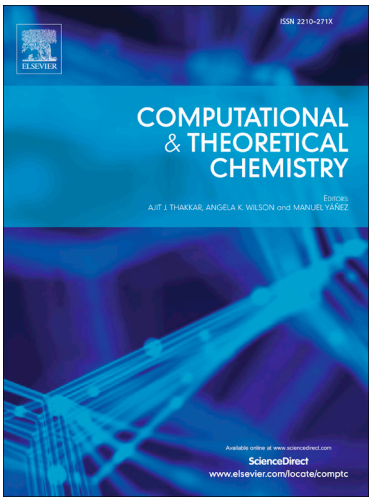

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Calculation of interaction energies in 2-butene and butane systems

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ABSTRACT

Benchmarking study on eighteen methods, including MP2, B2PLYP-D3, B2PLYP-D3BJ, ωB97xD, M05-D3, M06-D3, M052X-D3, M06HF-D3, PBE0-D3, PBE0-D3BJ, B3LYP-D3, B3LYP-D3DJ, TPSS-D3, TPSS-D3BJ, BP86-D3, BP86-D3BJ, BLYP-D3, BLYP-D3BJ and ten basis sets: cc-pVDZ, cc-pVTZ, aug-cc-pVDZ, cc-pVQZ, def2-SVP, def2-TZVP, def2-TZVPP, def2-QZVP, 6-311++G** and 6-31G**, for each method, have been performed, calculating interaction energies in (1) unsaturated/unsaturated systems (2-butene dimers), (2) unsaturated/saturated system (between butane and 2-butene) and (3) saturated/saturated (butane dimers). The calculated interaction energies are compared with accurate CCSD(T)/CBS energies. The data shows that most levels of theory have the highest errors for systems with butane dimers, and calculated interaction energies in these systems are overestimated. The best levels, overall for all systems, are BLYP-D3BJ/def2-QZVP and BLYP-D3BJ/cc-pVQZ with similar root mean square deviation (RMSD) values of 0.056 kcal mol^{-1} and 0.060 $kcalmol^{-1}$ compared to CCSD(T) values. The best level for (1) 2-butene dimers is B3LYP-D3BJ/aug-cc-pVDZ; for (2) interactions between 2-butene and butane is BLYP-D3BJ/def2-SVP; while for (3) butane dimers is BLYP-D3BJ/def2-QZVP. The difference in calculated energies among several method are not high, however, it is important that most of the DFT methods overestimate interactions in butane dimers.

Keywords: Benchmark, alkenes, alkanes, double bond, CCSD(T) calculations, DFT calculations