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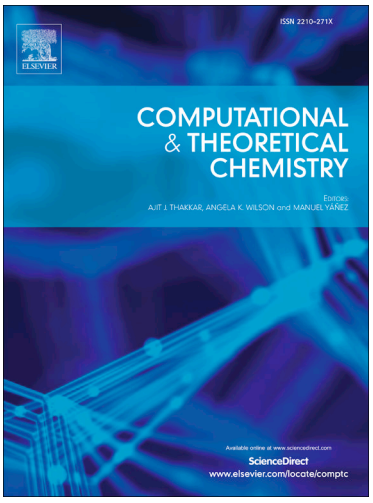

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Accurate theoretical method for homolytic cleavage of C-Sn bond: A benchmark approach

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Abstract

Stille coupling is a well-known cross coupling reaction, where the rate determination step is the dissociation of carbon stannous (C-Sn) bond. The organotin compounds are also used as precursors in the manufacturing of tin oxide films, solar cells, gas sensors, flat panel display technology and low emission glass materials *etc*. The reactivity of organotin compounds has direct relationship with the homolytic cleavage of C-Sn bond. Therefore, accurate determination of C-Sn bond has direct relevance in understanding many phenomena. The current benchmark study is aimed at finding out the accurate theoretical method for the homolytic cleavage (bond dissociation energy) of C-Sn bond. In this regard, nineteen DFs from eight different classes of DFT with two effective core potential basis sets (LANL2DZ and SDD) and two Karlsruhe basis sets (def2-SVP and def2-TZVP) are selected for the BDE calculation of C-Sn bond. Ten structurally diverse organotin compounds with experimentally known BDE of C-Sn bond are selected from the literature. The statistical [root mean square deviation (RMSD), standard deviation (SD), Pearson's correlation (R) and mean absolute error (MAE)] results are obtained by the comparison of theoretical data with the experimental BDE values of C-Sn bond of

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