?-strain-induced electrophilicity in small cycloalkynes: A DFT analysis of the polar cycloaddition of cyclopentyne towards enol ethers

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Small cycloalkynes possess a ?-strain-induced electrophilicity related to the bending of the Csp3-Csp-Csp bond angle. For cyclopentyne and benzyne, the electrophilicity index defined in the context of density functional theory gives a coherent rationale for the reactivity of these cycloalkynes, which may act as electrophiles in polar cycloaddition reactions toward enol ethers. © Wiley-VCH Verlag GmbH & Co. KGaA, 2006.