1A4b Generation and Spectroscopic Study on Tetraradical Species with Two Localized 1,3-Diradical Units

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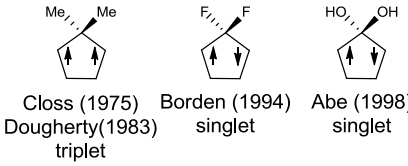
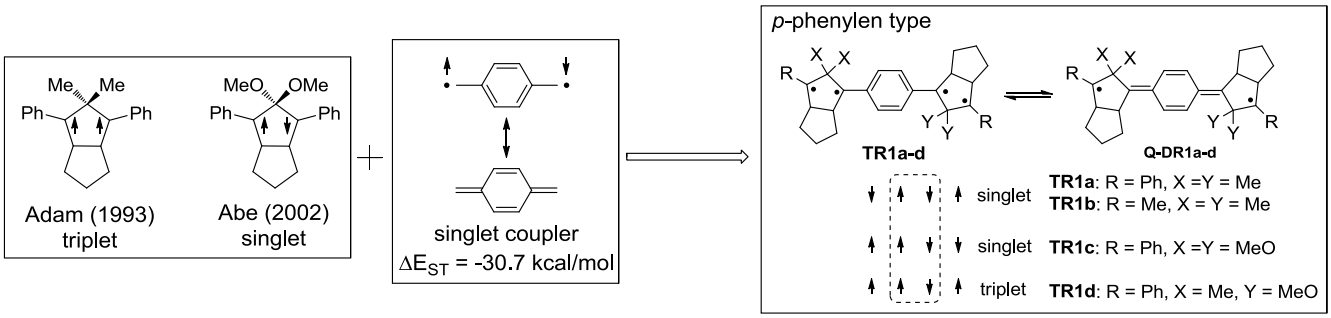
The direction of spins plays an important role in chemical reactions and physical property of open-shell molecules. So far, Borden and our group have found that the ground state of the spin-multiplicity of cyclopentane-1,3-diyls was controlled by the substituent effect at C(2) position[1-4].

In the present study, tetradicals **TR1a-d**, in which the two cyclopentane-1,3-diyl units were connected with para-phenylene coupler, were generated and their ground state spin-multiplicity was examined in detail using spectroscopic analyses including UV-vis and ESR measurements. When the tetraradical structure is important, the ground state spin-multiplicity is supposed to be controlled by the substituents X and Y on the diradical unit.





On the other hand, when the tetraradical **TR1a-d** have quinoidal structures, the substituents would be not sensitive to the ground state spin-multiplicity. Based on the ESR studies, the singlet ground state spin-multiplicity was found for all of the tetraradical species reported here.

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