

**SINTESIS MATERIAL *ZEOLITIC IMIDAZOLATE FRAMEWORK* (ZIF-67)
TERMODULASI ASAM BENZOAT SEBAGAI KATALIS DALAM
FIKSASI CO₂: KAJIAN EKSPERIMENTAL DAN TEORITIS**

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INTISARI

Sintesis *Zeolitic Imidazolate Framework* (ZIF-67), modifikasi ZIF-67 dengan asam benzoat, dan studi interaksi asam benzoat termodulasi ZIF-67 (asam benzoat@ZIF-67) menggunakan metode *Density Functional Theory* (DFT) telah dilakukan. Penelitian ini bertujuan untuk mengkaji pengaruh penambahan variasi molar asam benzoat pada sintesis ZIF-67 terhadap struktur dan morfologi kristal ZIF-67 serta potensi aplikasinya sebagai katalis pada fiksasi gas CO₂ serta mengetahui interaksi yang terjadi antara asam benzoat dan ZIF-67. ZIF-67 dan asam benzoat@ZIF-67 disintesis melalui metode suhu ruang dengan prekursor awal kobalt nitratheksahidrat dan 2-metilimidazol dalam pelarut metanol. Sintesis asam benzoat@ZIF-67 dilakukan dengan penambahan asam benzoat 0,5; 4; dan 10 mmol. Material hasil sintesis dikarakterisasi dengan FTIR, XRD, FE-SEM, SAA dan UV-VIS. Aplikasi ZIF-67 dan asam benzoat@ZIF-67 sebagai katalis dilakukan dengan menginteraksikan suatu epoksida dengan penambahan material katalis dan *co-catalyst* TBAB bersama gas CO₂ dalam sistem tertutup selama 6 jam, kemudian liquid hasil katalisis dilakukan karakterisasi ¹H-NMR untuk mengetahui konversi siklik karbonat yang terjadi. DFT digunakan untuk mempelajari pengaruh asam benzoat terhadap struktur dan morfologi ZIF-67.

Hasil karakterisasi menunjukkan bahwa ZIF-67 dan asam benzoat@ZIF-67 berhasil disintesis. Analisis menunjukkan bahwa kristal memiliki struktur dodekahedron dengan ukuran unit sel rata-rata sebesar 4975,856 Å serta ukuran kristal berkisar antara 200-650 nm. Uji ¹H-NMR menunjukkan bahwa konversi CO₂ menggunakan katalis ZIF-67 serta asam benzoat@ZIF-67 pada konsentrasi 0,5; 4; dan 10 mmol menghasilkan konversi siklik karbonat masing-masing sebesar 51%, 12,42%, 19,41%, dan 15,4%.

Kata kunci: asam benzoat@ZIF-67, DFT, fiksasi, karbon dioksida, ZIF-67

SYNTHESIS OF ZEOLITIC IMIDAZOLATE FRAMEWORK (ZIF-67) MODULATED BY BENZOIC ACID AS A CATALYST IN CO₂ FIXATION: EXPERIMENTAL AND THEORETICAL STUDIES

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ABSTRACT

The synthesis of Zeolitic Imidazolate Framework (ZIF-67), modification of ZIF-67 with benzoic acid, and the study of interactions between benzoic acid-modulated ZIF-67 (benzoic acid@ZIF-67) using Density Functional Theory (DFT) have been carried out. This research aims to examine the effect of varying molar amounts of benzoic acid added during the synthesis of ZIF-67 on the crystal structure and morphology of ZIF-67, as well as its potential application as a catalyst for CO₂ gas fixation, and to understand the interactions occurring between benzoic acid and ZIF-67. ZIF-67 and benzoic acid@ZIF-67 were synthesized via a room temperature method using kobalt nitrate hexahydrate and 2-methylimidazole as precursors in methanol solvent. The synthesis of benzoic acid@ZIF-67 was performed by adding benzoic acid at concentrations of 0,5, 4, and 10 mmol. The synthesized materials were characterized by FTIR, XRD, FE-SEM, surface area analysis (SAA), and UV-VIS spectroscopy. The application of ZIF-67 and benzoic acid@ZIF-67 as catalysts was conducted by reacting an epoxide with the catalyst material and the co-catalyst TBAB together with CO₂ gas in a closed system for 6 hours. The resulting liquid from the catalysis was analyzed by ¹H-NMR to determine the conversion of cyclic carbonate formed. DFT was used to study the effect of benzoic acid on the structure and morphology of ZIF-67.

The material characterization results showed that both ZIF-67 and benzoic acid@ZIF-67 were successfully synthesized. Analysis revealed that the crystals have a dodecahedral structure with an average unit cell size of 4975.856 Å and crystal sizes ranging from 200 to 650 nm. ¹H-NMR tests showed that the CO₂ conversion using ZIF-67 catalyst and benzoic acid@ZIF-67 at concentrations of 0,5, 4, and 10 mmol resulted in cyclic carbonate conversions of 51%, 12.42%, 19.41%, and 15.4%, respectively.

Keywords: benzoic acid@ZIF-67, carbon dioxide, DFT, fixation, ZIF-67