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12-Tungstoboric acid (H5BW12O40) as an efficient Lewis acid catalyst for the synthesis of chromenopyrimidine-2,5-diones and thioxochromenopyrimidin-5-ones: Joint experimental and computational study

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Abstract

H5BW12O40 (BWA), Keggin-type heteropoly acid was employed as an effective, eco-friendly and reusable Lewis acid catalyst for the high yielding synthesis of chromenopyrimidine-2,5-diones and thioxochromenopyrimidin-5-ones via multicomponent reaction (MCR) of differently substituted benzaldehydes, urea/thiourea, and 4-hydroxycoumarin in refluxing water. The BWA catalyst could be recovered by a simple filtration and applied in three successive runs with no noticeable decrease in the yield. Interestingly, this catalyst structure pattern may act as useful model for the design and assembly

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of the functional molecule-based catalysts, especially in the field of molecular sieve materials. Moreover, thermochemical properties in the synthesis of title compounds were assessed using density functional theory (DFT) calculations.

Keywords: H5BW12O40, Lewis acid, Heteropoly acids, Chromenopyrimidine-2,5-diones, Thioxochromenopyrimidin-5-ones, Multicomponent reaction, Density functional theory