

Nonadiabatic *ab initio* chemical reaction dynamics on photoisomerization reaction of 3,5-dimethylisoxazole via the S_1 electronic state

Kimura, Mizuki.^{1*}, Nanbu, Shinkoh.²

*presenter

¹m-kimura-0o3@eagle.sophia.ac.jp, Graduate School of Science and Technology, Sophia University, Japan

² Faculty of Science and Technology, Sophia University, Japan

Since the 1960s, research has been conducted on isoxazole, a versatile molecule used in pharmaceuticals, corrosion inhibitors, agrochemicals, and other fields. It is known to undergo isomerization when exposed to light¹. Nunes *et al.* proposed a reaction mechanism for photoisomerization by performing photoirradiation experiments on 3,5-dimethylisoxazole in an Ar matrix². The reaction mechanism is shown in Figure 1. Upon light irradiation of compound **1**, compounds **3**, **4**, **5**, and **6** were observed. In particular, the formation of **6** has attracted attention in recent years because of its role in pharmaceutical synthesis³. In this research, we aim to elucidate the photoexcited isomerization of 3,5-dimethylisoxazole to the S_1 state by full-degree-of-freedom *ab initio* molecular dynamics calculations, taking into account non-adiabatic transitions.

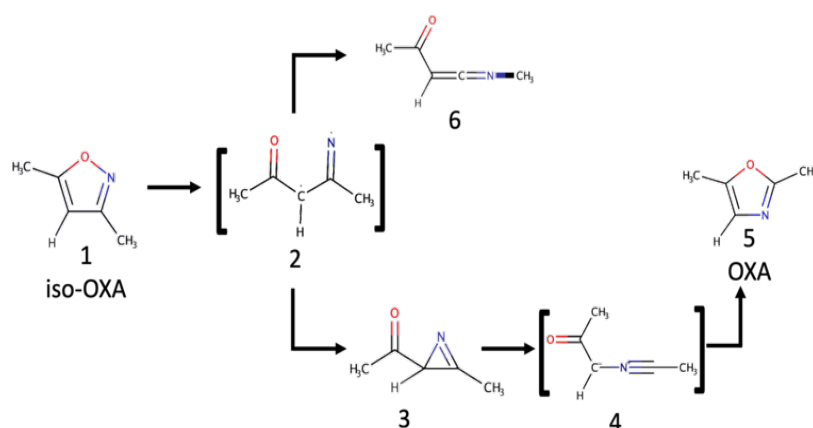


Fig 1 Isomerization process proposed by Nunes *et al.*

¹ B. J. Wakefield *et al.*, A.R. and Boulton, A.J., *Isoxazole Chemistry Since 1963*. Elsevier Science, **1981**, vol. 25, ch. 4, pp1293-1298

² C.M. Nunes *et al.*, Capture of an Elusive Nitrile Ylide as an Intermediate in Isoxazole–Oxazole Photoisomerization. *J.Org. Chem.*, **2013**, 78, 10657-10665

³ C. Brackman *et al.* Synthesis of Highly Reactive Ketenimines via Photochemical Rearrangement of Isoxazoles. *Org. Lett.*, **2023**, 25, 6593-6597