Cooperative and anticooperative effects in resonance assisted hydrogen bonds in merged structures of malondialhedyde

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Supporting Information

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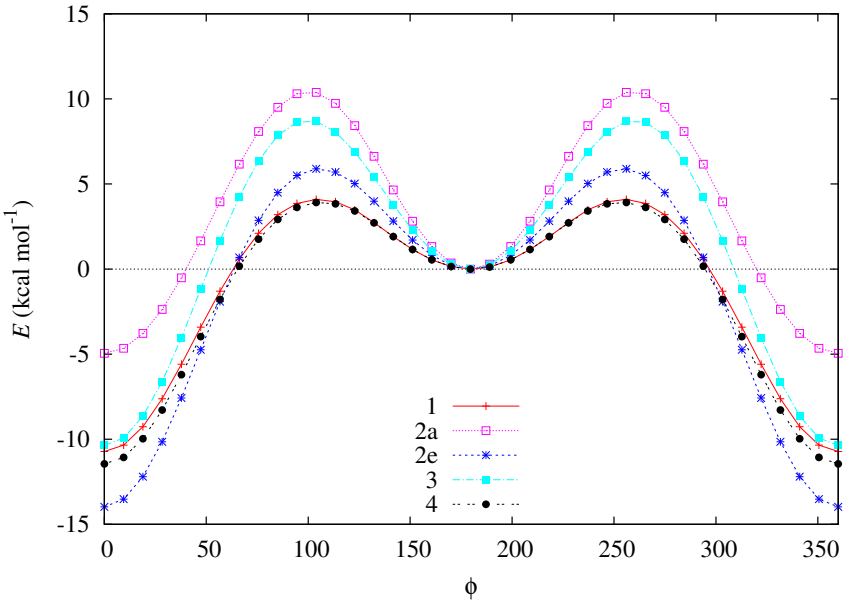

Figure S 1: Potential energy curves for the scan of the dihedral angles shown in equations (8)–(11) of the manuscript along with the corresponding plot for malondialdehyde. The approximation HF/aug-cc-pVTZ was used throughout.

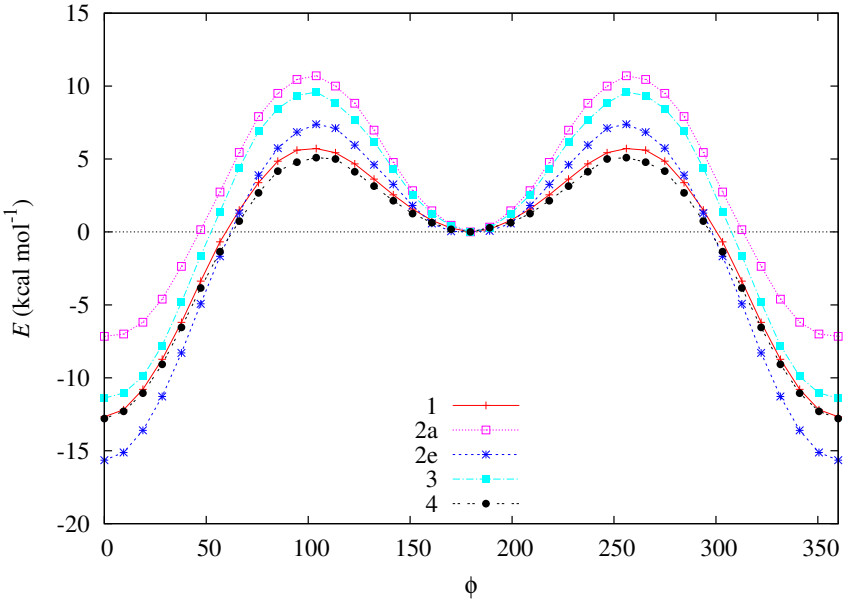

Figure S 2: Formation energies of the resonance assisted hydrogen bonds considered in this investigation given by the rotation of the dihedral angles specified in equations (8)–(11) of the body of the paper together with the corresponding curve of propanedial. The electronic energies were computed with the RIJCOSX-MP2/aug-cc-pVTZ level of theory.