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# Structure, thermal stability, antioxidant activity and DFT studies of trisphenols and related phenols

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**Abstract:** Two kinds of trisphenols have been successfully synthesized and their structures were confirmed by IR spectra, <sup>1</sup>HNMR, <sup>13</sup>CNMR, mass spectra and X-ray diffraction. They exhibited better thermal stability than both monophenol and bisphenols due to their higher molecular weight. Moreover, their antioxidant activities have been investigated in lubricant oil using PDSC and RBOT. The results showed that the *o*-trisphenol **3b** exhibited the best antioxidant activity while the *p*-trisphenol **3a** was the worst. In addition, their relationship between structures and properties has been further explored by a series of DFT calculations including the BDE values, the IP values and the Gibbs free energy barriers for the reaction between phenols and methylperoxyl radicals.

**Keywords:** Antioxidant activity; Trisphenol; Thermal stability; Lubricant; DFT

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