Title:	Insights on unimolecular and bimolecular reactivity patterns of pyridyl, pyridyl-N-oxide, and pyridinyl radicals through spin density
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Abstract:	Spin density is very vital in understanding the thermodynamic stability of radicals, biradicals, etc. To obtain insights on reactivity aspects of radicals using it, we carried out theoretical investigations on the unimolecular and bimolecular reactions of pyridyl 1a-c, pyridyl-N-oxide 2a-c, and pyridinyl 3a-c radical isomers. For all the radicals, we computed the C[sbnd]H bond dissociation energies (BDEs), isomerization reactions through the 1,2-H shift, unimolecular decomposition channels, and the bimolecular reactions with small molecules H2, H2O, CO, CO2, CH4, and CH3OH. Remarkably, spin density at the radical center or the transition state manifested the observed reactivity patterns.
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