Electronic Supplementary Information for Dalton Transactions

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SUPPLEMENTARY MATERIAL

Synthesis, structure and chiroptical study of chiral macrocyclic imine nickel(II) coordination compounds derived from camphor

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Table S1. Structural parameters determined by X-ray single crystal diffraction and theoretical calculations.

Bond Length	Exp.	Calc.	Bond Angles	Exp.	Calc.
1a					
N1-C1	1.411(3)	1.478	C1-N1-S1	115.37(16)	121.23
N2-C2	1.444(3)	1.485	C2-N2-S2	121.41(17)	122.08
N3-C3	1.475(3)	1.481	N1-C1-C2	118.44(19)	110.24
N4-C4	1.481(3)	1.478	C1-C2-N2	121.04(19)	116.17
N1-S1	1.6365(19)	1.682	N3-C3-C4	109.09(18)	111.03
N2-S2	1.6118(18)	1.672	C3-C4-N4	110.11(19)	110.64
S1-O1	1.4361(17)	1.517	O1-S1-O2	121.32(10)	121.11
S1-O2	1.4531(16)	1.511	O3-S2-O4	120.27(10)	121.49
S2-O3	1.3879(17)	1.514			
S2-O4	1.3879(17)	1.515			
C1-C2	1.504(3)	1.541			
C3-C4	1.511(3)	1.547			
1b					
N1-C1	1.429(5)	1.485	C1-N1-S1	125.9(3)	122.05
N2-C2	1.416(5)	1.478	C2-N2-S2	123.1(2)	121.23
N3-C3	1.454(5)	1.478	N1-C1-C2	116.0(3)	110.24
N4-C4	1.445(5)	1.481	C1-C2-N2	117.7(3)	116.18
N1-S1	1.608(3)	1.672	N3-C3-C4	111.4(3)	110.64
N2-S2	1.593(3)	1.682	C3-C4-N4	110.4(3)	111.03

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S1-O1	1.401(3)	1.515	O1-S1-O2	118.56(17)	121.49
S1-O2	1.401(3)	1.514	O3-S2-O4	118.93(17)	121.11
S2-O3	1.397(3)	1.511			
S2-O4	1.453(3)	1.517			
C1-C2	1.478(6)	1.541			
C3-C4	1.481(6)	1.547			
2a					
Ni(1)-N1	1.890(3)	1.902	N1-Ni1-N2	86.39(13)	85.89
Ni(1)-N2	1.890(3)	1.892	N1-Ni1-N3	97.55(13)	93.97
Ni(1)-N3	1.930(3)	1.963	N1-Ni1-N4	167.80(13)	176.32
Ni(1)-N4	1.888(3)	1.938	N2-Ni1-N3	94.64(13)	97.76
N1-C1	1.464(6)	1.479	N2-Ni1-N4	176.02(12)	164.49
N2-C2	1.452(6)	1.499	N3-Ni1-N4	81.62(12)	82.60
N3-C3	1.460(6)	1.502	N1-C1-C2	107.0(4)	108.21
N4-C4	1.489(6)	1.502	C1-C2-N2	109.7(4)	109.48
N1-S1	1.602(3)	1.673	N3-C3-C4	104.5(4)	104.06
N2-S2	1.595(3)	1.662	C3-C4-N4	107.9(4)	108.46
S1-O1	1.441(3)	1.532	C1-N1-S1	116.4(3)	113.99
S1-O2	1.433(3)	1.524	C2-N2-S2	112.6(2)	116.25
S2-O3	1.436(3)	1.520	O1-S1-O2	116.48(17)	116.83
S2-O4	1.444(3)	1.522	O3-S2-O4	113.7(2)	118.32
C1-C2	1.510(5)	1.533			
C3-C4	1.514(5)	1.545			
2b					
Ni(1)-N1	1.882(4)	1.902	N1-Ni1-N2	86.63(18)	85.89

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Ni(1)-N2	1.872(4)	1.892	N1-Ni1-N3	97.36(19)	93.97
Ni(1)-N3	1.887(4)	1.962	N1-Ni1-N4	168.1(2)	176.31
Ni(1)-N4	1.931(4)	1.938	N2-Ni1-N3	175.92(18)	164.49
N1-C1	1.482(4)	1.502	N1-C1-C2	104.8(3)	104.06
N2-C2	1.463(4)	1.503	C1-C2-N2	108.3(3)	108.46
N3-C3	1.482(4)	1.499	N3-C3-C4	109.1(3)	108.21
N4-C4	1.459(4)	1.479	C3-C4-N4	106.6(3)	109.48
N1-S1	1.608(5)	1.673	N2-Ni1-N4	94.06(19)	97.77
N2-S2	1.587(5)	1.662	N3-Ni1-N4	82.23(18)	82.61
S1-O1	1.442(3)	1.524	C1-N1-S1	116.0(3)	113.98
S1-O2	1.429(4)	1.532	C2-N2-S2	111.3(3)	116.25
S2-O3	1.434(4)	1.520	O1-S1-O2	116.5(2)	116.83
S2-O4	1.448(4)	1.523	O3-S2-O4	113.4(3)	118.32
C1-C2	1.517(7)	1.534			
C3-C4	1.520(7)	1.545			

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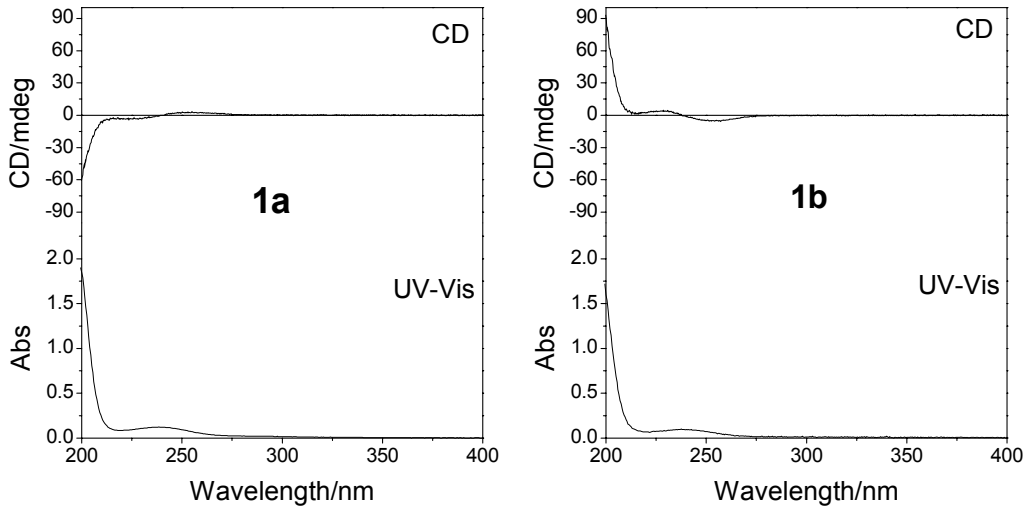

Figure S1. Electronic absorption and CD spectra measured in MeOH of **1**a and **1**b

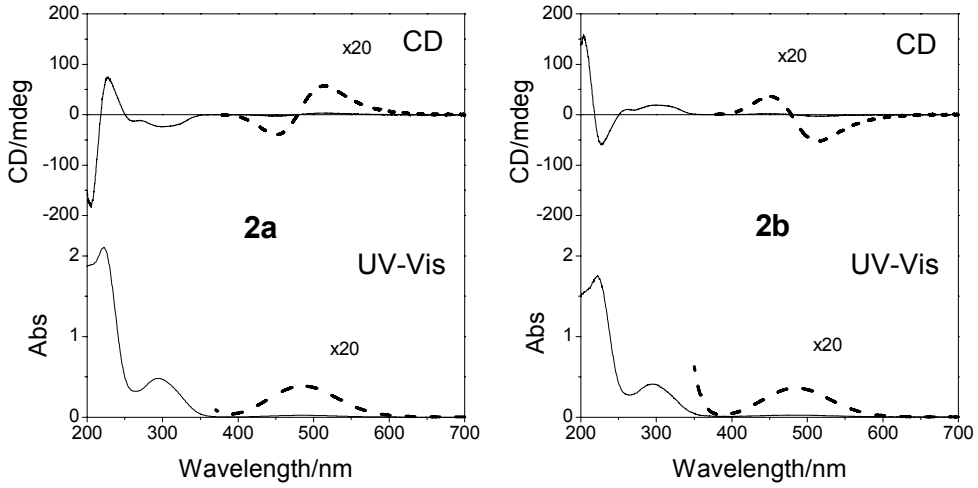

Figure S2. Electronic absorption and CD spectra measured in MeOH of **2**a and **2**b

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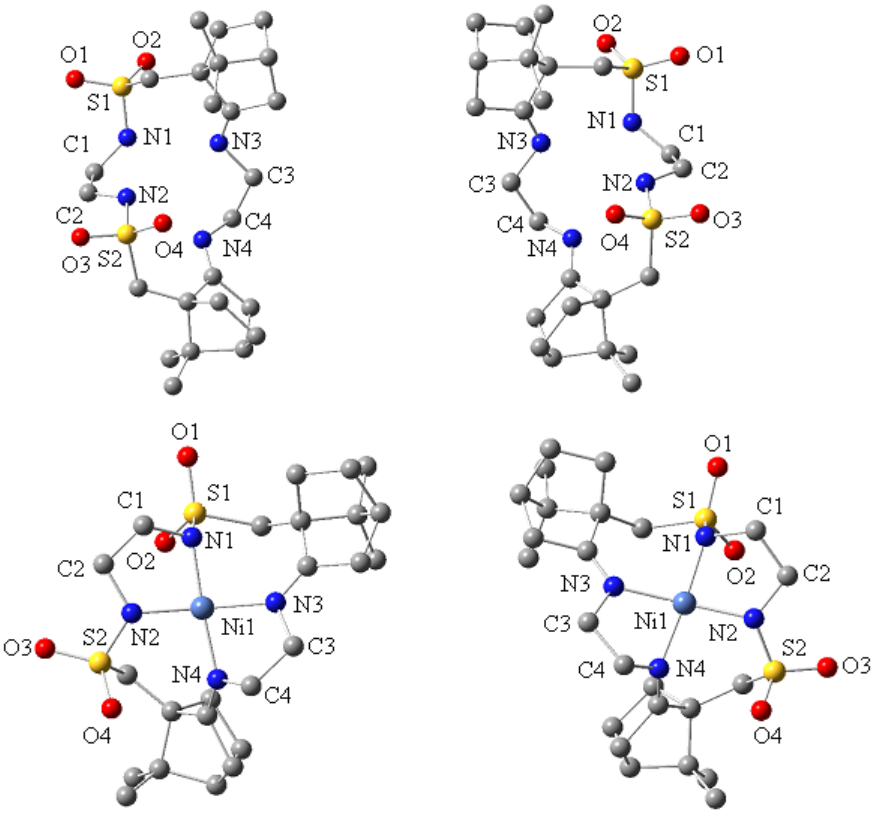

Figure S3. Optimized molecular structure of ligands(upper) and nickel coordination compounds(lower).