2B2b

Spin Alignment in Tetraradicals, based on the Substituent Effect on the Ground State Spin-Multiplicity of Localized 1,3-Diyls

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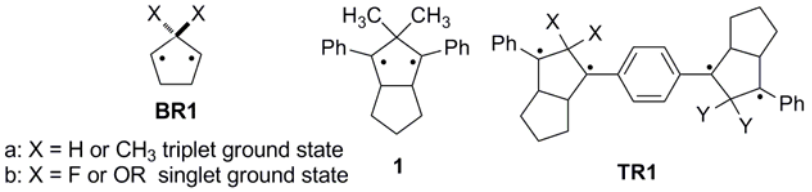
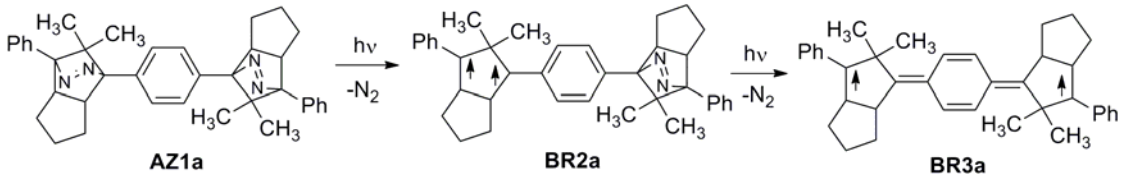
【Introduction】 In our previous study, we have found notable substituent effects at the C(2) position on the ground state spin-multiplicity of localized 1,3-biradicals, i.e. cyclopentane-1,3-diyls **BR1**. In this study, we examined whether the substituent effects can be applied for the spin alignment in tetraradical species **TR1** in which two 1,3-biradical units are connected in a *p*-phenylene fashion.



【Results and Discussion】 The photodenitrogenation of **AZ1a** (X = Y = CH_3, λ_{max} = 365 nm) was performed by irradiating with a 500 W Xenon lamp (λ_{irr} = 300 – 400 nm) in a 2-methyltetrahydrofuran (MTHF) glass at 80 K, which was monitored by measuring the electronic absorption spectrum. Just after photoirradiation, the species which absorb the light around 320 - 360 nm were observed in the denitrogenation. Two species were identified by the ESR measurements. The compound A has a typical triplet ESR signals, and the compound B has a strong ESR signal at ca. g = 2.03.



Since the *D* parameter of the compound A was determined to be 520 G, which is nearly the same value for the biradical **1**, the distance between the two spins was estimated to be 3.5Å. Thus, the compound A was assigned to be **BR2a.** To identify the spin-multiplicity of compound B, the 2D-ESTN measurement has been done (Figure 1). The measurements clearly indicate that the compound B is also the triplet species, since the ESR signals was observed at the same nutation frequency of the compound A, i.e. **BR2a**. The *D* parameter of the compound B determined to be 19G. The calculated distance between the two spins was estimated to be 11Å. The spectroscopic analysis suggest that the compound B is the triplet biradical **BR3a**.

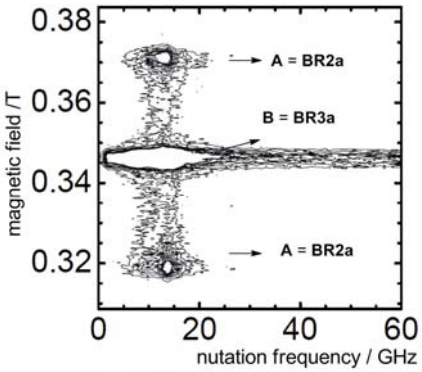


Figure 1 2D-ESTN spectral analysis