Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

The Coordination Structure of the Extracted Nickel(II) Complex with a Synergistic Mixture Containing Dinonylnaphthalene Sulfonic Acid and 2-Ethylhexyl-4-Pyridine carboxylate Ester

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Outline

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^{1}H-NMR Spectra

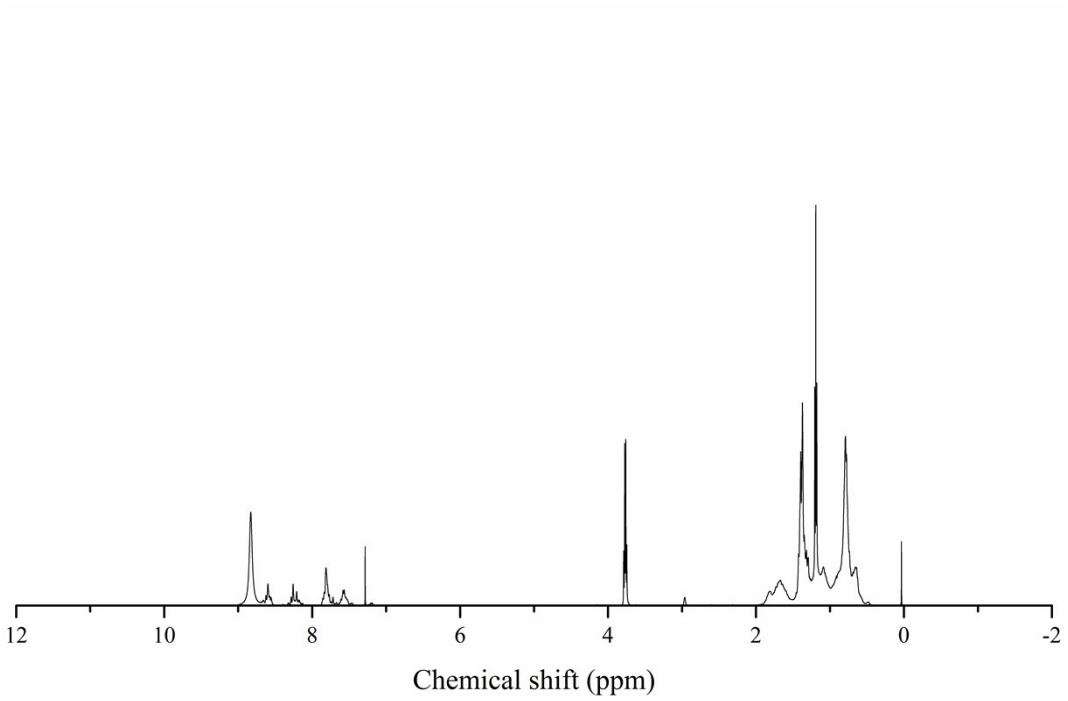

Figure S1 ^{1}H-NMR spectrum of purified HDNNS

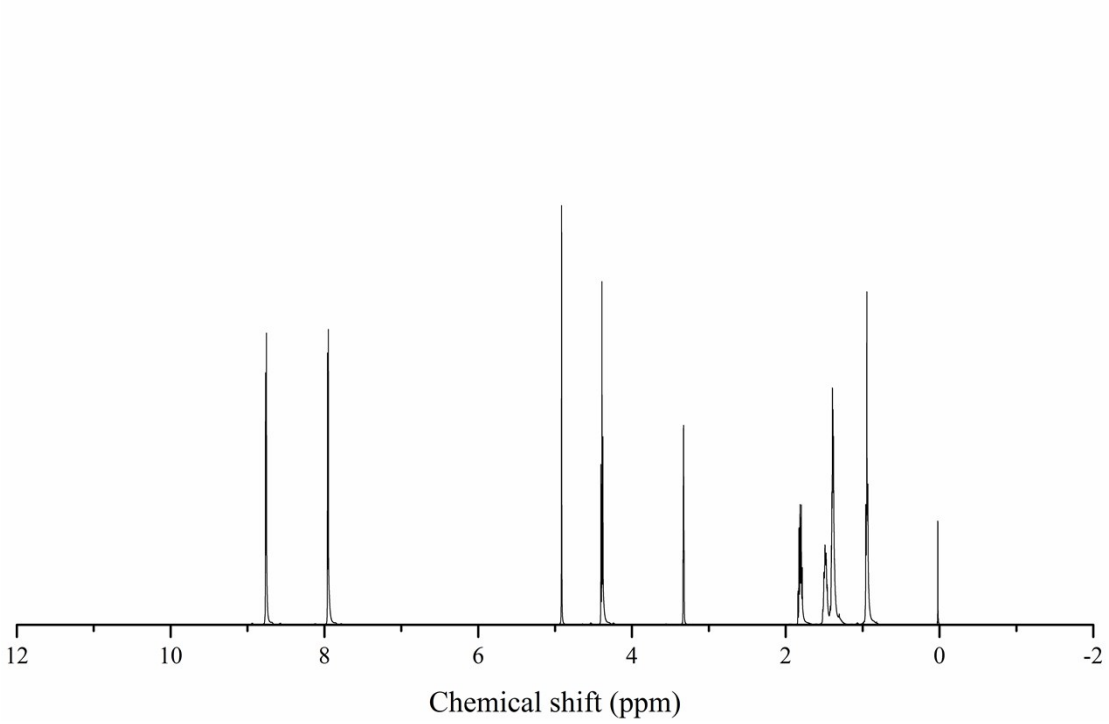

Figure S2 ^{1}H-NMR spectrum of n-hexyl -4-pyridinecarboxylate ester (L^{I})

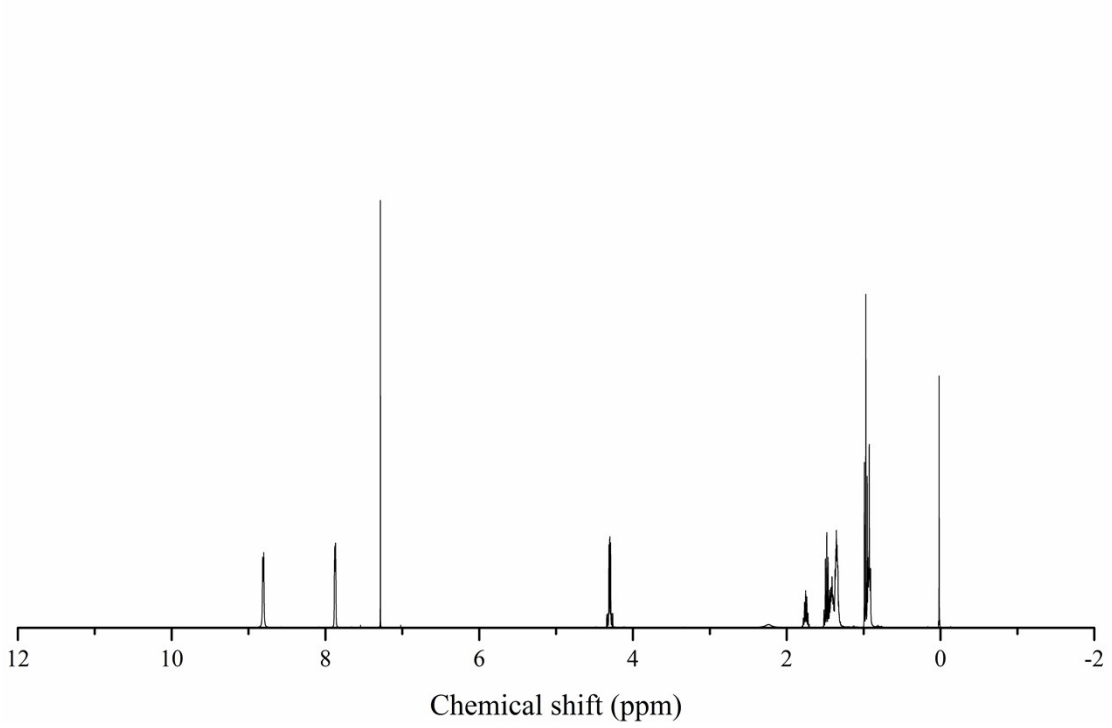

Figure S3 ^{1}H-NMR spectrum of 2-ethylhexyl 4-pyridinecarboxylate ester (4PC, L^{II})

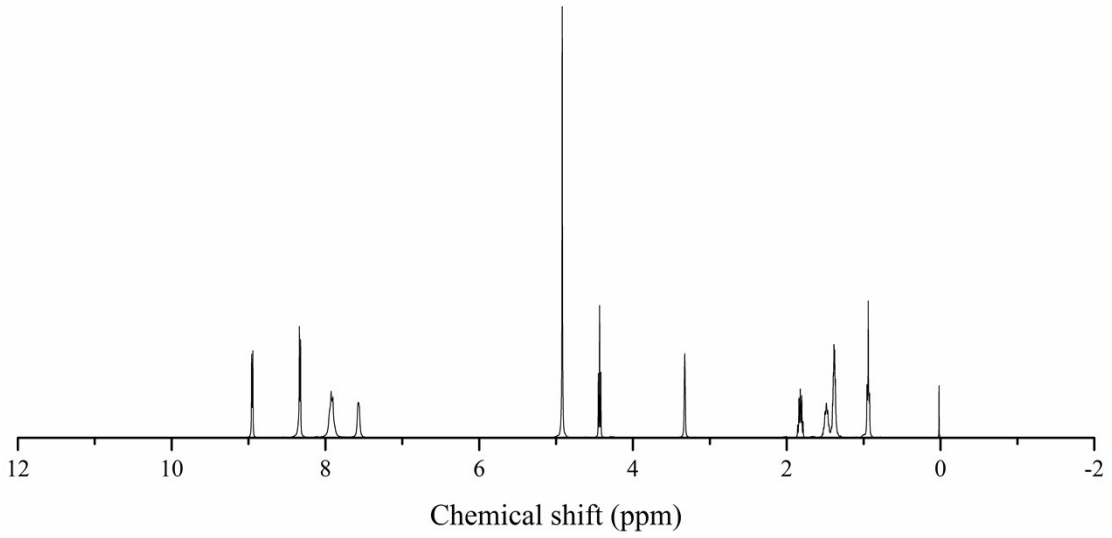

Figure S4 ^{1}H-NMR spectrum of the nickel synergist complex

Crystallographic details

Table S1 Important bond lengths (Å) and angles (°)

Ni1-O1W	2.063(3)	Ni1-O2W	2.071(3)
Ni1-N1	2.104(3)		
O1W-Ni1-O1W^{a}	180.0	O2W-Ni1-N1	88.66(11)
O1W-Ni1-O2W	91.35(11)	O2W^{a}-Ni1-N1	91.34(11)
O1W^{a}-Ni1-O2W	88.65(11)	O1W-Ni1-N1^{a}	88.18(10)
O1W-Ni1-O2W^{a}	88.65(11)	O1W^{a}-Ni1-N1^{a}	91.82(10)
O1W^{a}-Ni1-O2W^{a}	91.35(11)	O2W-Ni1-N1^{a}	91.34(11)
O2W^{a}-Ni1-O2W	180.0	O2W^{a}-Ni1-N1^{a}	88.66(11)
O1W-Ni1-N1	91.82(10)	N1-Ni1-N1^{a}	180.00(5)
O1W^{a}-Ni1-N1	88.18(10)		

Symmetry code: ^{a}-x, -y+1, -z+2.

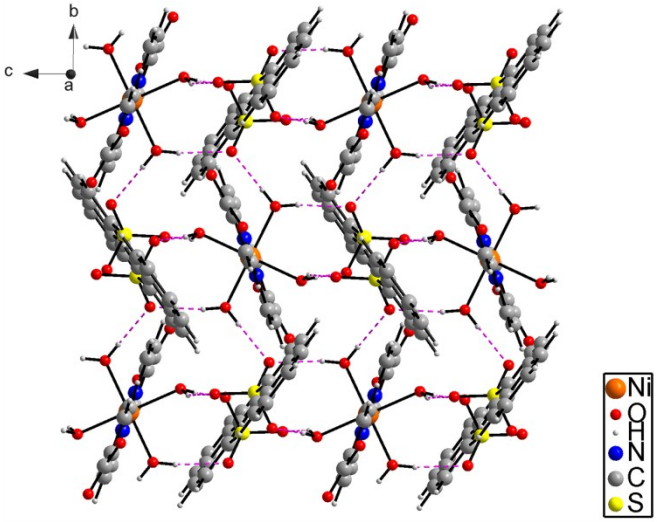

Figure S5 2D plane for alternating rows of $Ni(H_2O)_4(L^I)_2^{2+}$ cations linked by naphthalene-2-sulfonate anions spacers in the nickel synergist complex as viewed along the a-axis

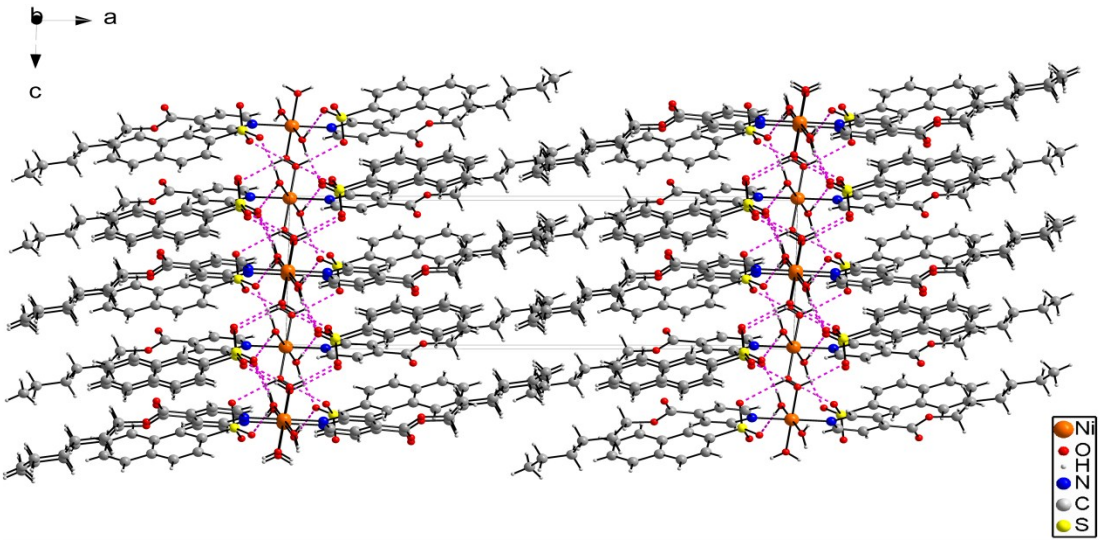

Figure S6 The packing structure of the nickel synergist complex viewed down the b-axis.

Table S2 Summary of hydrogen bonding (Å and °) for the nickel synergist complex

D-H...A	Symmetry operation on A	D-H (Å)	H…A (Å)	D…A (Å)	D-H…A (°)
O1W-H11…O5	-x, -y+1,-z+1	0.815	1.940	2.755	177.30
O1W-H12…O6	x, y, z	0.816	1.998	2.795	165.44
O2W-H21…O7	-x, y+1/2, -z+3/2	0.822	1.975	2.798	179.16
O2W-H22…O7	-x, -y+1, -z+1	0.815	2.031	2.829	166.22

FI-IR details

Table S3 Infrared frequencies and assignments of L^{I}, HNS, the nickel synergist complex, L^{II}, HDNNS and the extracted Ni(II) complex in the non-polar organic phase

Vibrstional modes	L^{I}	HNS	The nickel synergist complex	L^{II}	HDNNS	The extracted Ni(Ⅱ) complex
$\nu_{as}(CH_3)$	2957		2956	2960	2960	2959
$\nu_{as}(CH_2)$	2858		2861	2866	2870	2868
$\nu_{s}(CH_3)$	2928		2928	2929	2928	2929
ν(C=O)	1728		1731	1730		1731
$\delta_{as}(CH_3)$	1462		1465	1463	1464	1462
$\delta_{s}(CH_3)$	1383		1383	1383	1382	1382
ν(py)	1407		1417	1407		1417
ν(C=C)	1638	1644	1638	1636	1631	1634
	1561	1501	1562	1562	1502	1562
			1503			1502
ν(C-O)	1279		1287	1281		1280
ν_{s}(S=O)		1043	1034		1051	1040

ESI-MS Spectra

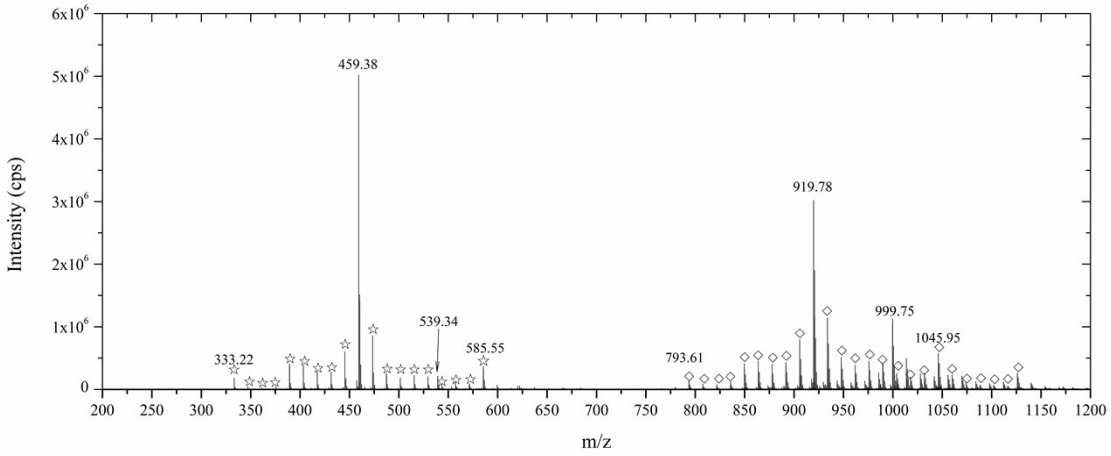

Figure S7 The ESI-MS spectrum of the purified HDNNS in n-hexane with a final concentration of 10^{-3} mol L^{-1}; ☆ represents species of monomer HDNNS homologues and ◇ represents species of dimer $(HDNNS)_2$ where one of HDNNS was replaced by HDNNS homologues.

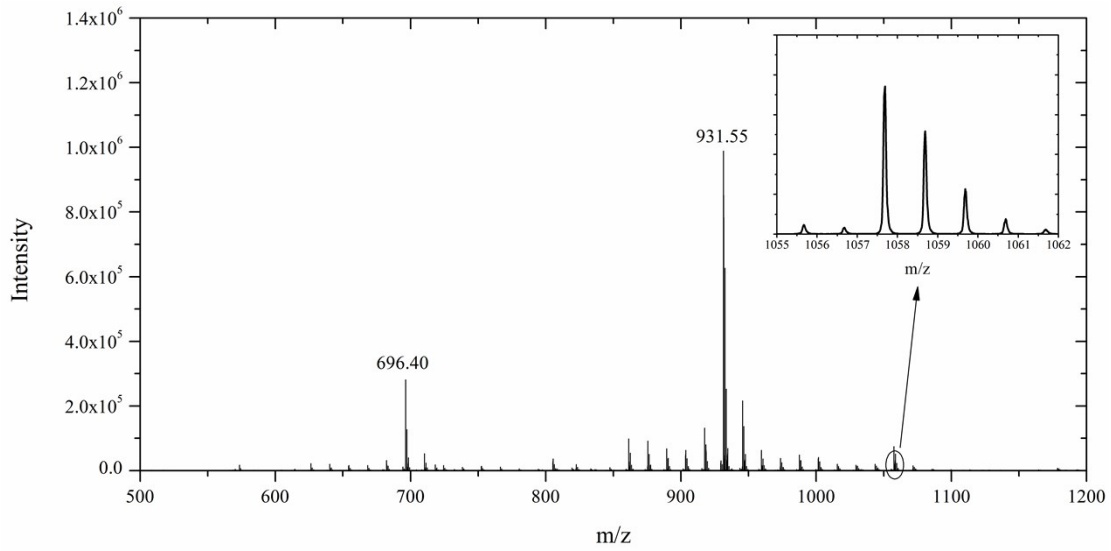

Figure S8 The ESI-MS spectrum of the synergistic extractants in the non-polar organic phase.