

Supporting Information

Synthesis and Properties of the 3-*tert*-Butyl-7-trifluoromethyl-1,4-dihydro-1-phenyl-1,2,4-benzotriazin-4-yl Radical

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UV-Vis spectra

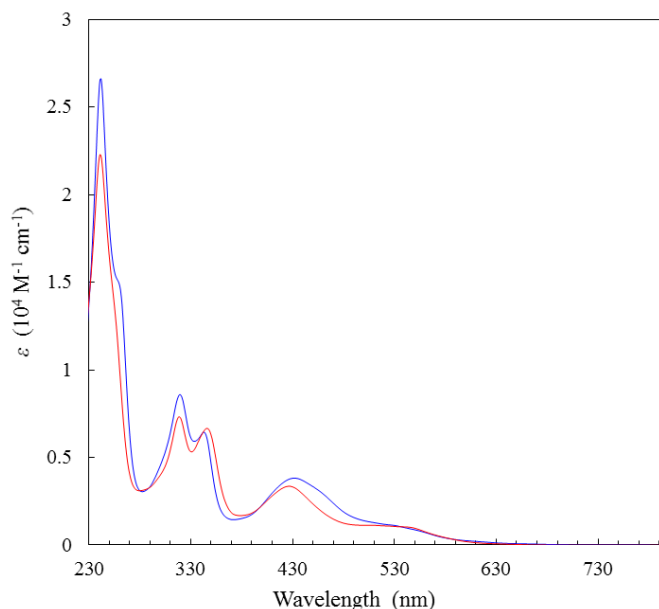


Figure S1. UV-Vis spectra of **1**(red) and **2**(blue) in CH₂Cl₂.

Crystallographic analysis

Table S1 Crystallographic data of **1** and **2**.

	1	2
Chemical formula	C ₁₇ H ₁₈ N ₃	C ₁₈ H ₁₇ F ₃ N ₃
Formula weight	264.34	332.34
Temperature / K	296	296
Crystal size / mm ³	0.85 × 0.73 × 0.20	0.78 × 0.32 × 0.12
Space group	<i>P</i> 2 ₁ / <i>n</i> (No. 14)	<i>Cc</i> (No. 9)
<i>a</i> / Å	9.6624(13)	5.592(2)
<i>b</i> / Å	9.8119(11)	18.904(7)
<i>c</i> / Å	15.7422(18)	15.882(5)
β / °	104.595(4)	92.487(11)
<i>V</i> / Å ³	1444.3(3)	1677.3(11)
<i>Z</i>	4	4
<i>d</i> _{calc} / g cm ⁻³	1.216	1.316
μ / mm ⁻¹	0.074	0.103
<i>F</i> (000)	564	692
θ (min, max) / °	2.469, 29.355	2.508, 22.273
Index ranges	-13 ≤ <i>h</i> ≤ 13, -10 ≤ <i>k</i> ≤ 13, -21 ≤ <i>l</i> ≤ 17	-6 ≤ <i>h</i> ≤ 7, -19 ≤ <i>k</i> ≤ 24, -17 ≤ <i>l</i> ≤ 20
Measured reflection	13831	4642
Independent reflection (<i>R</i> _{int})	3762 (0.0357)	2871 (0.0559)
Observed reflection (<i>I</i> ≥ 2σ(<i>I</i>))	2323	1725
Goodness of fit on <i>F</i> ²	0.860	1.060
<i>R</i> , <i>R</i> _w (<i>I</i> ≥ 2σ(<i>I</i>))	0.0523, 0.1345	0.0662, 0.1736
<i>R</i> , <i>R</i> _w (all data)	0.0929, 0.1683	0.1132, 0.2069
Resd density (min, max) / e Å ⁻³	-0.345, 0.192	-0.264, 0.348

DFT output data of 2

Archive data for doublet

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26.3109674,3,179.69666548,0|C,2,1.36847704,1,89.53100047,5,179.9158756
7,0|C,4,1.41100184,3,122.17799176,1,-178.23522057,0|H,7,0.93082205,4,1
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86,0|C,9,1.47014886,7,119.10774099,4,178.65144275,0|C,6,1.39227986,2,1
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2,3,176.49075442,1,-7.8681205,0|H,17,0.93152676,14,178.60935886,3,16.2
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.29718523,0|C,13,1.52022933,5,111.73685395,2,-156.26489911,0|H,35,0.96
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Table S2 Calculated energies of triplet and broken symmetry singlet for **2** at UB3LYP/6-31G(d) level.

	E (HF)	S^2	S^2_{Λ}
Triplet state	-2319.1453881	2.02689	2.000421
Broken symmetry singlet state	-2319.1453862	1.026865	0.216298