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Title:	Thermal unimolecular reactivity pathways in dehydro-diazines radicals
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Abstract:	<p>In this work, we investigated the detailed reactivity of dehydro-diazine radicals through unimolecular dissociation pathways. Aromatic six-membered rings with two nitrogens as heteroatoms are classified as diazines, which include pyrimidine 1, pyridazine 2, and pyrazine 3. The C–H bond scission in pyrimidine, pyridazine, and pyrazine leads to three (1a–1c), two (2a and 2b), and one (3a) radical isomers, respectively. Through quantum chemical calculations, reactivity aspects of all the six radical isomers have been investigated by considering different modes of unimolecular reactions. On the basis of the computations at (U)B3LYP/cc-pVTZ, (U)M06-2X/cc-pVTZ, and (U)CCSD(T)/cc-pVTZ/(U)B3LYP/cc-pVTZ levels of theory and analysis, we found out that ring-opening pathways were kinetically more favorable compared with isomerization (1,2-H shift) pathways or C–H bond dissociation leading to biradicals. In all the cases, ring-opening via C–N bond cleavage has a lower energy barrier compared with C–C bond cleavage owing to the stabilizing interaction between radical electron and the nitrogen lone pair. Moreover, the unimolecular decomposition channels can lead to several fragmentation products, which are interesting in the astrochemical context. On the basis of these investigations and also the impact of three centered–five electrons (3c–5e) interactions on the reactivity aspects, we determined the kinetic stability order among the six isomeric dehydrodiazine radicals.</p>
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