

Article

α -Tocopherol and Trolox as Effective Natural Additives for Polyurethane Foams: A DFT and Experimental Study

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Abstract: In this work, α -tocopherol and trolox were studied as compounds that have high biological activity. α -Tocopherol is considered a food additive because the refining process of vegetable oils causes the depletion of this vitamin, and thus, its inclusion is required to keep them from oxidizing. Computational tools have determined the antioxidant activity of these additives. The geometries of the studied molecules were optimized using two density functional methods, including M05-2X and M06-2X, in combination with the 6-311++G(2d,2p) basis set. The results indicated that when comparing the antioxidant activity of α -tocopherol and trolox, they were very similar to each other, but α -tocopherol had an antioxidant activity slightly higher, around 1.2 kJ/mol, than trolox. Thus, these additives can be used as polymer additives to protect materials from free-radical-induced stress. To test their applicability in polymeric formulations, flexible polyurethane foams were prepared with varying α -tocopherol ratios and NCO indices (1.0 and 1.1). Increasing the α -tocopherol content reduced the compressive force and altered the mechanical properties, likely due to its presence in the foam structure. This additive not only fine-tuned the mechanical properties but also provided antioxidant effects, enabling multiple enhancements in polymeric products with a single additive.

Keywords: DFT; bond dissociation enthalpy; HAT; ionization potential; vitamin E; FPUF

Citation: Thbayh, D.K.; Mentés, D.; Boros, Z.R.; Palusiak, M.; Farkas, L.; Viskolcz, B.; Fiser, B. α -Tocopherol and Trolox as Effective Natural Additives for Polyurethane Foams: A DFT and Experimental Study. *Molecules* **2024**, *29*, 6037. <https://doi.org/10.3390/molecules29246037>

Received: 24 November 2024

Revised: 18 December 2024

Accepted: 19 December 2024

Published: 21 December 2024

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1. Introduction

Free radicals are produced not only as a result of normal metabolic processes in the human body (endogenous sources) but also as a result of environmental variables (exogenous sources), including ozone radiation, stress, industrial chemicals, pesticides, and pollution [1–5]. There are three categories of plant-based antioxidants: phenolic chemicals, vitamins, and carotenoids [6]. The molecules of phenolic compounds range from simple structures such as ferulic acid, vanillin, gallic acid, caffeic acid, and butylated hydroxytoluene to polyphenols like tannins and flavonoids [7].