Supplementary Materials

Ni(II) dimers of NNO donor tridentate reduced Schiff base ligands as alkali metal ion capturing agents: Syntheses, crystal structures and magnetic properties

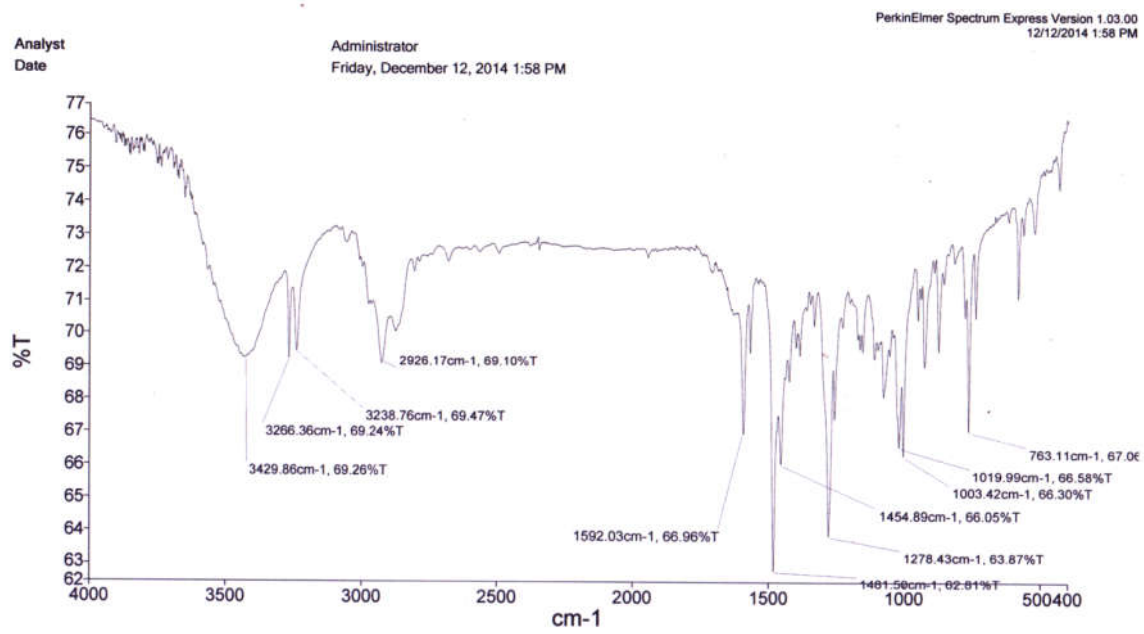

Figure S1. IR spectrum of complex **1.**

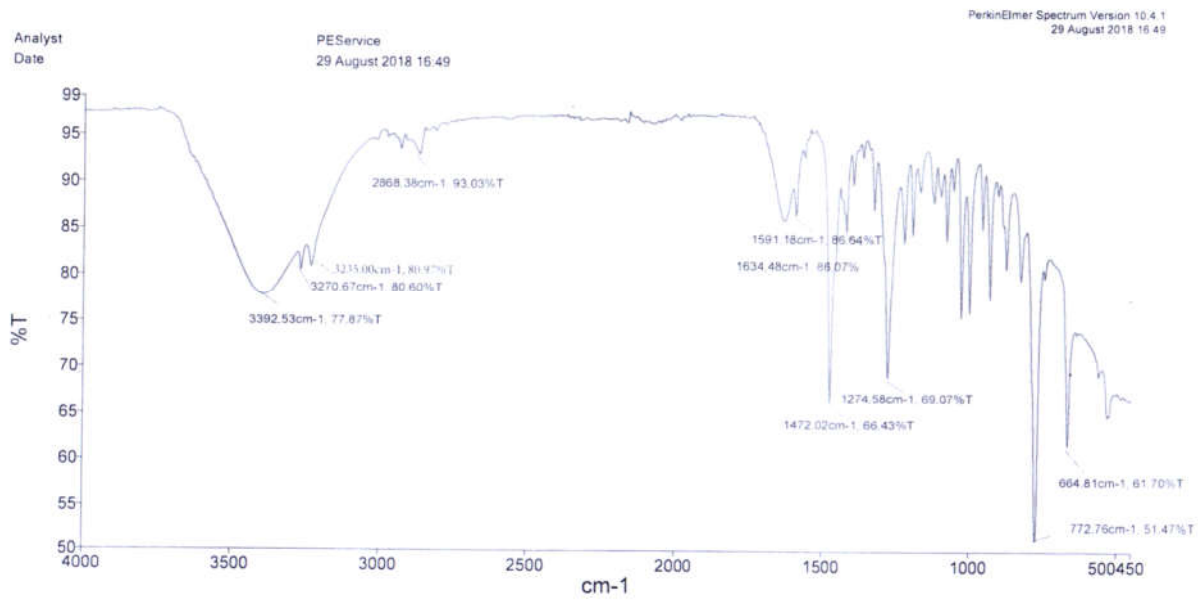

Figure S2. IR spectrum of complex **2.**

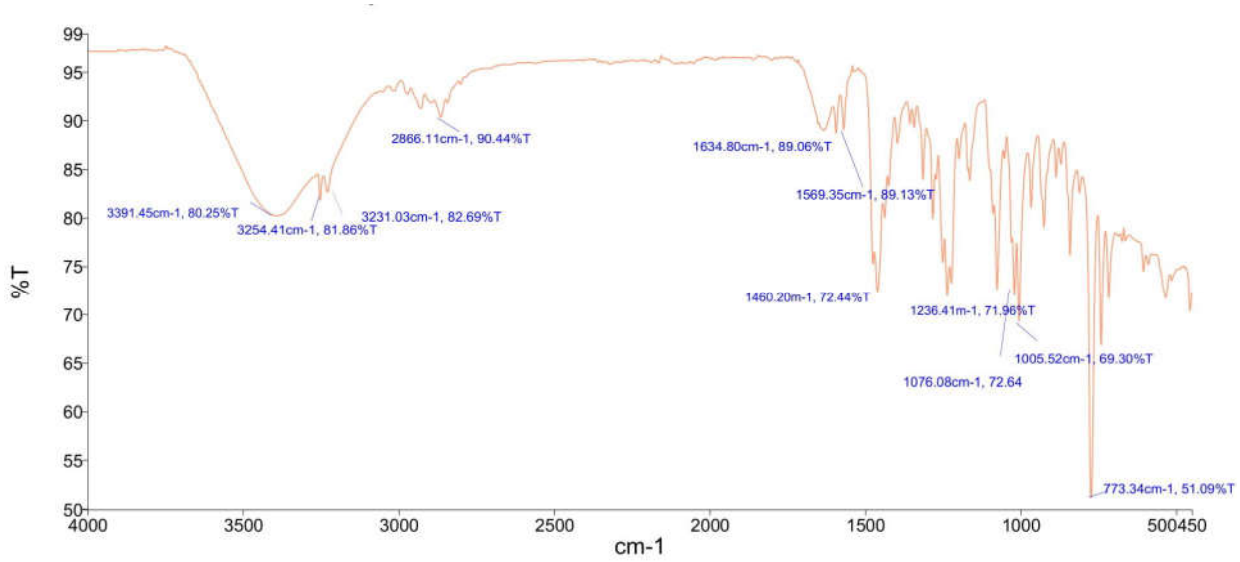

Figure S3. IR spectrum of complex **3.**

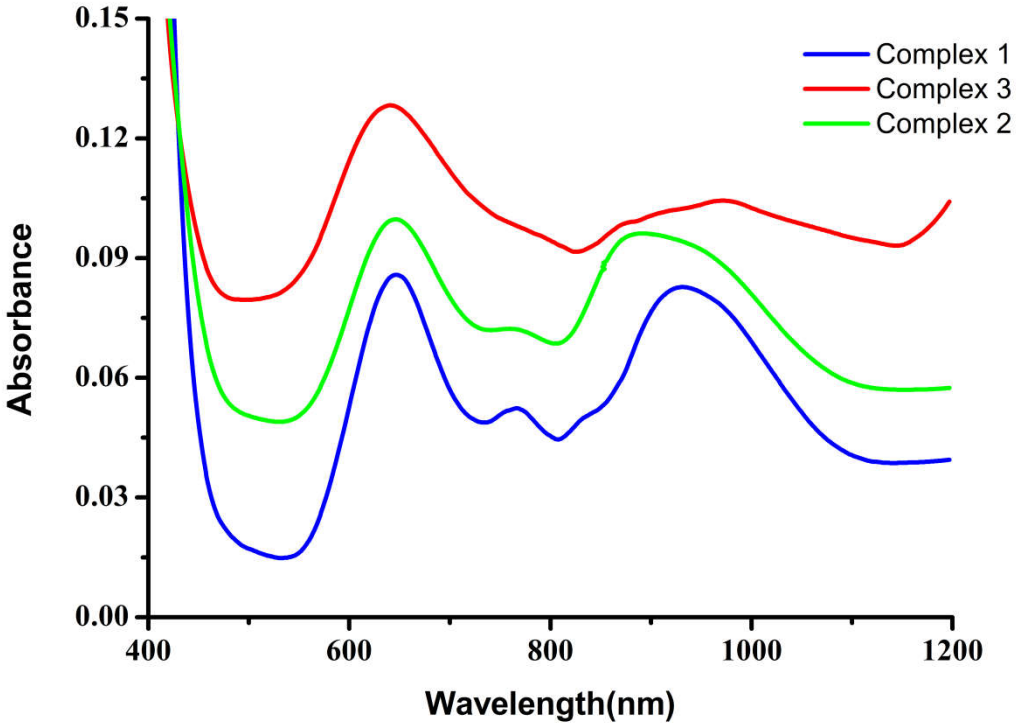

Figure S4. Electronic spectrum of complexes **1-3**.

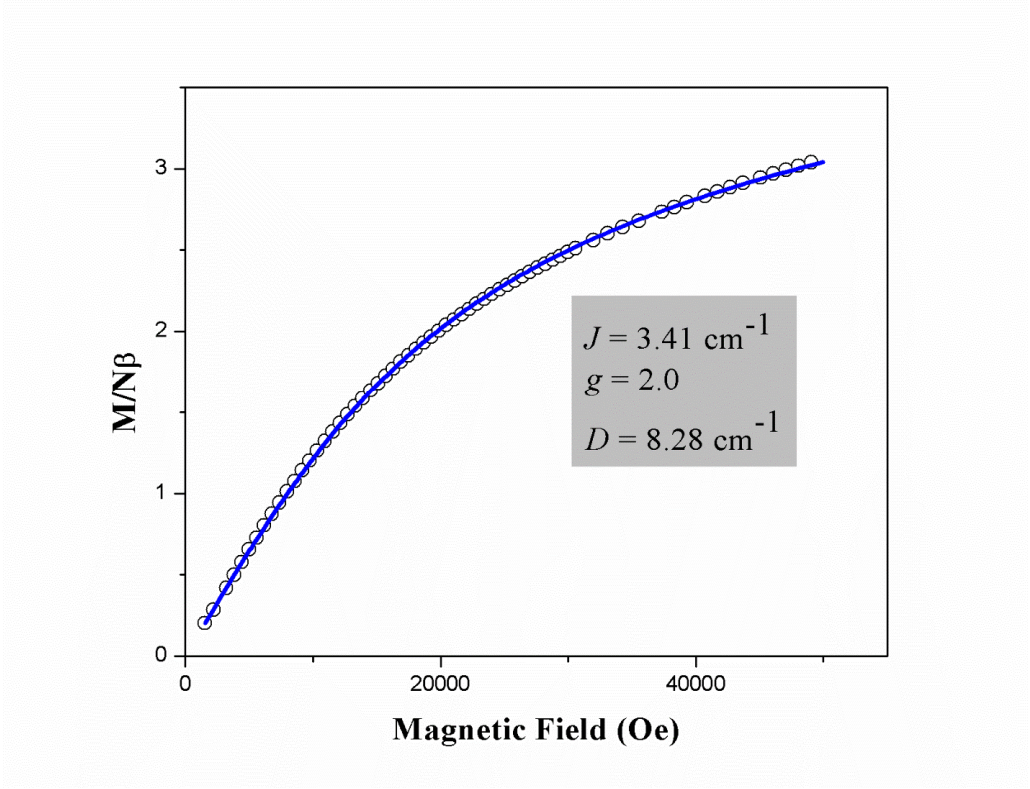

Figure S5. Magnetic field dependence of molar magnetizations for complex **1** at 2 K fitted with PHI software [1], *g* value was taken as 2.0.

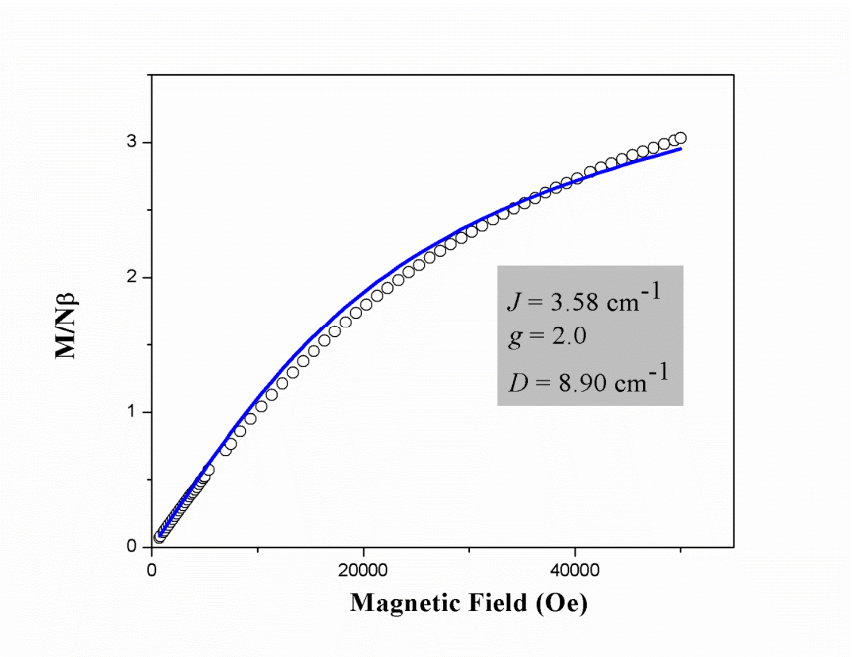

Figure S6. Magnetic field dependence of molar magnetizations for complex **2** at 2 K fitted with PHI software [1], *g* value was taken as 2.0.

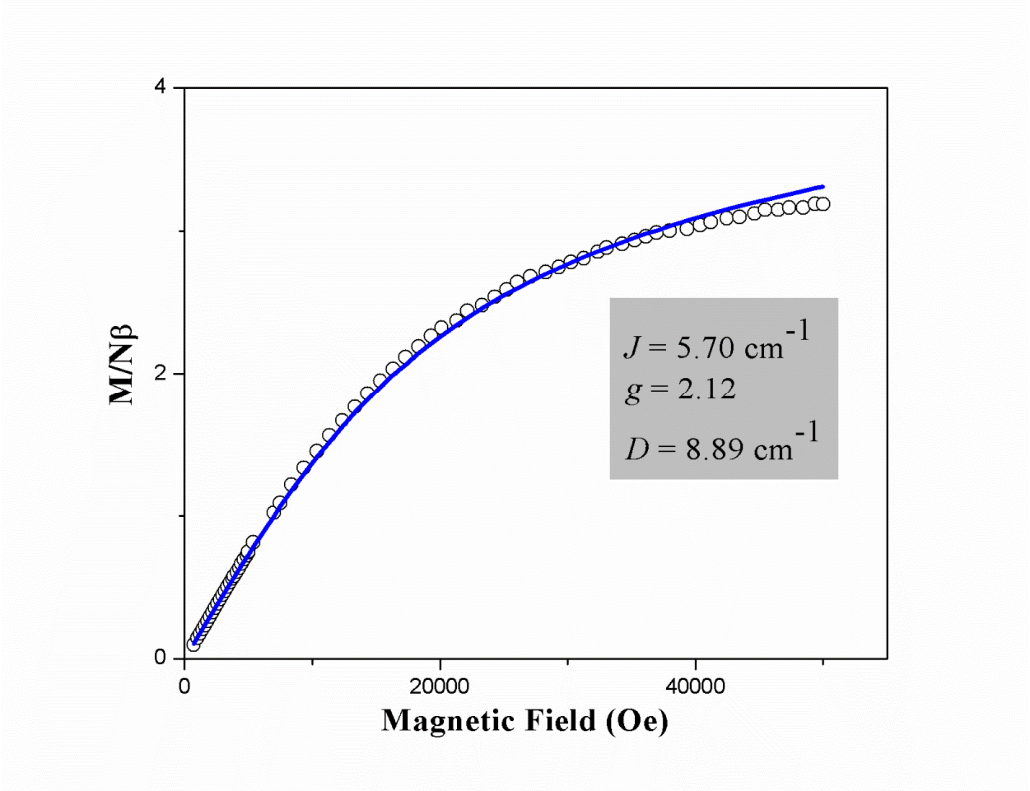

Figure S7. Magnetic field dependence of molar magnetizations for complex **3** at 2 K fitted with PHI software [1].

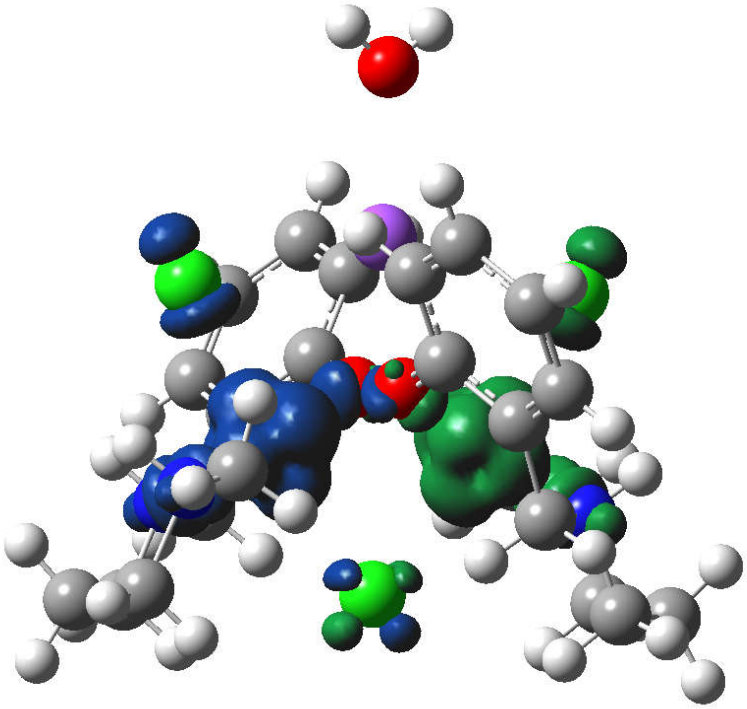

Figure S8. SD in the BS state of complex **1** (blue and green surfaces – α and β spin, iso value 0.002).

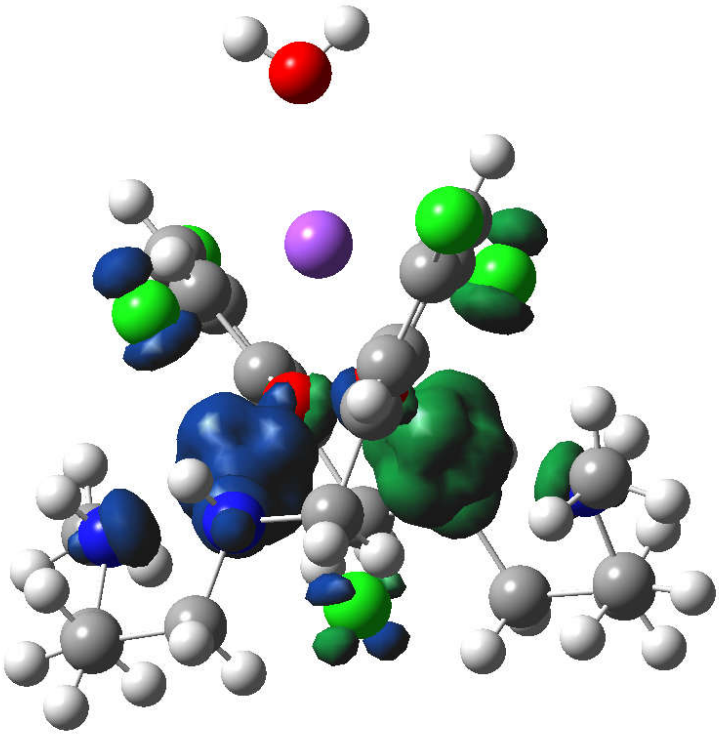

Figure S9. SD in the BS state of complex **2**(blue and green surfaces – α and β spin, iso value 0.002).

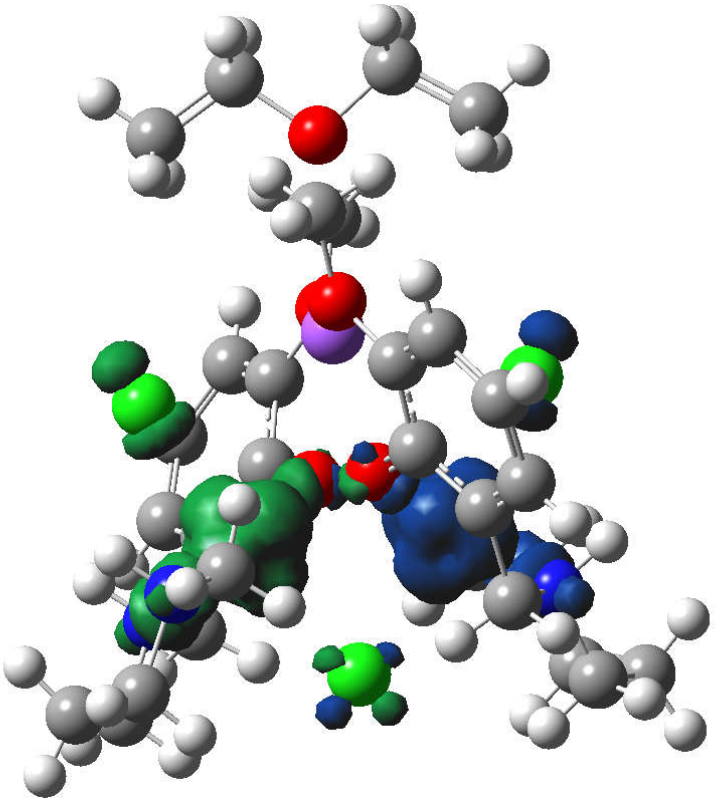

Figure S10. SD in the BS state of complex **3**(blue and green surfaces – α and β spin, iso value 0.002).

Table S1. Molecular dimensions (distances, Å, angles, °) in **1**, **2** and **3**.

Compound	**1**	**2**	**3**
Ni(1)−O(11)	2.049(2)	2.053(2)	2.0335(11)
Ni(1)−N(19)	2.080(3)	2.083(2)	2.0864(14)
Ni(1)−N(23)	2.085(3)	2.079(2)	2.0887(15)
Ni(1)−O(11)$1	2.164(2)	2.164(2)	2.3178(11)
Ni(1)−Cl(1)	2.4782(10)	2.4626(8)	2.45640(5)
Ni(1)−Cl(2)	2.4300(10)	2.4497(7)	2.4106(5)
Na(1)−O(11)	2.388(3)	2.400(2)	2.4164(15)
Na(1)−O(1)	2.293(6)	2.296(6)	2.775(4)
Na(1)−Cl(2)	2.7532(11)	2.7525(8)	2.8930(5)
Na(1)−O(131)			2.4265(13)
O(11)−Ni(1)−N(19)	93.13(10)	92.36(7)	93.72(5)
O(11)−Ni(1)−N(23)	174.25(11)	174.75(8)	172.49(6)
N(19)−Ni(1)−N(23)	92.01(12)	92.84(8)	92.42(6)
O(11)−Ni(1)−O(11)$1	74.70(10)	74.36(8)	74.58(5)
N(19)−Ni(1)−O(11)$1	165.91(10)	166.05(7)	163.94(5)
N(23)−Ni(1)−O(11)$1	100.50(11)	100.51(8)	100.18(5)
O(11)−Ni(1)−Cl(2)	90.53(7)	90.91(6)	89.27(4)
N(19)−Ni(1)−Cl(2)	95.58(9)	94.02(6)	97.26(4)
N(23)−Ni(1)−Cl(2)	86.42(10)	87.99(7)	85.68(5)
O(11)−Ni(1)−Cl(1)	84.12(7)	83.95(5)	86.63(4)
N(19)−Ni(1)−Cl(1)	89.99(8)	92.82(6)	87.70(4)
N(23)−Ni(1)−Cl(1)	98.45(10)	96.52(7)	97.93(5)
O(11)$1−Ni(1)−Cl(1)	81.84(6)	81.73(7)	80.77(3)
Cl(2)−Ni(1)−Cl(1)	172.49(3)	171.60(2)	173.76(2)
O(11)−Na(1)−O(11)$1	64.75(12)	64.18(9)	66.39(6)
O(11)−Na(1)−O(131)			67.37(4)
O(11)−Na(1)−O(131)$1			130.39(6)
O(131)−Na(1)−O(131)$1			161.91(8)
O(11)−Na(1)−O(1)	147.63(6)	147.91(5)	146.81(3)
O(131)−Na(1)−O(1)			80.95(4)
O(11)−Na(1)−Cl(2)	76.42(7)	77.06(5)	71.71(3)
O(11)-Na(1)-Cl(2)$1	79.53(7)	78.83(5)	80.44(4)

O(131)−Na(1)−Cl(2)$1			83.96(4)
O(131)−Na(1)−Cl(2)			101.26(4)
O(1)−Na(1)−Cl(2)	104.27(5)	104.27(4)	106.66(2)
Cl(2)−Na(1)−Cl(2)$1	151.45(10)	151.46(7)	146.68(4)

$1= 1-x, y, 3/2-z.

Reference

1. Chilton, N.F., Anderson, R.P., Turner, L.D., Soncini, A. Murray, K.S. PHI: A powerful new program for the analysis of anisotropic monomeric and exchange-coupled polynuclear d-and f-block complexes. *J. comput. Chem.* **2013**, *34*, 1164-1175.