

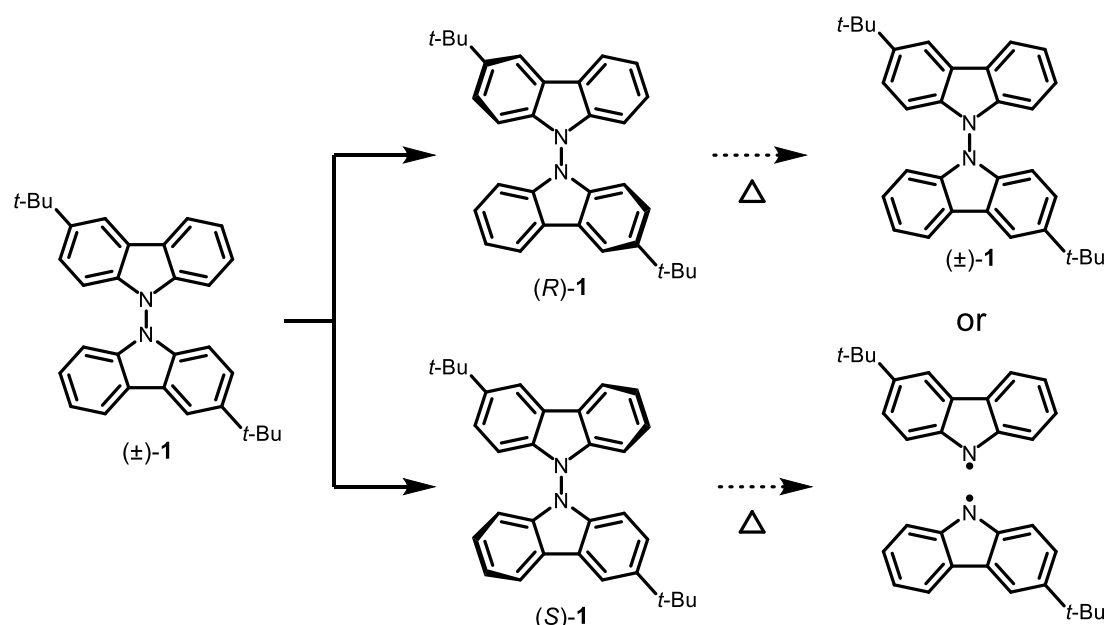
## The elucidation for thermal stability in atropisomers of substituted carbazole dimer linked by N-N bond

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Among many biaryl compounds with axial chirality, only two biaryl compounds with axial chirality linked by a N-N bond have been reported to date. The stability of the axial chirality of these N-N linked biaryl compounds has not been precisely understood yet. In addition, it is known that this class of compounds undergoes thermal decomposition through N-N bond cleavage. In this study, we elucidated the thermal stability of axial chirality of substituted carbazole dimer and the decomposition through N-N bond cleavage by experiment and DFT calculation.<sup>[1]</sup>

Racemic 9,9'-bicarbazole (**1**) was resolved by HPLC with chiral stationary phase. The enantiomerically enriched (*R*)-**1** and the decomposition of ( $\pm$ )-**1** were investigated at high temperature. The energies of racemization and cleavage were also evaluated by DFT theory [B3LYP/6-31G(d)]. The results will be presented in detail.



[1] T. Kobayashi, F. Ishiwari, T. Fukushima, K. Hanaya, T. Sugai, S. Higashibayashi, *Eur. J. Org. Chem.* doi.org/10.1002/ejoc.202001385