# Structural Insights into Dibrominated 2,3-Benzaldehyde Compounds with Potential as Antioxidant Agents in Biodiesel

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Biodiesel is a promising renewable fuel that has the potential to reduce negative aspects associated with fossil fuels, such as pollution, greenhouse gas emissions and resource depletion. However, biodiesel is more prone to oxidation, limiting its shelf life and effectiveness as a fuel. To address this issue, three variations of dibrominated 2,3- dimethoxybenzaldehyde (DMB)[1,2] have been developed to reduce the rate of oxidation and preserve the physical-chemical properties of biodiesel. This study explores 4,5-bromo-2,3- dimethoxybenzaldehyde (4,5DMB), 4,6-bromo-2,3-dimethoxybenzaldehyde (4,6DMB) and 5,6-bromo-2,3-dimethoxybenzaldehyde (5,6DMB) potential as additive to improve the oxidative stability of biodiesel[3]. The research involves the synthesis, crystallization, and comprehensive structural characterization of DMB compounds. The 4,5DMB ($C_9H_8Br_2O_3$ – I2/a; $R_1$ = 0.0475; Goof = 1.049), the 4,6DMB ($C_9H_8Br_2O_3$ – $P2_1/c$; $R_1$ = 0.0318; Goof = 1.036) and 5,6DMB ($C_9H_8Br_2O_3$ – $P2_1/c$; $R_1$ = 0.0391; Goof = 1.023). Theoretical calculations by the density functional theory (DFT), at M06-2X/6-311++G(d,p) level of theory were conducted to explore the dibrominated compound electronic properties, as well as the supramolecular arrangements that may contribute to their antioxidant potential. To identify the dibrominated compound reactive sites were used the Fukui functions[4]. Finally, machine learning models were implemented using pySiRC to estimate kinetic parameters of the oxidation process. The –OH radical reaction rate constant from an aqueous model was used to demonstrate that the dibrominated 2,3-benzaldehyde compounds effectively reduce the rate of oxidation and improve the stability of biodiesel.

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