Application of design of experiment for optimization of MOF-235 synthesis

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Statistical design of experiments was performed to optimize the MOF-235 synthesis process. The concentrations of terephthalic acid (TPA), iron (Ⅲ) chloride hexahydrate, N, N-dimethylformamide (DMF) and ethanol were important factors to develop the crystal structure of MOF-235. MOF-235 was synthesized with various concentrations, and then crystallinity was measured by XRD. The effect of the composition on the synthesis of MOF-235 was evaluated using the statistical analysis. In the analysis of variance using the F-test, the concentration of ethanol had the greatest effect on the crystallinity and the TPA was the least influential. A regression model for predicting the crystallinity of MOF-235 was derived and the prediction results for the two synthetic variables were presented using contour plots. Finally, crystallinity was predicted by the mixture method with FeCl3, ethanol and DMF.