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Electronic Supplementary Information

Adsorption of water induces a reversible structural phase transition and colour change in new nickel (II) macrocyclic complexes forming flexible supramolecular networks

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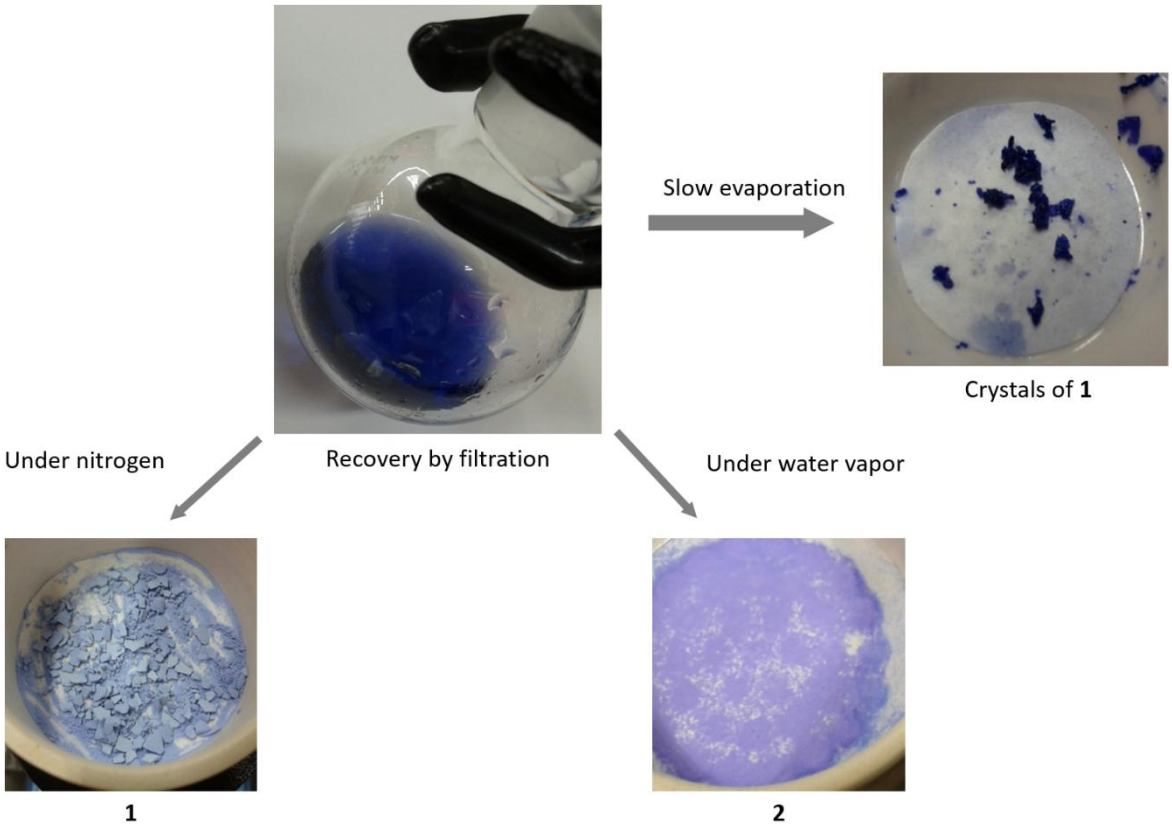

Fig. S1: Schematic representation of the recovery of products **1** and **2**.

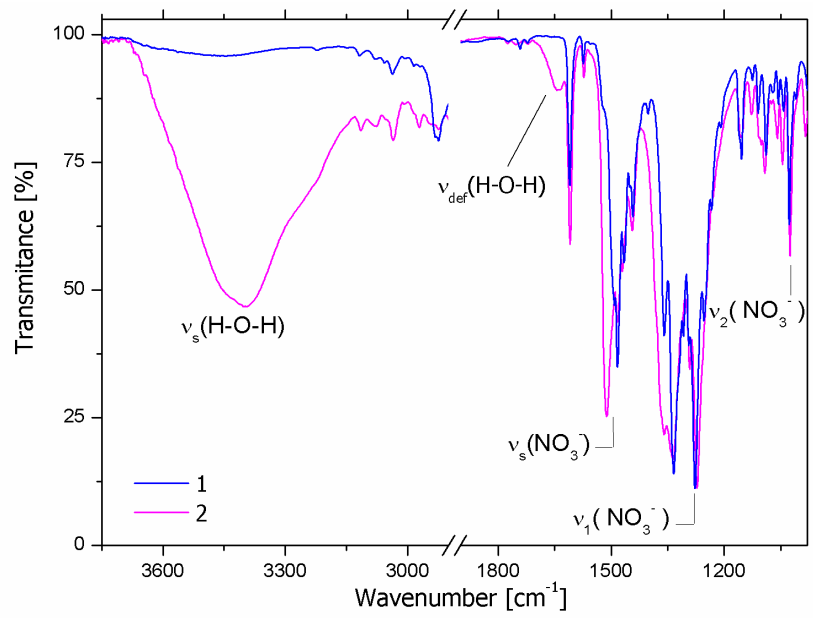

Fig. S2: Mid-infrared spectra of compounds **1** and **2**.

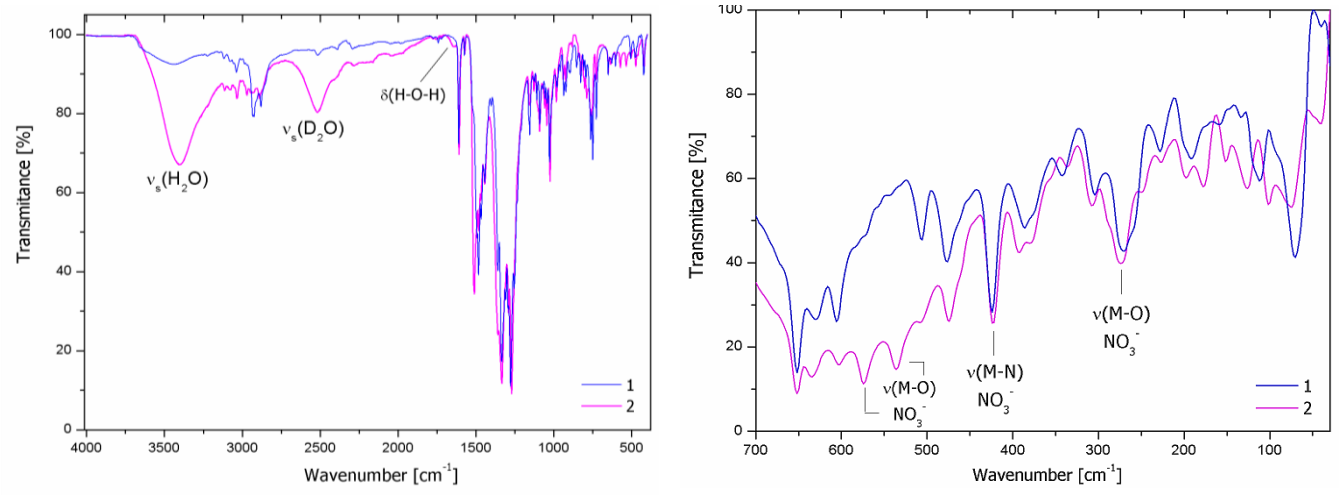

Fig. S3: Comparison of mid-infrared spectra (left) and far-infrared spectra (right) of deuterated compounds **1** and **2**.

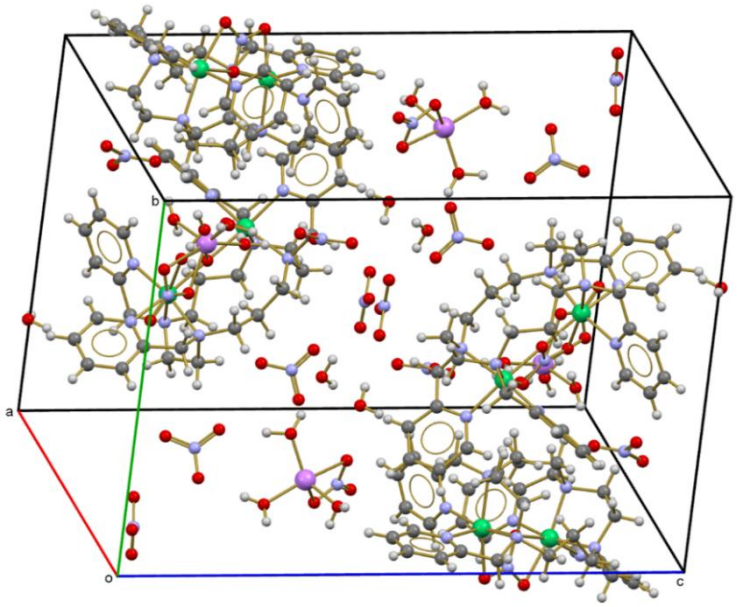

Fig. S4: a) Unit cell of compound **1**. Perspective view of the molecular structure, C (black); H (white); O (red); N (blue); Ni (green) and Li (pink). Thermal ellipsoids are shown at the 50% probability level.

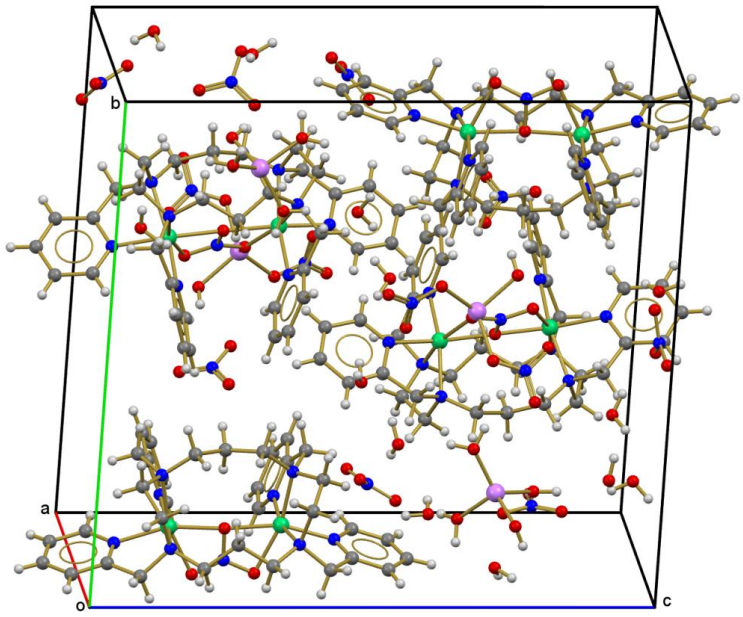

Fig. S5: a) Unit cell of compound **2**. Perspective view of the molecular structure, C (black); H (white); O (red); N (blue); Ni (green) and Li (pink). Thermal ellipsoids are shown at the 50% probability level.

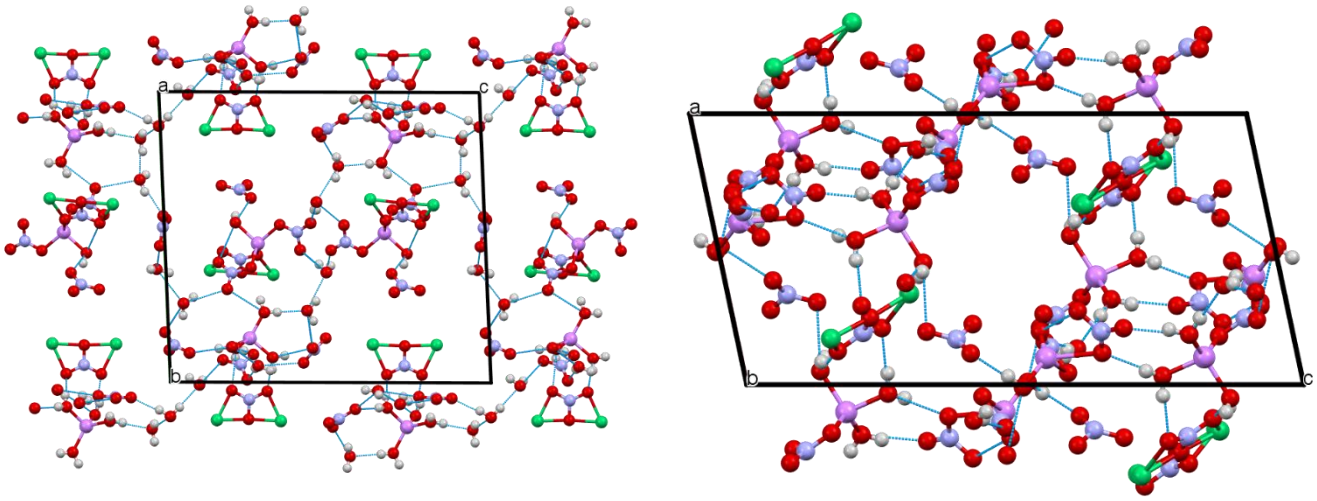

Fig. S6: Perspective of the intermolecular interactions present in compound **2**, along the planes b-c (left) and a-c (right). For clarity only nitrates, water molecules and lithium complexes are shown.

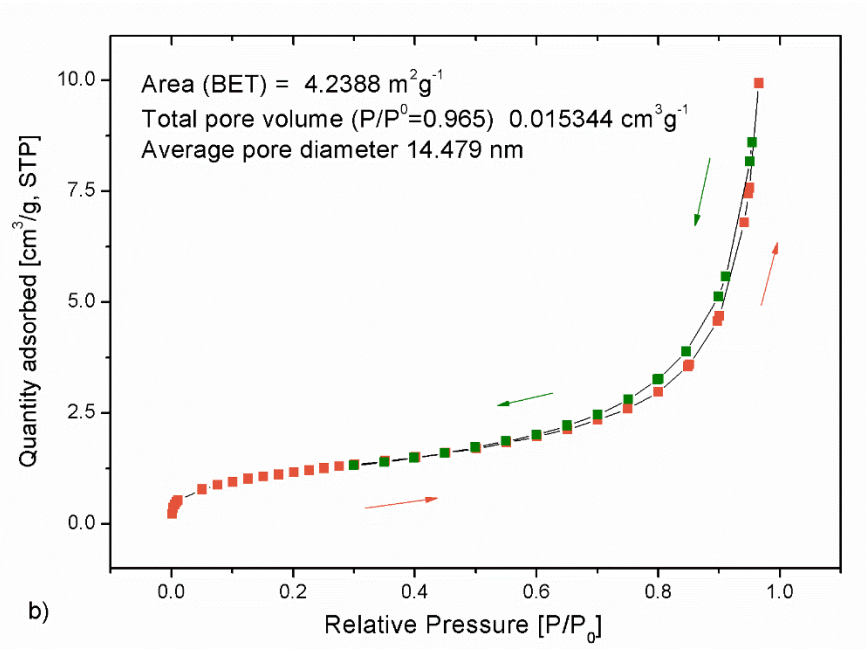

Fig. S7: Adsorption-desorption isotherms of compound **1**, measured at relative low pressure, under N_2.

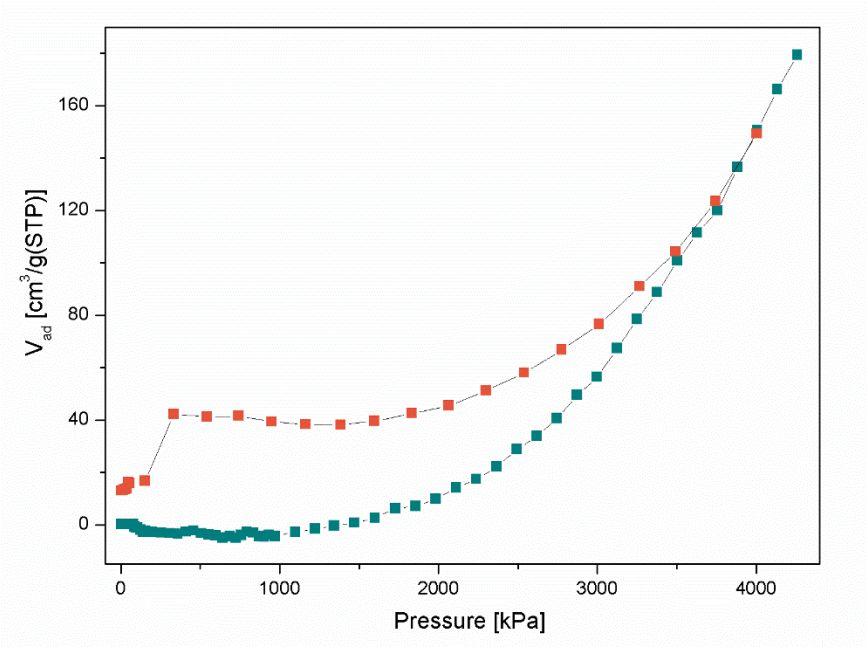

Fig. S8: Adsorption-desorption isotherms of compound **1**, measured at high pressure, under CO_2.

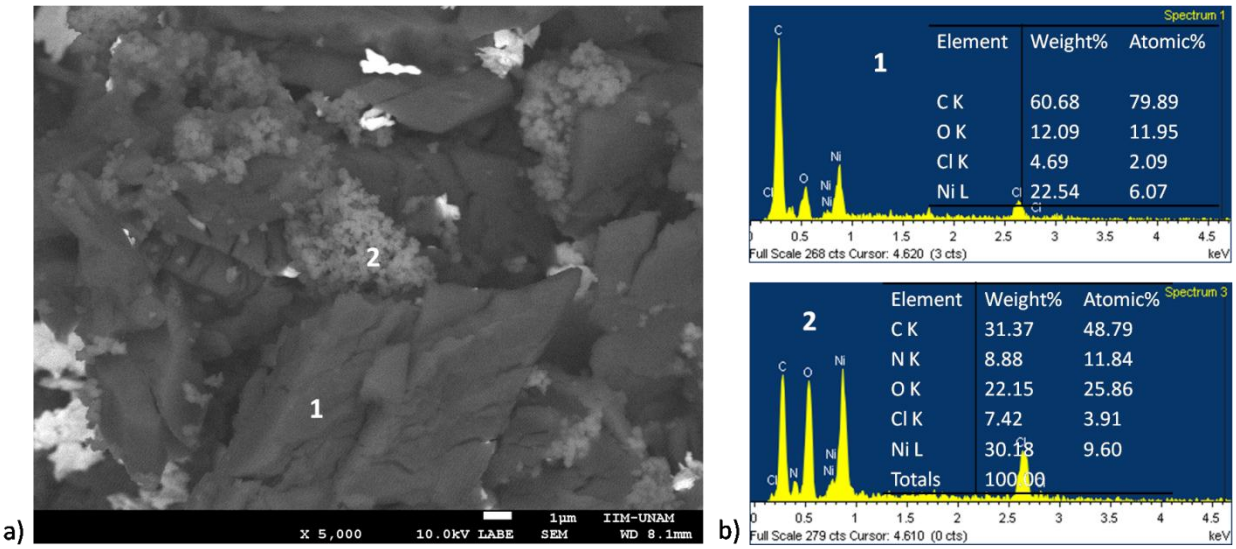

Fig. S9: a) Backscattered electron image for the violet binuclear nickel (II) compound (after adsorption process). b) Elemental analysis made by EDS. The different phases observed correspond to compounds **1** and **2**.

Table S1. Selected bond lengths [Å] and angles [°] for the equivalent nickel atoms in compound **1**, and the non-equivalent nickel atoms in compound **2**. Comparison of centres Ni(1) and Ni(2) of compound **1** with centres Ni(1) and Ni(2) of compound **2.**

1		**2**	
Bond lengths [Å]			
O(1)-Ni(1)	2.072(2)	Ni(2)-O(203)	2.077(6)
O(2)-Ni(1)	2.164(2)	Ni(1)-O(201)	2.167(6)
O(1)-Ni(2)	2.060(2)	Ni(1)-O(203)	2.068(6)
O(3)-Ni(2)	2.165(2)	Ni(2)-O(202)	2.154(6)
Ni(1)-N(5)	2.060(3)	Ni(1)-N(15)	2.071(7)
Ni(1)-N(6)	2.068(3)	Ni(1)-N(22)	2.087(8)
Ni(1)-N(1)	2.105(3)	Ni(1)-N(4)	2.131(8)
Ni(1)-N(2)	2.147(3)	Ni(1)-N(1)	2.137(8)
Ni(2)-N(8)	2.049(3)	Ni(2)-N(29)	2.050(8)
Ni(2)-N(7)	2.078(3)	Ni(2)-N(36)	2.094(7)
Ni(2)-N(4)	2.115(3)	Ni(2)-N(8)	2.127(8)
Ni(2)-N(3)	2.134(3)	Ni(2)-N(11)	2.157(8)
Angles [°]			
Ni(2)-O(1)-Ni(1)	174.92(13)	Ni(1)-O(203)-Ni(2)	174.4(4)
N(5)-Ni(1)-N(6)	93.90(12)	O(203)-Ni(1)-N(15)	162.7(3)
N(5)-Ni(1)-O(1)	91.88(10)	O(203)-Ni(1)-N(22)	90.7(3)
N(6)-Ni(1)-O(1)	161.37(11)	N(15)-Ni(1)-N(22)	94.9(3)
N(5)-Ni(1)-N(1)	81.60(12)	O(203)-Ni(1)-N(4)	101.1(3)
N(6)-Ni(1)-N(1)	95.41(11)	N(15)-Ni(1)-N(4)	96.1(3)
O(1)-Ni(1)-N(1)	102.96(10)	N(22)-Ni(1)-N(4)	80.6(3)
N(5)-Ni(1)-N(2)	165.51(12)	O(203)-Ni(1)-N(1)	97.4(3)
N(6)-Ni(1)-N(2)	81.47(11)	N(15)-Ni(1)-N(1)	81.3(3)
O(1)-Ni(1)-N(2)	96.82(10)	N(22)-Ni(1)-N(1)	164.3(3)
N(1)-Ni(1)-N(2)	85.17(12)	N(4)-Ni(1)-N(1)	84.6(3)
O(1)-Ni(1)-O(2)	62.15(9)	O(203)-Ni(1)-O(201)	62.5(2)
N(5)-Ni(1)-O(2)	97.68(11)	N(15)-Ni(1)-O(201)	100.4(3)
N(6)-Ni(1)-O(2)	99.49(10)	N(22)-Ni(1)-O(201)	98.7(3)
N(1)-Ni(1)-O(2)	165.10(10)	N(4)-Ni(1)-O(201)	163.5(2)
N(2)-Ni(1)-O(2)	96.63(11)	N(1)-Ni(1)-O(201)	97.0(3)
Angles [°]			
N(8)-Ni(2)-N(7)	92.34(11)	N(29)-Ni(2)-O(203)	94.4(3)
N(8)-Ni(2)-O(1)	91.24(10)	N(29)-Ni(2)-N(36)	91.2(3)
O(1)-Ni(2)-N(7)	164.19(10)	O(203)-Ni(2)-N(36)	162.3(3)
N(8)-Ni(2)-N(4)	82.33(12)	N(29)-Ni(2)-N(8)	82.4(3)
N(7)-Ni(2)-N(4)	95.29(11)	O(203)-Ni(2)-N(8)	101.4(3)
O(1)-Ni(2)-N(4)	100.45(10)	N(36)-Ni(2)-N(8)	96.0(3)
N(8)-Ni(2)-N(3)	166.09(11)	N(29)-Ni(2)-N(11)	164.4(3)
N(7)-Ni(2)-N(3)	80.95(11)	O(203)-Ni(2)-N(11)	96.3(3)
O(1)-Ni(2)-N(3)	98.52(10)	N(36)-Ni(2)-N(11)	81.9(3)
N(4)-Ni(2)-N(3)	86.15(12)	N(8)-Ni(2)-N(11)	84.4(3)
O(1)-Ni(2)-O(3)	62.69(9)	N(29)-Ni(2)-O(202)	96.5(3)
N(8)-Ni(2)-O(3)	97.58(10)	O(203)-Ni(2)-O(202)	62.3(2)
N(7)-Ni(2)-O(3)	101.56(10)	N(36)-Ni(2)-O(202)	100.4(3)
N(4)-Ni(2)-O(3)	163.14(10)	N(8)-Ni(2)-O(202)	163.6(2)
N(3)-Ni(2)-O(3)	95.71(11)	O(202)-Ni(2)-N(11)	98.5(3)

Table S2. Selected bond lengths [Å] and angles [°] for the lithium entities in compounds **1** and **2.**

1		**2**	
Bond lengths [Å]			
O(3W)-Li(1)	1.972(8)	Li(1)-O(201)	1.972(17)
O(4W)-Li(1)	1.921(8)	Li(1)-O(1)	1.983(19)
O(5W)-Li(1)	1.973(7)	Li(1)-O(216)	2.01(2)
O(7A)-Li(1)	2.429(9)	Li(1)-O(213)	2.03(2)
O(9A)-Li(1)	2.110(8)		
Angles [°]			
O(4W)-Li(1)-O(3W)	127.7(4)	O(201)-Li(1)-O(1)	101.1(8)
O(3W)-Li(1)-O(5W)	97.3(3)	O(201)-Li(1)-O(216)	125.8(10)
O(5W)-Li(1)-O(9A)	99.8(3)	O(1)-Li(1)-O(213)	113.2(9)
O(4W)-Li(1)-O(7A)	89.9(3)	O(216)-Li(1)-O(213)	112.4(8)
O(9A)-Li(1)-O(7A)	54.7(2)		