

SINTESIS DAN KARAKTERISASI KERANGKA LOGAM ORGANIK Co/Zr-UiO-66 DENGAN PERLAKUAN ASAM SULFAT SERTA POTENSINYA SEBAGAI KATALIS DALAM FIKSASI CO₂

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INTISARI

Sintesis dan karakterisasi kerangka logam organik Co/Zr-UiO-66 dengan perlakuan asam sulfat serta potensinya sebagai katalis dalam fiksasi CO₂ menjadi siklik karbonat telah dilaksanakan. Variasi perlakuan Co/Zr-UiO-66 dilakukan untuk melihat perubahan struktur kristal, morfologi, serta interaksi antara Co(NO₃)₂ dan kerangka Zr-UiO-66 yang dianalisis melalui pendekatan DFT. Uji aktivitas katalitik dilakukan untuk mengevaluasi efektivitas material hasil sintesis dalam mengkonversi CO₂ menjadi produk yang bernilai tambah yaitu senyawa siklik karbonat.

Sintesis Co/Zr-UiO-66 dilakukan menggunakan metode solvotermal, kemudian diberi perlakuan menggunakan larutan H₂SO₄ 0,1 M dan 0,5 M untuk mengkaji perubahan struktur Co/Zr-UiO-66. Karakterisasi dilakukan menggunakan XRD, FE-SEM, FTIR, dan XRF, sementara uji aktivitas katalitik pada reaksi fiksasi CO₂ dilakukan dengan mereaksikan epiklorohidrin dan CO₂ dalam reaktor tertutup pada suhu 80 °C selama 6 jam. Selain itu, kajian komputasi dengan metode DFT dilakukan untuk mengkaji interaksi antara ion Co²⁺ dan kerangka Zr-UiO-66.

Material Co/Zr-UiO-66 dan Co/Zr-UiO-66 dengan perlakuan H₂SO₄ berhasil disintesis melalui metode solvotermal dengan struktur kristal tetap terjaga meskipun mengalami perubahan komposisi dan morfologi akibat perlakuan dengan H₂SO₄ yang dikuatkan dari nilai *unit cell* hasil analisis XRD. Nilai *unit cell* Co/Zr-UiO-66 dan Co/Zr-UiO-66 dengan perlakuan H₂SO₄ 0,1 M serta 0,5 M berturut turut sebesar a = b = c = 20,79; 20,74, dan 20,74 (Å). Kajian komputasi menunjukkan bahwa penambahan Co(NO₃)₂ tidak mengganggu struktur kristal dengan energi ikat yang cenderung negatif untuk menghasilkan kompleks Co/Zr-UiO-66 yang stabil. Aktivitas katalitik tertinggi diperoleh pada variasi Co/Zr-UiO-66 menggunakan perlakuan H₂SO₄ 0,1 M dengan konversi 64,85%.

Kata kunci : asam sulfat, DFT, karakterisasi, kobalt, Zr-UiO-66

***SYNTHESIS AND CHARACTERIZATION OF METAL ORGANIC
FRAMEWORK Co/Zr-UiO-66 WITH SULFURIC ACID TREATMENT AND
ITS POTENTIAL AS A CATALYST IN CO₂ FIXATION***

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ABSTRACT

Research on the synthesis and characterization of a Co/Zr-UiO-66 metal-organic framework with sulfuric acid treatment has been done to assess its potential as a catalyst for CO₂ fixation. The aim of this study was to synthesize and characterize Co/Zr-UiO-66 material treated with H₂SO₄ as a catalyst in the CO₂ fixation reaction. Several Co/Zr-UiO-66 variations was performed to observe changes in the crystal structure, morphology, and interactions between Co(NO₃)₂ and the Zr-UiO-66 framework, which were analyzed using a DFT approach. Catalytic activity tests were conducted to evaluate the effectiveness of the synthesized material in converting CO₂ into value-added products.

The synthesis of Co/Zr-UiO-66 was carried out via a solvothermal method using ZrCl₄, BDC, and Co(NO₃)₂·6H₂O as precursors, followed by treatment with 0.1 M and 0.5 M H₂SO₄ to enhance catalytic properties. Characterization was performed using XRD, FE-SEM, FTIR, and XRF, while catalytic activity in the CO₂ fixation reaction was tested by reacting epichlorohydrin and (C₄H₉)₄NBr in a sealed reactor at 80 °C for 6 hours. Additionally, computational studies employing DFT with the CP2K software were carried out to examine interactions between Co²⁺ ions and the UiO-66 framework.

The Co/Zr-UiO-66 material and its H₂SO₄-treated variants were successfully synthesized via a solvothermal method, maintaining their crystalline structure despite changes in composition and morphology due to H₂SO₄ treatment, as confirmed by unit cell parameters from XRD analysis. The unit cell values for Co/Zr-UiO-66 and Co/Zr-UiO-66 treated with 0.1 M and 0.5 M H₂SO₄ were a = b = c = 20,79; 20,74, and 20,74 Å, respectively. Computational studies showed that the addition of Co(NO₃)₂ did not disrupt the crystal structure, with binding energy values tending to be negative, indicating the formation of a stable Co/Zr-UiO-66 complex. The highest catalytic activity was observed for the Co/Zr-UiO-66 sample treated with 0.1 M H₂SO₄, achieving a conversion rate of 64.85%. This demonstrates that H₂SO₄ treatment effectively enhances the catalytic performance of Co/Zr-UiO-66.

Keywords: characterization, cobalt, DFT, sulfuric acid, Zr-UiO-66.