Turkish Journal of Chemistry

Turkish Journal

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Chemistry

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Bromination of 1-Cyclopent-1-en-1-ylbenzene and 1-(5-Bromocyclopent-1-en-1-yl)benzene and Theoretical Investigation of the Products

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Abstract: The bromination of 1-cyclopent-1-en-1-ylbenzene (4) in different solvents and at different temperatures was accompanied by the evolution of hydrogen bromide and yielded 1-(5-bromocyclopent-1-en-1-yl)benzene (8). Further bromination of 8 gave exclusively 2R(S),5R(S)-1-(1,2,5-tribromocyclopentyl)benzene (11). The experimental results were compared with the theoretical ones based on semi-empirical (MM+ and AM1), Hartree-Fock (HF) and density functional theory (DFT). The formation of 11 was explained by the formation of a weakly bridged bromoniun ion of type 9.

Key Words: Bromination, Olefins, MM+, AM1, Hartree-Fock (HF) and Density Functional Theory (DFT) calculations

Turk. J. Chem., **27**, (2003), 287-294.
Full text: pdf
Other articles published in the same issue: Turk. J. Chem.,vol.27,iss.3.