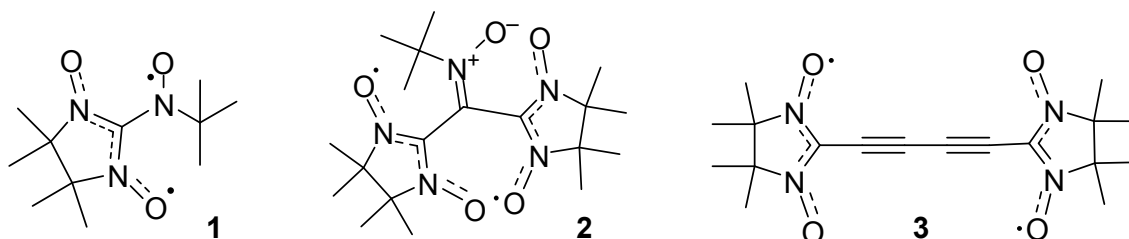


Triplet, Singlet and Nearly Degenerate Nitroxide Diradicals

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Being curious by the report on theoretical construction of hydrocarbon polyradicals published by W. Borden and E. Davidson in 1977, we explored the feasibility of preparing stable nitroxide diradicals with the low-lying triplet or singlet state, as well as a nearly degenerate state. We succeeded in isolating a triplet ground state nitroxide diradical **1** that is persistent at room temperature, possesses a singlet-triplet energy gap that is greater than the thermal energy at room temperature ($J/k_B \sim 390\text{K}$, $H = -2JS_{1/2} \cdot S_{1/2}$), and can be sublimed.¹ We prepared and studied another class of stable nitroxide diradicals (**2** as an example) with singlet ground state and low singlet-triplet energy splitting ($J/k_B = -7.4\text{K}$).² The diradical **3** with the diacetylene coupler was found to have singlet ground state with strong antiferromagnetic coupling and a high kinetic stability at ambient conditions ($J/k_B = -104\text{K}$).³



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