Title:	Photochemistry of 3,6-Didehydropyridazine Biradical—An Untraceable Para Benzyne Analogue
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Abstract:	We report matrix isolation infrared spectroscopic studies to characterize 3,6-didehydropyridazine 6, a heterocyclic analogue of para benzyne, combined with computations. In this regard, we have utilized 3,6-diiodopyridazine 11 as a photolytic precursor. The experiments toward the generation of the biradical are carried out in argon and nitrogen matrices at 4 K. Instead of the elusive biradical, we have observed a ring-opening product maleonitrile (Z)-7 upon irradiation at 254 nm. In contrast, prolonged irradiation at 254 nm leads only to Z-E isomerization, forming fumaronitrile (E)-7. The mechanistic aspects of ring-opening, product selectivity, and Z-E photoisomerization steps have been investigated in detail using high-level ab initio computations. These studies have found that 3,6-didehydropyridazine 6 is an untraceable intermediate, and the ring-opening step leading to maleonitrile is barrierless. In addition, we have proposed the involvement of the S1 (π–π*) state via conical intersection in the Z-E photoisomerization of maleonitrile.
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