Effect of substituents on dehydrogenation enthalpy of dibenzyl toluene

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Liquid organic hydrogen carriers (LOHCs) have tremendously attracted attention owing to their advantages in the storage and transport of hydrogen at ambient conditions. Dibenzyl toluene (DBT) is one of the most prominent candidates which has been investigated since its favorable properties as a LOHC. But the only disadvantage of DBT is the releasing hydrogen occurs at high temperatures. In this study, the effect of various substituents on the dehydrogenation of DBT was elucidated using density functional theory (DFT) methods. In specific, the charge distribution of DBT was investigated to understand the effect of the modified DBT. This study will facilitate the use of DBT as a LOHC, allowing hydrogen energy to be used more easily and ensuring the hydrogen economy in the future.

Keywords — Dibenzyl toluene, density functional theory, liquid organic hydrogen carriers.