Nonacethrene as a magnetic photoswitch: can one methyl group change the game?

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In this project we aim to design a new all organic chiral magnetic photoswitch. The target compound is called nonacethrene and is the bigger homolog of cethrene, a chiroptical diradicaloid photoswitch. Pristine cethrene is too reactive but functionalization with two methyl groups in the fjord region leads to dimethylcethrene, which can be switched between an open and a closed form via light but does not possess an electron paramagnetic resonance (EPR) signal at room temperature. By expanding the π-backbone and therefore lowering the singlet-triplet gap, nonacethrene is EPR active. Nonacethrene undergoes an unwanted cascade reaction and dimethylnonacethrene is not reactive enough to act as a photoswitch. The adjustment of the steric bulk in the fjord region with only one methyl group represents an opportunity for further optimization to achieve bistability and is a viable strategy to realize a magnetic photoswitch operating at ambient temperature.