Cross-linked poly (dimethylaminoethyl acrylamide) coated magnetic nanoparticles: A high loaded, retrievable, and stable basic catalyst for the synthesis of benzopyranes in water

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Calculations of CHN

FT-IR and HNMR of selected compounds:
1- Calculation of loading amount of MPS on the surface of MNP@MPS

\[ n = \frac{C\%}{100 \times 0.012 \times m} \]

\( m = \) The number of carbon atom in MPS

\[ n = \frac{3.19}{100 \times 0.012 \times 7} = 0.38 \text{ mmol/g} \]

2- Calculation of loading amount of cross-linker MBA in MNP@PMA

Since the only source of N atom in MNP@PMA is MBA, it can be calculated by followed;

\[ n = \frac{N\%}{100 \times 0.014 \times m} \]

\( m = \) The number of nitrogen atom in cross-linker MBA

Note: The nitrogen content in MNP@MPS should be considered in next calculations. However MPS has no N atom but 0.09% can be attributed to NH₃ molecule in MNP.

\[ n = \frac{(0.87 - 0.09)}{100 \times 0.014 \times 2} = 0.28 \text{ mmol/g} \]  \( \text{(Loading of cross-linker in MNP@PMA)} \)

\( \%_{\text{MBA in MNP@PMA}} = 0.28 \left( \frac{\text{mmol}}{g} \right) \times 0.154 \left( \frac{g}{\text{mmol}} \right) \times 100 = 4.3\% \)

3- Calculation of loading amount of CO₂Me in MNP@PMA
Amount of methyl acrylate units in PMA and subsequently the loading amount of CO$_2$Me in MNP@PMA can be calculated by followed:

After subtracting of C% of MPS (from CHN MNP@MPS) and %C of MBA (from calculated loading amount) carbon content of PMA can be concluded.

\[
\text{the loading amount for MBA} = \frac{C\%}{100 \times 0.012 \times m}
\]

\( m = \) The number of carbon atom in cross-linker MBA

Which;

\[
0.28 = \frac{C\%}{100 \times 0.012 \times 7} \quad \text{and} \quad \%C \text{ in MBA}=2.35\%
\]

then

13.27= total C% in MNP@PMA

3.19= C% in MNP@MPS

2.35= C% of MBA

Which

\%C in poly(methylacrylate) or acrylate units= 13.27-3.19-2.35= 7.73%

\[
n = \frac{C\%}{100 \times 0.012 \times m}
\]

\( m = \) The number of carbon atom in methyl acrylate unite
and \( n = 1.61 \text{ mmol/g} \) (the loading amount of methyl acrylate acrylate units or loading amount of CO\(_2\)Me units on the surface of MNP@PMA)

**4- Calculation of loading amount of \(-\text{NMe}_2\) in MNP@PDMA**

Since the cross-linker amount in MNP@PMA and MNP@PDMA is same, by subtracting N\% of MNP@PMA (which is corresponded to MBA) from \%N of MNP@PDMA we can calculate the loading amount of dimethylamino ethyl acrylamide and subsequently the loading amount of \(-\text{NMe}_2\).

\[
N\% = 5.05 - 0.87 = 4.18\% \quad (\text{N content of dimethylaminoethyl acrylamide units})
\]

\[
n = \frac{N\%}{100 \times 0.014 \times m}
\]

\[m= \text{The number of nitrogen atom in dimethylaminoethyl acrylamide unit}
\]

\[
n = \frac{4.18\%}{100 \times 0.014 \times 2} = 1.49 \left( \frac{\text{mmol}}{g} \right)
\]

(Loading of dimethylaminoethyl acrylamide unit or \(-\text{NMe}_2\) unit)