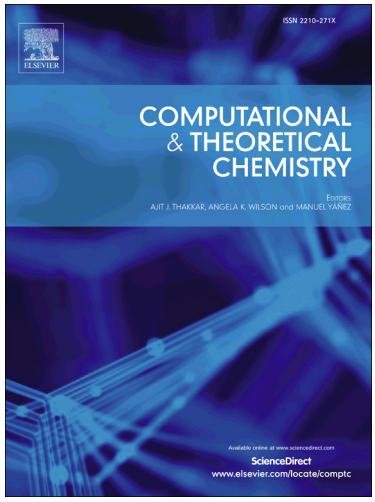

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On Structure and Stability of Pyrimidine Ylidenes and Their Homologues

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ABSTRACT: Structure of six-membered cyclic aminoiminocarbenes (pyrimidine ylidenes) and their group 13-15 homologues was studied by quantum chemical calculations. Isodesmic and dimerization reaction energies, NICS values, frontier molecular orbitals, as well as NBO, Bader's "atoms in molecules" and Laplacian bond order (LBO) analyses were employed for estimating relative stability of the studied carbenes (carbene homologues). They show a low degree of aromatic delocalization and considerable variation of electronic structure depending on the nature of divalent element. The predicted stability for the series of interest is lower than that for the corresponding five-membered Arduengo carbenic structures, but comparable with Alder's bis(dimethylamino)carbene.

KEYWORDS: DFT, N-heterocyclic carbene, pyrimidine ylidene, isodesmic reaction, stability.