

MODEL INTERAKSI ETER 15-MAHKOTA-5 TERSUBSTITUSI DENGAN KATION Ni^{2+} dan Co^{2+} BERDASARKAN TEORI FUNGSI KERAPATAN

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INTISARI

Pemodelan molekul terhadap interaksi eter 15-mahkota-5 dengan kation Ni^{2+} dan Co^{2+} telah dilakukan menggunakan metode *Density Functional Theory* (DFT) pada tingkat teori B3LYP. Kajian difokuskan untuk mempelajari pengaruh substituen dan keberadaan molekul air dalam sistem kompleks. Pemodelan dilakukan pada fasa gas dan fasa larutan. Substituen penarik elektron (-Br, -COOH) menyebabkan penurunan energi interaksi kompleks dan sebaliknya gugus pendonor elektron (-NH₂, -CH₂CH₃, -OH, -CH₃, -OCH₃) mampu meningkatkan energi interaksi kompleks pada fasa gas. Pada fasa gas, kestabilan kompleks 15-mahkota-5 dengan $\text{Ni}^{2+} > \text{Co}^{2+}$. Pola kenaikan kestabilan kompleks tersebut sesuai dengan hasil analisis energi interaksi, ukuran kavitas, transfer muatan, dan visualisasi kerapatan elektron.

Keberadaan molekul air pada fasa gas dimodelkan menggunakan mikrosolvasi menunjukan bahwa dua molekul air terikat pada kation Ni^{2+} dan Co^{2+} . Pada fasa gas substituen -NH₂ memberikan kestabilan kompleks paling tinggi untuk kompleks dengan Ni^{2+} atau Co^{2+} . Pengaruh pelarut air pada fasa larutan dimodelkan dengan *Polarized Continuum Model* (PCM). Energi interaksi pada fasa larutan sesuai dengan nilai kestabilan kompleks $\text{Co}^{2+} < \text{Ni}^{2+}$. Pola peningkatan kestabilan kompleks fasa larutan tersebut dikaji berdasarkan parameter energi interaksi dan momen dwi kutubnya. Pada fasa larutan kompleks [Ni^{2+} .benzo-15-mahkota-5-CH₃] dan [Co^{2+} .benzo-15-mahkota-5-CH₂CH₃] memberikan kestabilan kompleks paling tinggi.

Kata kunci: 15-mahkota-5, DFT, mikrosolvasi, PCM.

INTERACTION MODELLING Ni^{2+} AND Co^{2+} CATIONS BY 15-CROWN-5 ETHER DERIVATIVES BASED ON DENSITY FUNCTIONAL THEORY

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ABSTRACT

A molecular modeling on the interaction of the 15-crown-5 ether derivatives toward Ni^{2+} and Co^{2+} cations has been conducted by Density Functional Theory method at B3LYP. The effects of substituent groups and water molecules were the major focus of this theoretical study. This molecular modelling was carried out in gas and solvent phases. The electron withdrawing substituents (-Br, -COOH) reduced the interaction energies and the electron donating substituents (-NH₂, -CH₂CH₃, -OH, -CH₃, -OCH₃) gives the opposite results. The gas-phase complex stabilization $\text{Co}^{2+} < \text{Ni}^{2+}$. This result was confirmed by interaction energy, the amount of charge transfer and the electron density visualization.

The effects of water molecules on gas-phase was modeling with microsolvation showed that two molecules water addition to complexes with Ni^{2+} or Co^{2+} . In the gas-phase it found that -NH₂ substituen gave highest stabilization complexes. The interaction 15-crown-5 ethers in solvent phase was studied by Polarized Continuum Model (PCM). The order of the solvent phase following stabilitation complex $\text{Co}^{2+} < \text{Ni}^{2+}$. This stabilization complex trend was systematically studied from the interaction energy and the momen dipole of the complex in solvent phase. In the solvent phase gives result that [Ni^{2+} .benzo-15-crown-5-CH₃] and [Co^{2+} .benzo-15-crown-5-CH₂CH₃] has highest complex stabilization.

Keyword: 15-crown-5, DFT, mikrosolvation, PCM