

## SUPPLEMENTARY INFORMATION

### Preparation and characterization of Au nanoparticles capped with mercaptocarboranyl clusters

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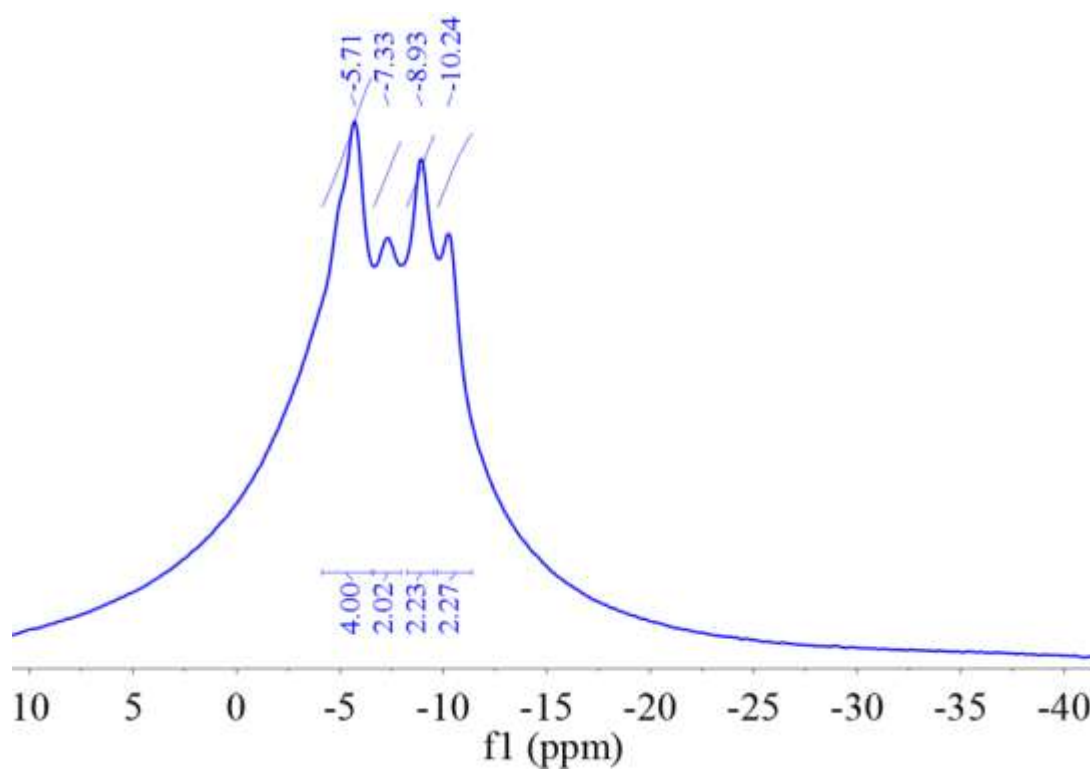
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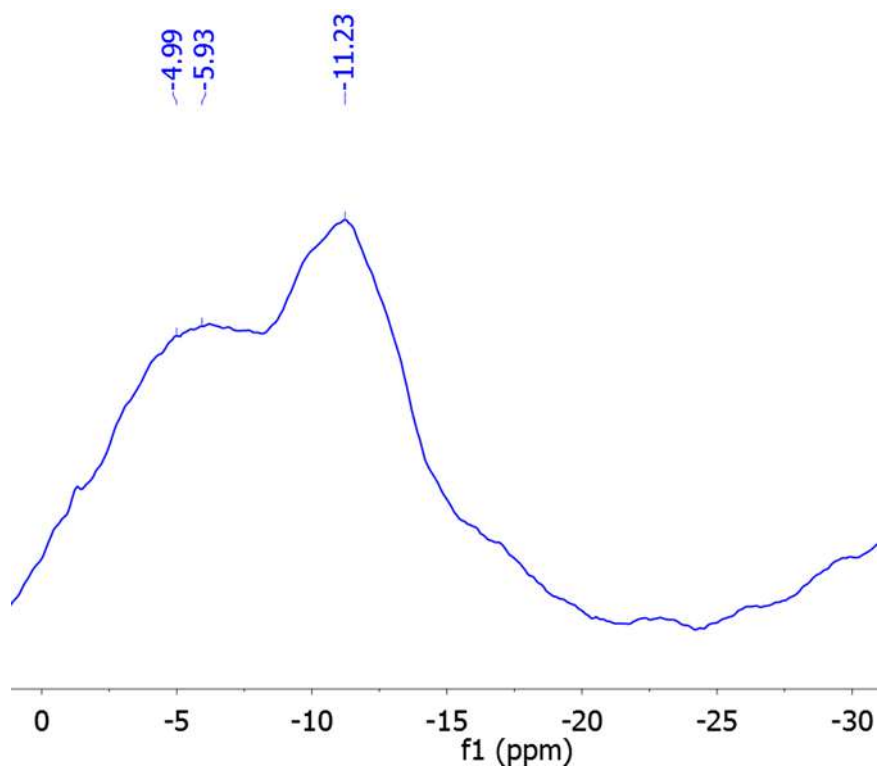
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- Figure S10.** FTIR spectra of ligand **2** (black) and its corresponding 10 nm MPCs (red).
- Figure S11.** FTIR spectra of ligand **3** (black) and its corresponding 10 nm MPCs (red).

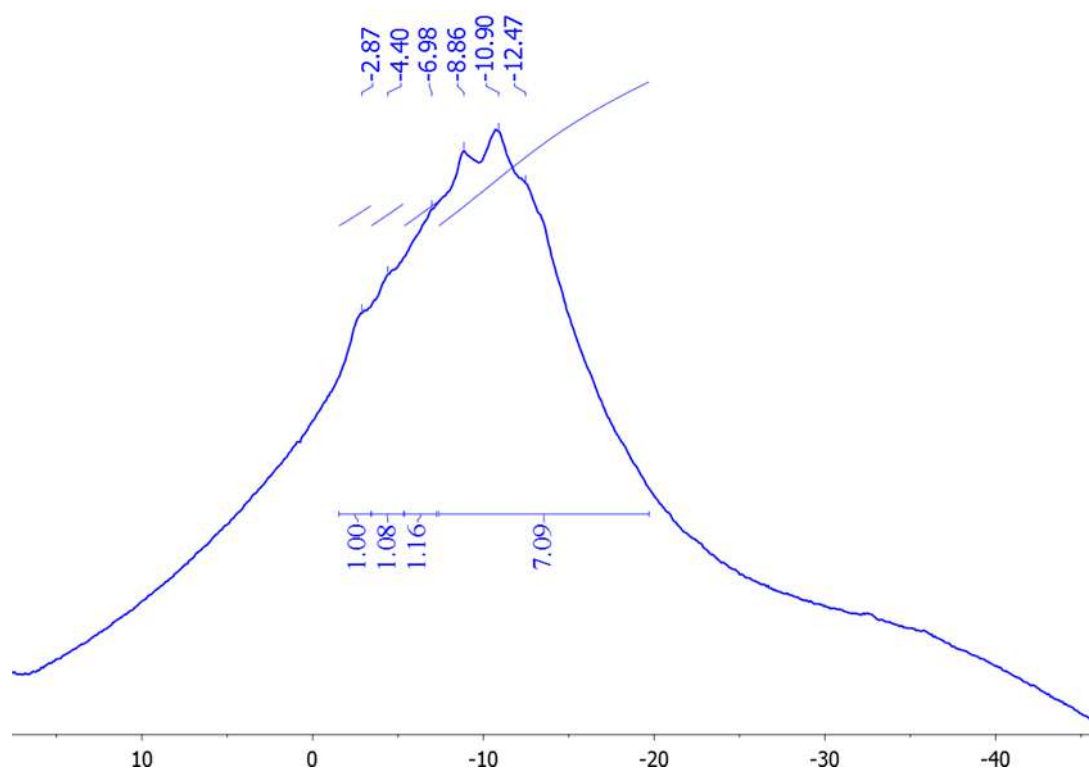
**Figure S1.**  $^{11}\text{B}\{^1\text{H}\}$ -NMR spectrum (recorded in  $\text{d}_6$ -acetone) of MPCs modified with ligand **1**.



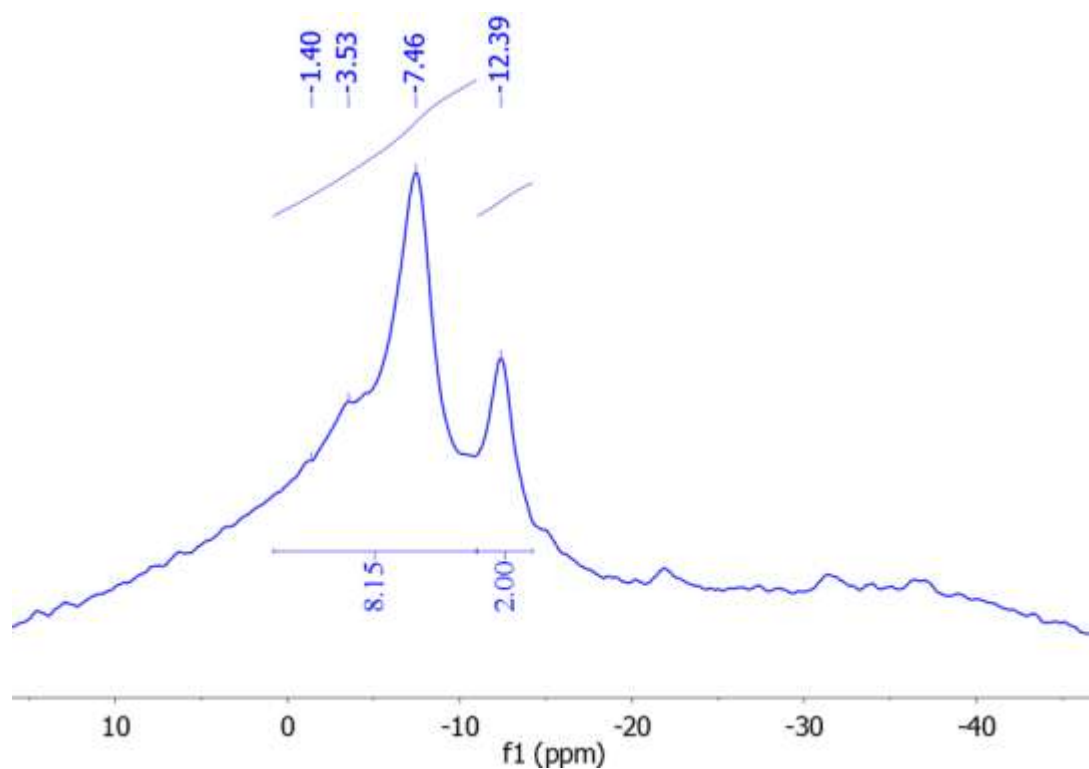
**Figure S2.**  $^{11}\text{B}$ -NMR spectrum (recorded in  $\text{d}_6$ -acetone) of MPCs modified with ligand **1**.



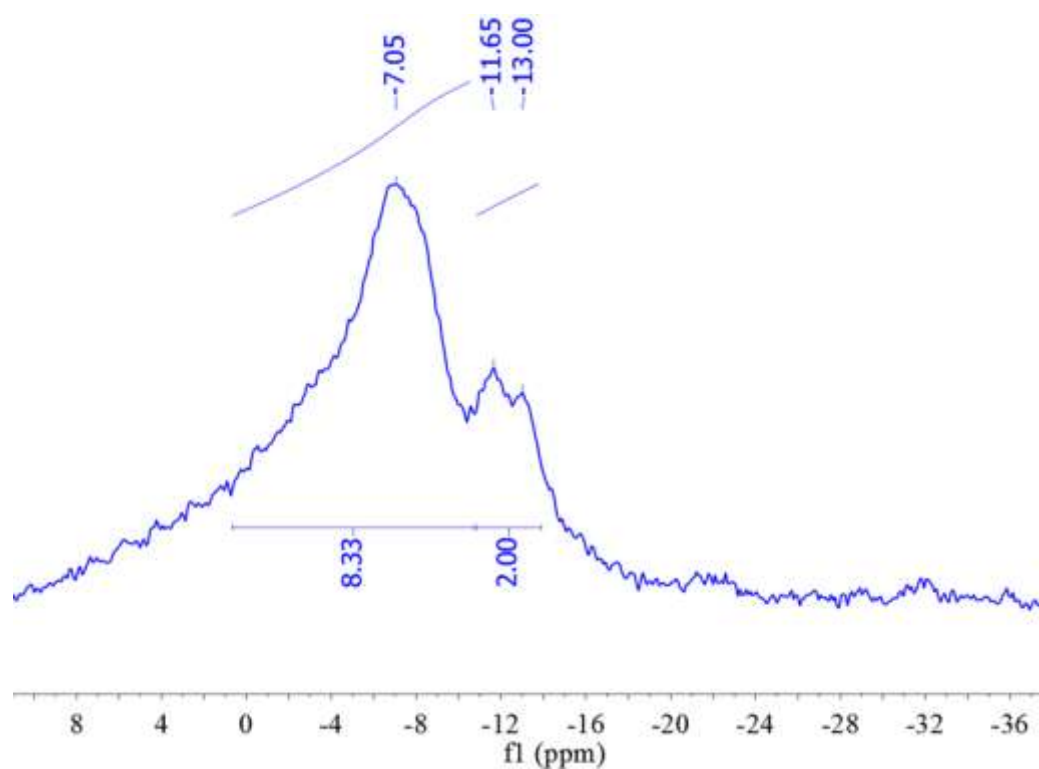
**Figure S3.**  $^{11}\text{B}\{^1\text{H}\}$ -NMR spectrum (recorded in  $\text{d}_6$ -acetone) of MPCs modified with ligand **2**.



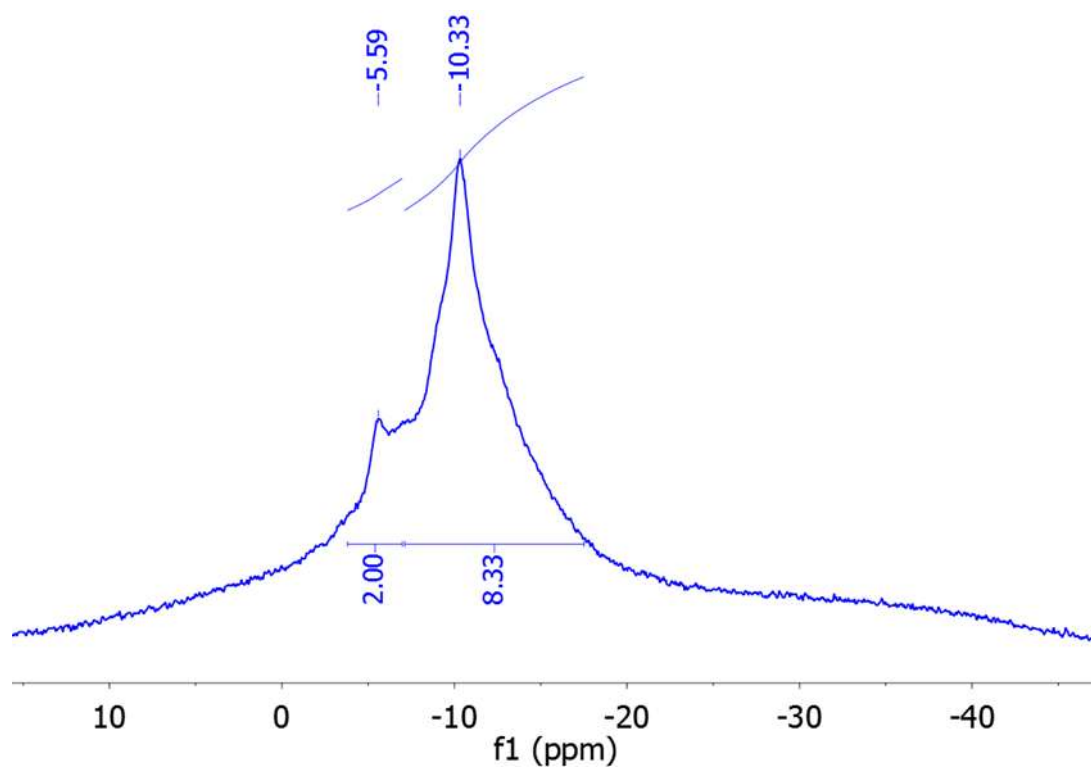
**Figure S4.**  $^{11}\text{B}\{^1\text{H}\}$ -NMR spectrum (recorded in  $\text{d}_6$ -acetone) of MPCs modified with ligand **3**.



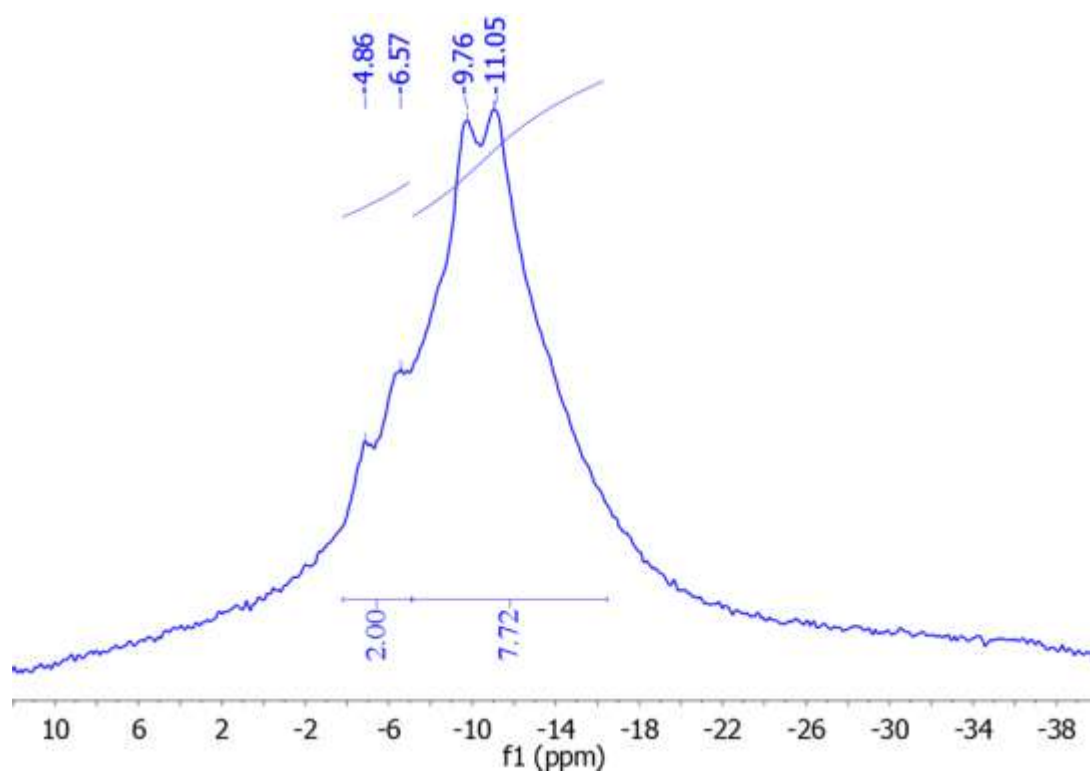
**Figure S5.**  $^{11}\text{B}$ -NMR spectrum (recorded in  $\text{d}_6$ -acetone) of MPCs modified with ligand **3**.



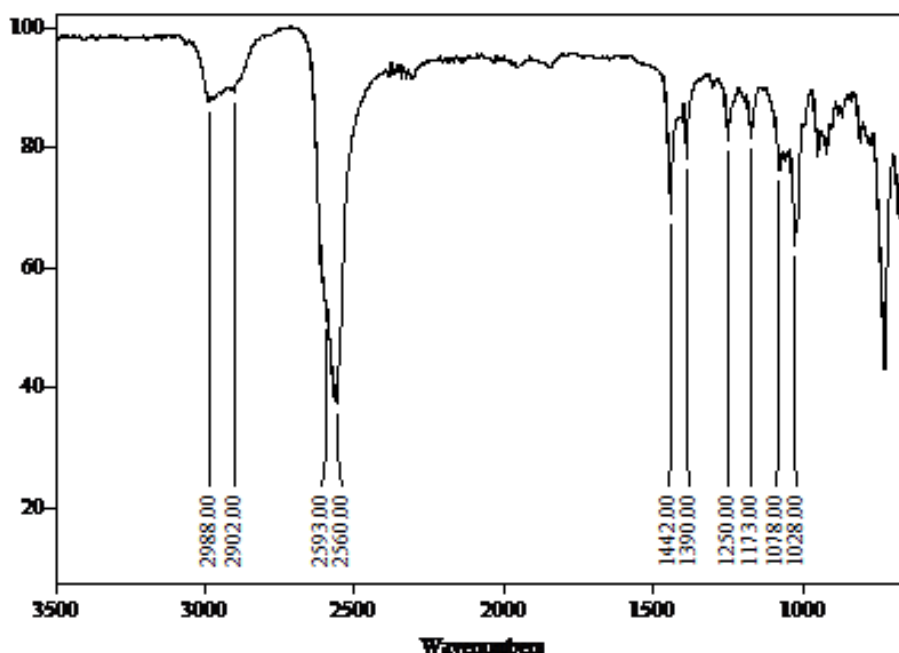
**Figure S6.**  $^{11}\text{B}\{^1\text{H}\}$ -NMR spectrum (recorded in  $\text{d}_6$ -acetone) of MPCs modified with ligand **5**.



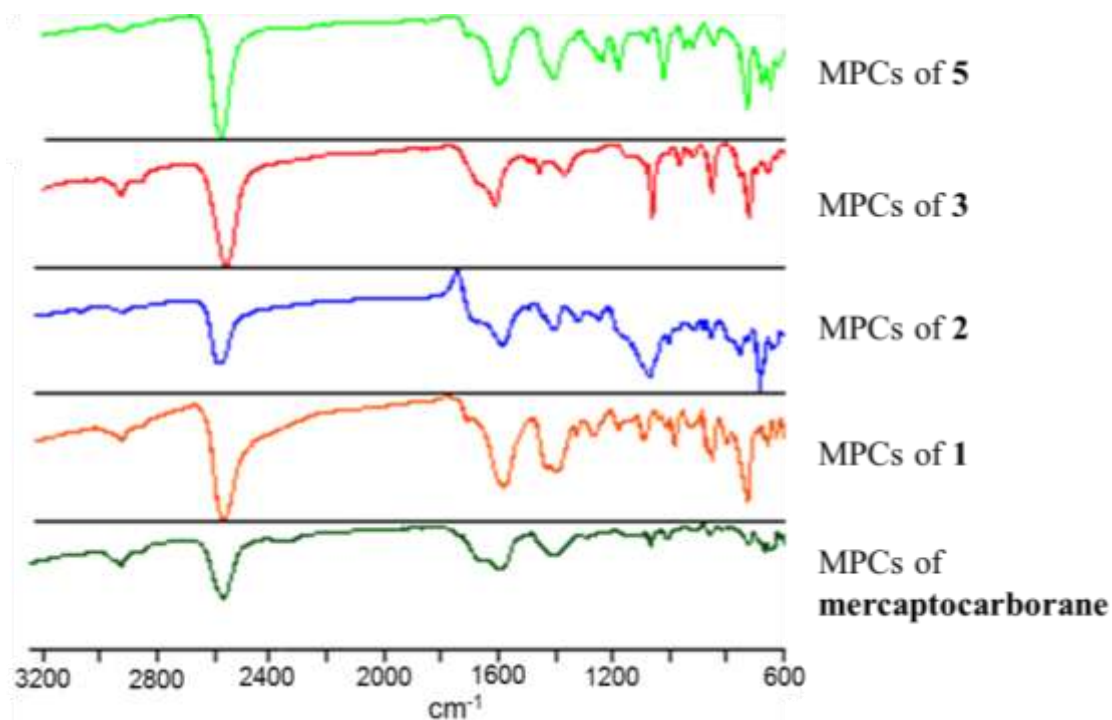
**Figure S7.**  $^{11}\text{B}$ -NMR spectrum (recorded in  $\text{d}_6$ -acetone) of MPCs modified with ligand **5**.



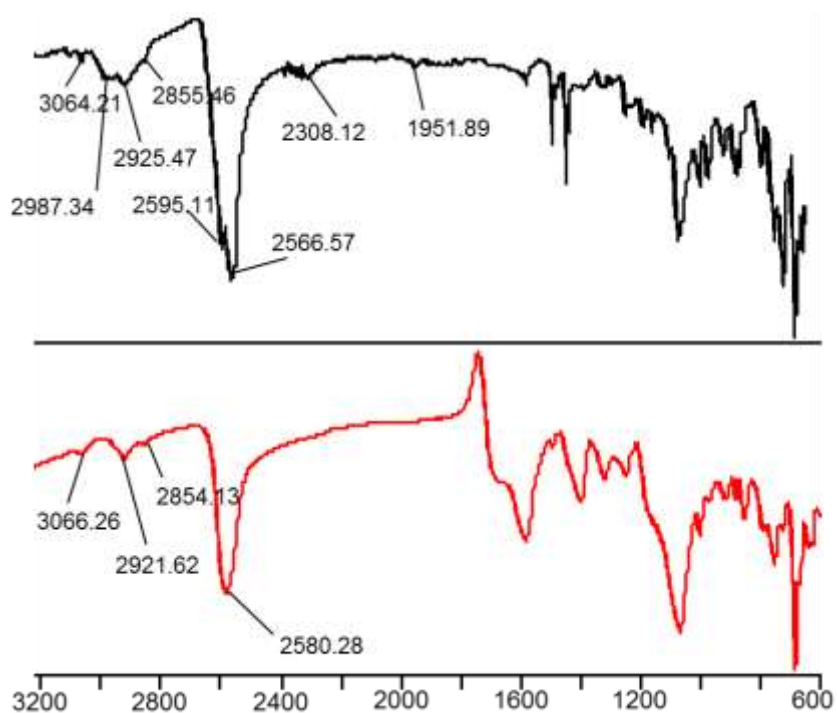
**Figure S8.** FTIR for compound **5**.



**Figure S9.** FTIR of 3 nm MPCs capped with mercaptocarborane (1-SH-2-Me-1,2-*closo*-C<sub>2</sub>B<sub>10</sub>H<sub>10</sub>), ligand **1** (1-SH-2-Ph-1,2-*closo*-C<sub>2</sub>B<sub>10</sub>H<sub>10</sub>), ligand **2** (1,2-(SH)<sub>2</sub>-1,2-*closo*-C<sub>2</sub>B<sub>10</sub>H<sub>10</sub>), ligand **3** (1-SH(CH<sub>2</sub>)<sub>2</sub>-2-Me-1,2-*closo*-C<sub>2</sub>B<sub>10</sub>H<sub>10</sub>) and ligand **5** (1-SH(CH<sub>2</sub>)<sub>3</sub>-2-Me-1,2-*closo*-C<sub>2</sub>B<sub>10</sub>H<sub>10</sub>).



**Figure S10.** FTIR spectra of ligand **2** (black) and its corresponding 10 nm MPCs (red).



**Figure S11.** FTIR spectra of ligand **3** (black) and its corresponding 10 nm MPCs (red).

