Normal coordinate and vibrational analyses of 2-aza- and 2-phosphabutadienes.
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Abstract

The structural stability of 2-azabutadiene CH2:CHN:CH2 and 2-phosphabutadiene CH2:CHP:CH2 were studied by DFT-B3LYP and ab initio MP2 calcns. with the 6-311+G** basis set. From the calcns. the two compds. were predicted to exist predominantly in a planar trans structure. The calcn. at MP2 level of 2-azabutadiene was consistent with the possibility of very low abundance of secondary high energy gauche conformation (taking into consideration the double degeneracy of the nonplanar structure). From MP2 calcns. the equil. const. for the gauche .tautm. trans interconversion in 2-azabutadiene is 0.111 at 298.15 K, which corresponds to an equil. mixt. of 10% gauche and 90% trans of the aza compd. The vibrational frequencies were computed at the MP2 level for each of the two mols. in their trans conformation. Complete vibrational assignments were made on the basis of normal coordinate analyses for 2-aza- and 2-phosphabutadienes.