)-C(74)	1.393(11)
C(61)-C(62)	1.382(11)	C(74)-C(75)	1.395(17)
C(62)-C(63)	1.385(12)	C(74)-H(74)	0.9300
C(62)-H(62)	0.9300	C(75)-C(76)	1.35(2)

C(75)-H(75)	0.9300	C(88)-H(88)	0.9300
C(76)-C(77)	1.38(2)	C(89)-C(90)	1.383(12)
C(76)-H(76)	0.9300	C(89)-H(89)	0.9300
C(77)-C(78)	1.387(14)	C(90)-H(90)	0.9300
C(77)-H(77)	0.9300	C(91)-C(92)	1.422(15)
C(78)-H(78)	0.9300	C(91)-O(16)	1.453(11)
C(79)-O(14)	1.359(8)	C(91)-H(91A)	0.9700
C(79)-C(84)	1.393(11)	C(91)-H(91B)	0.9700
C(79)-C(80)	1.399(10)	C(92)-C(93)	1.452(15)
C(80)-C(81)	1.397(11)	C(92)-H(92A)	0.9700
C(80)-H(80)	0.9300	C(92)-H(92B)	0.9700
C(81)-C(82)	1.362(14)	C(93)-C(94)	1.491(13)
C(81)-H(81)	0.9300	C(93)-H(93A)	0.9700
C(82)-C(83)	1.360(15)	C(93)-H(93B)	0.9700
C(82)-H(82)	0.9300	C(94)-O(16)	1.406(10)
C(83)-C(84)	1.376(13)	C(94)-H(94A)	0.9700
C(83)-H(83)	0.9300	C(94)-H(94B)	0.9700
C(84)-H(84)	0.9300	C(95)-O(17)	1.385(10)
C(85)-O(15)	1.377(8)	C(95)-C(96)	1.428(13)
C(85)-C(86)	1.385(10)	C(95)-H(95A)	0.9700
C(85)-C(90)	1.384(10)	C(95)-H(95B)	0.9700
C(86)-C(87)	1.387(11)	C(96)-C(97)	1.473(15)
C(86)-H(86)	0.9300	C(96)-H(96A)	0.9700
C(87)-C(88)	1.367(13)	C(96)-H(96B)	0.9700
C(87)-H(87)	0.9300	C(97)-C(98)	1.315(14)
C(88)-C(89)	1.367(14)	C(97)-H(97A)	0.9700

C(97)-H(97B)	0.9700	C(105)-H(10L)	0.9700
C(98)-O(17)	1.447(11)	C(106)-O(19)	1.439(11)
C(98)-H(98A)	0.9700	C(106)-H(10M)	0.9700
C(98)-H(98B)	0.9700	C(106)-H(10N)	0.9700
C(99)-O(18)	1.441(10)	C(107)-O(20)	1.385(11)
C(99)-C(100)	1.501(13)	C(107)-C(108)	1.447(13)
C(99)-H(99A)	0.9700	C(107)-H(10O)	0.9700
C(99)-H(99B)	0.9700	C(107)-H(10P)	0.9700
C(100)-C(101)	1.484(16)	C(108)-C(109)	1.511(12)
C(100)-H(10A)	0.9700	C(108)-H(10Q)	0.9700
C(100)-H(10B)	0.9700	C(108)-H(10R)	0.9700
C(101)-C(102)	1.435(15)	C(109)-C(110)	1.497(11)
C(101)-H(10C)	0.9700	C(109)-H(10S)	0.9700
C(101)-H(10D)	0.9700	C(109)-H(10T)	0.9700
C(102)-O(18)	1.412(12)	C(110)-O(20)	1.441(10)
C(102)-H(10E)	0.9700	C(110)-H(11A)	0.9700
C(102)-H(10F)	0.9700	C(110)-H(11B)	0.9700
C(103)-O(19)	1.433(9)	C(111)-O(21)	1.432(9)
C(103)-C(104)	1.527(13)	C(111)-C(112)	1.498(10)
C(103)-H(10G)	0.9700	C(111)-H(11C)	0.9700
C(103)-H(10H)	0.9700	C(111)-H(11D)	0.9700
C(104)-C(105)	1.543(15)	C(112)-C(113)	1.513(12)
C(104)-H(10I)	0.9700	C(112)-H(11E)	0.9700
C(104)-H(10J)	0.9700	C(112)-H(11F)	0.9700
C(105)-C(106)	1.459(14)	C(113)-C(114)	1.505(11)
C(105)-H(10K)	0.9700	C(113)-H(11G)	0.9700

C(113)-H(11H)	0.9700	C(121)-H(12D)	0.9700
C(114)-O(21)	1.443(9)	C(122)-O(23)	1.449(10)
C(114)-H(11I)	0.9700	C(122)-H(12E)	0.9700
C(114)-H(11J)	0.9700	C(122)-H(12F)	0.9700
C(115)-O(22)	1.426(10)	C(123)-O(24)	1.414(12)
C(115)-C(116)	1.491(13)	C(123)-C(124)	1.422(18)
C(115)-H(11K)	0.9700	C(123)-H(12G)	0.9700
C(115)-H(11L)	0.9700	C(123)-H(12H)	0.9700
C(116)-C(117)	1.506(15)	C(124)-C(125)	1.435(18)
C(116)-H(11M)	0.9700	C(124)-H(12I)	0.9700
C(116)-H(11N)	0.9700	C(124)-H(12J)	0.9700
C(117)-C(118)	1.378(14)	C(125)-C(126)	1.487(15)
C(117)-H(11O)	0.9700	C(125)-H(12K)	0.9700
C(117)-H(11P)	0.9700	C(125)-H(12L)	0.9700
C(118)-O(22)	1.453(10)	C(126)-O(24)	1.399(13)
C(118)-H(11Q)	0.9700	C(126)-H(12M)	0.9700
C(118)-H(11R)	0.9700	C(126)-H(12N)	0.9700
C(119)-O(23)	1.415(9)	O(1)-Fe(1)	1.908(5)
C(119)-C(120)	1.469(13)	O(1)-Li(1)	1.916(15)
C(119)-H(11S)	0.9700	O(2)-Li(2)	1.945(15)
C(119)-H(11T)	0.9700	O(2)-Li(1)	2.025(14)
C(120)-C(121)	1.509(14)	O(2)-Fe(1)	2.059(5)
C(120)-H(12A)	0.9700	O(3)-Fe(1)	1.891(5)
C(120)-H(12B)	0.9700	O(3)-Li(2)	1.934(15)
C(121)-C(122)	1.496(12)	O(4)-Li(3)	1.901(13)
C(121)-H(12C)	0.9700	O(4)-Fe(1)	1.917(5)

O(5)-Fe(1)	1.886(5)	O(18)-Li(3)	1.935(14)
O(5)-Li(3)	1.922(14)	O(19)-Li(4)	1.894(14)
O(6)-Li(4)	1.849(14)	O(20)-Li(5)	1.875(14)
O(6)-Fe(2)	1.910(5)	O(21)-Li(6)	1.919(13)
O(7)-Li(5)	1.974(13)	O(22)-Li(7)	1.886(14)
O(7)-Fe(2)	2.038(5)	O(23)-Li(8)	1.930(13)
O(7)-Li(4)	2.127(14)	O(24)-Li(9)	1.921(15)
O(8)-Fe(2)	1.910(5)	Cl(1)-Li(4)	2.351(14)
O(8)-Li(5)	1.945(13)	Cl(1)-Li(3)	2.349(12)
O(9)-Fe(2)	1.920(5)	Cl(1)-Li(5)	2.351(12)
O(9)-Li(6)	1.939(12)	Cl(2)-Li(7)	2.351(12)
O(10)-Fe(2)	1.888(5)	Cl(2)-Li(6)	2.357(12)
O(10)-Li(6)	1.931(13)	Cl(2)-Li(8)	2.358(12)
O(11)-Li(7)	1.885(14)	Cl(3)-Li(1)	2.341(13)
O(11)-Fe(3)	1.915(5)	Cl(3)-Li(9)#1	2.352(11)
O(12)-Li(8)	1.929(13)	Cl(3)-Li(2)	2.374(12)
O(12)-Fe(3)	2.043(5)	Fe(1)-Li(3)	2.858(13)
O(12)-Li(7)	2.045(15)	Fe(1)-Li(1)	2.935(14)
O(13)-Fe(3)	1.885(5)	Fe(1)-Li(2)	2.941(15)
O(13)-Li(8)	1.929(15)	Fe(2)-Li(6)	2.868(12)
O(14)-Fe(3)	1.921(4)	Fe(2)-Li(4)	2.920(13)
O(14)-Li(9)	1.935(14)	Fe(2)-Li(5)	2.964(12)
O(15)-Fe(3)	1.902(5)	Fe(3)-Li(9)	2.872(13)
O(15)-Li(9)	1.905(13)	Fe(3)-Li(8)	2.914(13)
O(16)-Li(1)	1.884(15)	Fe(3)-Li(7)	2.914(15)
O(17)-Li(2)	1.904(15)	Li(1)-Li(2)	2.836(19)

Li(4)-Li(5)	2.904(18)	Li(9)-Cl(3)#2	2.352(11)
Li(7)-Li(8)	2.799(17)		

Symmetry transformations used to generate equivalent atoms:

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

Table S3.: Bond lengths [Å] for compound **3**

O(8)-C(44)	1.337(15)	Fe(1)-O(5)	1.902(4)
O(8)-C(41)	1.403(13)	Fe(1)-O(2)	1.902(4)
O(8)-Li(1)	1.921(13)	Fe(1)-O(3)	1.916(4)
C(43)-C(44)	1.332(17)	Fe(1)-O(1)	1.944(4)
C(43)-C(42)	1.380(19)	Fe(1)-O(4)	2.019(4)
C(43)-H(43A)	0.9700	Fe(1)-Li(1)	2.917(10)
C(43)-H(43B)	0.9700	Fe(1)-Li(3)	2.939(10)
C(42)-C(41)	1.53(2)	Fe(1)-Li(2)	2.952(10)
C(42)-C(44)	1.98(3)	O(4)-C(19)	1.351(7)
C(42)-H(42A)	0.9700	O(4)-Li(3)	1.974(11)
C(42)-H(42B)	0.9700	O(4)-Li(2)	2.111(12)
C(41)-H(41A)	0.9700	O(5)-C(25)	1.377(7)
C(41)-H(41B)	0.9700	O(5)-Li(3)	1.947(10)
C(44)-H(44A)	0.9700	O(1)-C(1)	1.351(7)
C(44)-H(44B)	0.9700	O(1)-Li(1)	1.935(12)

O(6)-C(31)	1.330(7)	C(1)-C(2)	1.403(9)
O(6)-Li(3)#1	1.937(10)	C(14)-C(15)	1.396(12)
O(6)-Li(3)	1.966(10)	C(14)-H(14)	0.9300
O(6)-Li(2)	1.994(11)	C(8)-C(7)	1.366(9)
O(3)-C(13)	1.367(8)	C(8)-C(9)	1.426(10)
O(3)-Li(2)	1.938(11)	C(8)-H(8)	0.9300
O(2)-C(7)	1.373(7)	C(2)-C(3)	1.389(11)
O(2)-Li(1)	1.955(11)	C(2)-H(2)	0.9300
O(9)-C(45)	1.406(8)	C(25)-C(26)	1.352(9)
O(9)-C(48)	1.449(8)	C(7)-C(12)	1.385(9)
O(9)-Li(2)	1.932(12)	C(45)-C(46)	1.491(12)
C(13)-C(18)	1.389(10)	C(45)-H(45A)	0.9700
C(13)-C(14)	1.391(10)	C(45)-H(45B)	0.9700
C(19)-C(24)	1.384(9)	C(26)-C(27)	1.371(10)
C(19)-C(20)	1.393(9)	C(26)-H(26)	0.9300
C(19)-Li(2)	2.553(13)	C(6)-C(5)	1.390(10)
C(24)-C(23)	1.379(10)	C(6)-H(6)	0.9300
C(24)-H(24)	0.9300	C(27)-C(28)	1.376(10)
C(30)-C(25)	1.385(9)	C(27)-H(27)	0.9300
C(30)-C(29)	1.391(10)	C(48)-C(47)	1.463(11)
C(30)-H(30)	0.9300	C(48)-H(48A)	0.9700
C(31)-C(32)	1.377(10)	C(48)-H(48B)	0.9700
C(31)-C(36)	1.411(9)	C(36)-C(35)	1.385(11)
C(31)-Li(2)	2.560(12)	C(36)-H(36)	0.9300
C(31)-Li(3)#1	2.780(12)	C(28)-C(29)	1.364(11)
C(1)-C(6)	1.371(9)	C(28)-H(28)	0.9300

C(18)-C(17)	1.418(11)	C(20)-C(21)	1.384(10)
C(18)-H(18)	0.9300	C(20)-H(20)	0.9300
C(12)-C(11)	1.358(9)	C(29)-H(29)	0.9300
C(12)-H(12)	0.9300	C(17)-C(16)	1.401(14)
Li(3)-O(6)#1	1.937(10)	C(17)-H(17)	0.9300
Li(3)-Li(3)#1	2.566(19)	C(21)-H(21)	0.9300
Li(3)-Li(2)	2.689(15)	C(3)-H(3)	0.9300
Li(3)-C(31)#1	2.780(12)	C(11)-H(11)	0.9300
C(35)-C(34)	1.343(13)	C(16)-H(16)	0.9300
C(35)-H(35)	0.9300	C(33)-C(34)	1.365(13)
C(4)-C(5)	1.368(11)	C(33)-H(33)	0.9300
C(4)-C(3)	1.371(12)	C(34)-H(34)	0.9300
C(4)-H(4)	0.9300	C(46)-C(47)	1.370(13)
C(32)-C(33)	1.382(11)	C(46)-H(46A)	0.9700
C(32)-H(32)	0.9300	C(46)-H(46B)	0.9700
C(15)-C(16)	1.339(13)	C(23)-H(23)	0.9300
C(15)-H(15)	0.9300	C(47)-H(47A)	0.9700
C(9)-C(10)	1.344(11)	C(47)-H(47B)	0.9700
C(9)-H(9)	0.9300	O(7)-C(37)	1.397(11)
C(5)-H(5)	0.9300	O(7)-C(40)	1.422(11)
Li(1)-O(7)	1.943(12)	C(38)-C(39)	1.303(16)
C(22)-C(23)	1.367(12)	C(38)-C(37)	1.420(15)
C(22)-C(21)	1.390(12)	C(38)-H(38A)	0.9700
C(22)-H(22)	0.9300	C(38)-H(38B)	0.9700
C(10)-C(11)	1.382(10)	C(37)-H(37A)	0.9700
C(10)-H(10)	0.9300	C(37)-H(37B)	0.9700

C(39)-C(40)	1.520(14)	C(40)-H(40A)	0.9700
C(39)-H(39A)	0.9700	C(40)-H(40B)	0.9700
C(39)-H(39B)	0.9700		

Symmetry transformations used to generate equivalent atoms:

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