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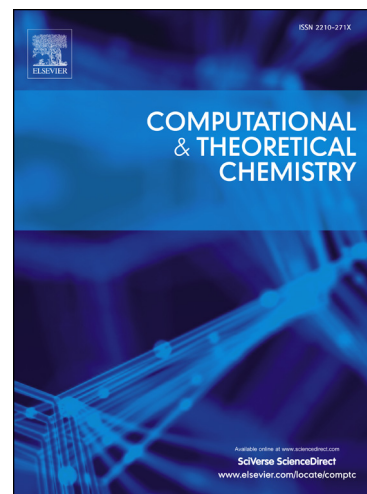
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Computational study of the rotational pathways of the amino group in 2-chloroaniline, azines and formamide: one or two rotational barriers?

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Abstract

Rotation of the amino group in five different molecular systems, 2-aminopyridine, 2-aminopyrimidine, 2-chloroaniline, N-methylamino-1,3,5-triazine, and formamide, has been studied at B3LYP/6-311++G(2d,2p), MP2/6-311++G(2d,2p), and CCSD(T)/6-311++G(2d,2p)//B3LYP/6-311++G(2d,2p) levels of density functional, MP2, and coupled cluster theories. To this end, detailed rotation energy profiles for the above amino systems were obtained in two different ways: 1) by computing the energy-values as a function of only one torsion angle; and 2) by taking into account that the pyramidal nature of the NH₂ group changes as rotation progresses so that energy profiles should be defined by two torsion angles. In the first case, saw-toothed energy profiles exhibiting two rotational barriers were always obtained. Conversely, by using two torsion angles as reaction coordinates smooth pathways were found where a rotation cycle can be completed passing only through the lowest energy barrier. Implications of these conflicting pathways are discussed.

Keywords: amino group, rotational pathways, rotational barriers

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