Semiempirical study of methoxy- and (un)substituted amino-methylene ethylidene propane dinitriles

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Abstract:
The geometry optimization of methoxy- and (un)substituted amino-methylene/ethylidene propanedinitriles, vinylamine, vinylalcohol and ethylene has been carried out with semiempirical AM1 and MINDO3 methods. Our results point out the conjugation of x-molecular systems with the inclusion of a lone pair of amino nitrogen (or etheric oxygen). This conjugation leads to the planar structure of the (un)substituted amino group, shortening of the C-N (or C-O) bond length and elongation of the C=C bond.

KeyWords Plus:
GROUND-STATES, MINDO-3 CALCULATIONS, MOLECULES

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