Ab initio study of (un)substituted amino- and methoxymethylene/ethyldene propanedinitriles
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Abstract:
The geometry optimization of (un)substituted amino- and methoxy-methylene/ethyldene propane-dinitriles, vinylamine and its N-methyl derivatives and vinyl alcohol and its O-methyl derivative has been carried out at ab initio DZP HF level. MP2 calculations have been performed for all molecules at the SCF geometry. Our results indicate the conjugation of pi -molecular systems with inclusion of lone pair of amino nitrogen (or ether oxygen). The conjugation enforces planar structure in (un)substituted amino group, shortening the C-N (or C-O) bond lengths and elongating the C=C double bond.

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