Supporting information

Thiolate-Protected Ni_{39} and Ni_{41} Nanoclusters: Synthesis, Self-Assembly and Magnetic Property

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Figures:

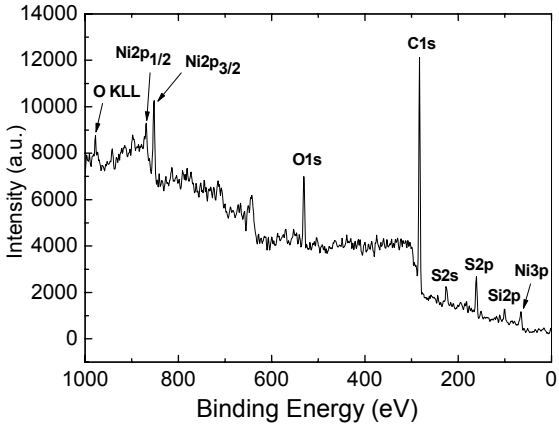

Fig. S1 Survey scan of XPS analysis of the nickel clusters.

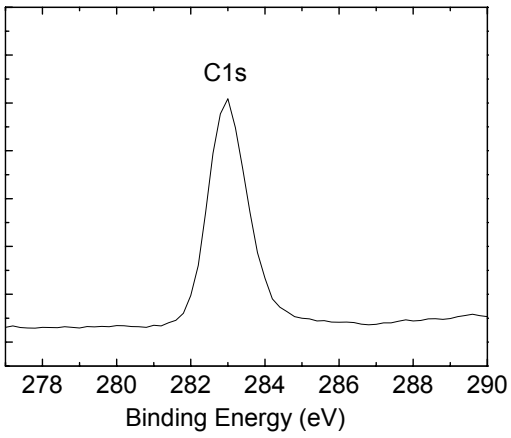

Fig. S2 XPS analysis of Ni nanoclusters: C1s electrons.

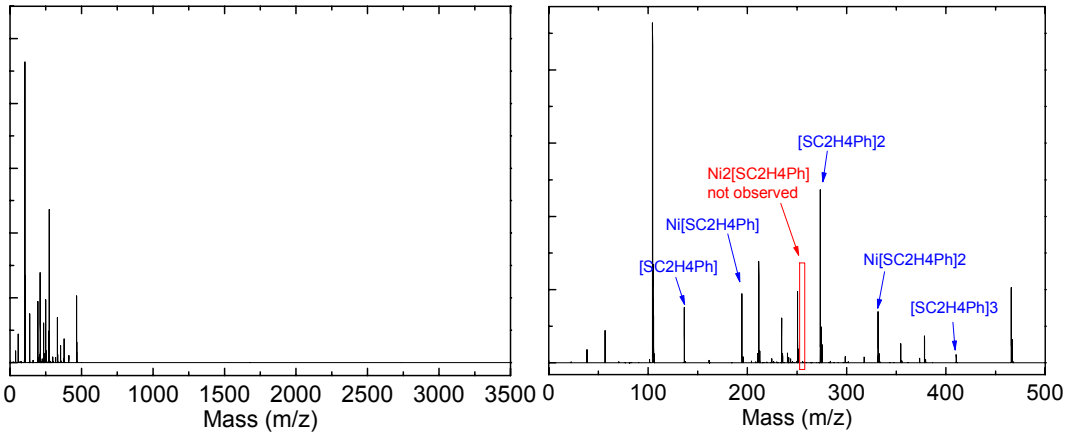

Fig. S3 MALDI-TOF mass spectrum of Ni cluster sample in m/z range of 0–3500.

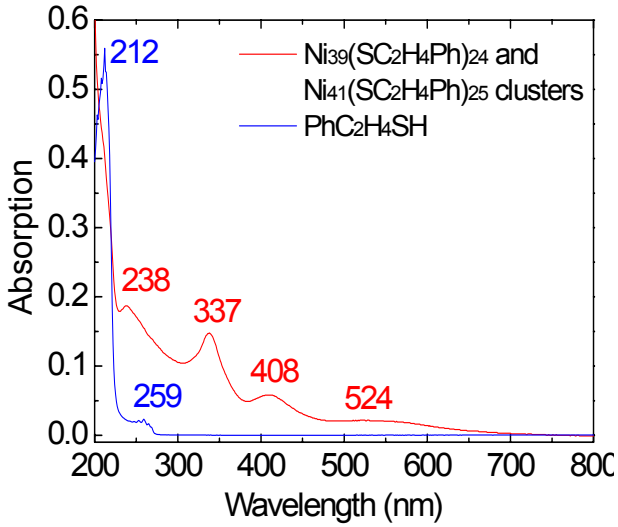

Fig. S4 UV-vis spectrum of the nickel clusters and pure ligand of PhC_2H_4SH in cyclohexane.

Table S1 Possible structural models of the $Ni_{39}(SC_2H_4Ph)_{24}$ and $Ni_{41}(SC_2H_4Ph)_{25}$. (SR= SC_2H_4Ph)

$Ni_{39}(SC_2H_4Ph)_{24}$			$Ni_{41}(SC_2H_4Ph)_{25}$		
Num. of $Ni_2(SR)_3$ Staples	Num. of $Ni(SR)_2$ Staples	Ni Core	Num. of $Ni_2(SR)_3$ Staples	Num. of $Ni(SR)_2$ Staples	Ni Core
8	0	23	7	2	25
6	3	24	5	5	26
4	6	25	3	8	27
2	9	26	1	11	28
0	12	27			

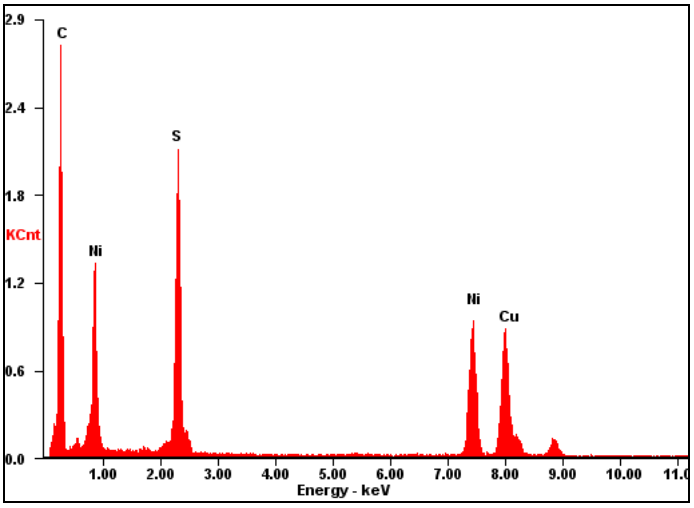

Fig. S5 EDS spectrum of the Ni clusters. No Na, Cl or B element is detected. The Cu is from the background of TEM copper grid.

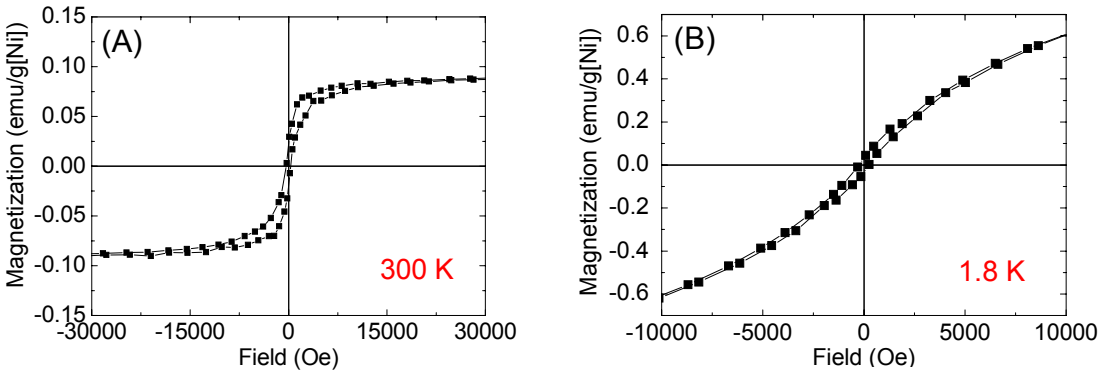

Fig. S6 Magnetization hysteresis loops of the nickel clusters measured at (A) 300 K, (B) 1.8 K.

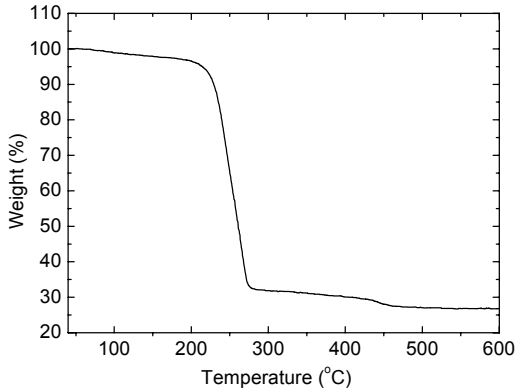

Fig. S7 TGA of the $Ni_{39}(SC_2H_4Ph)_{24}$ and $Ni_{41}(SC_2H_4Ph)_{25}$ clusters carried out under N_2 at a heating rate of 10 °C/min.

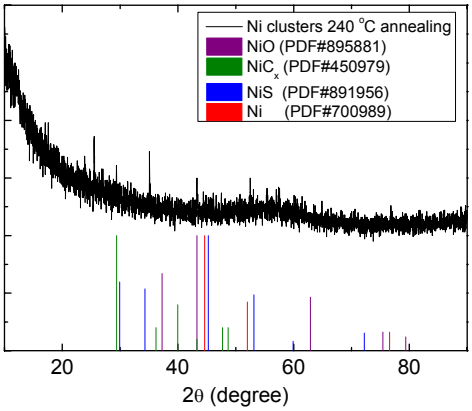

Fig. S8 XRD spectra of the $Ni_{39}(SC_2H_4Ph)_{24}$ and $Ni41(SC_2H_4Ph)_{25}$ clusters annealed in Ar at 240 ºC for 2 hrs. No material phase can be clearly identified.

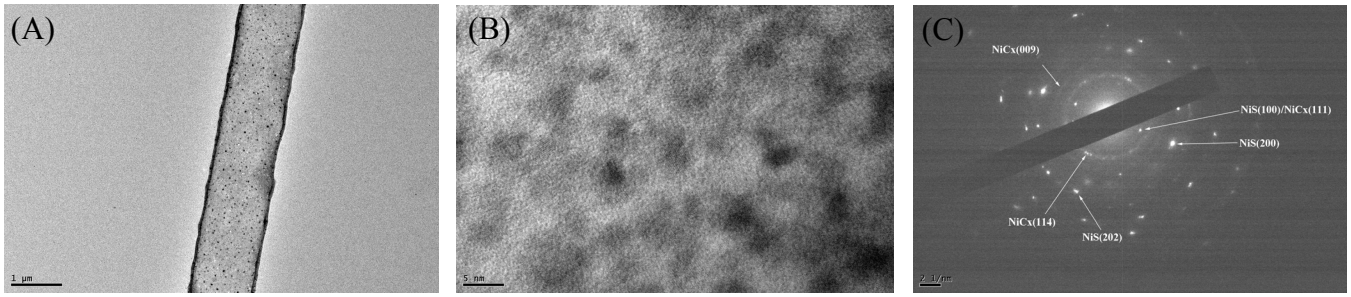

Fig. S9 (A) TEM image of the a assembled $Ni_{39}(SC_2H_4Ph)_{24}$ and $Ni_{41}(SC_2H_4Ph)_{25}$ cluster rod annealed in Ar at 240 ºC for 2 hrs (scale bar: 1μm), and corresponding (B) HRTEM image (scale bar: 5 nm). (C) The selected area electron diffraction (SAED) indicates the existence of NiS and NiC_x nanocrystals.