1-(2-Methoxyphenyl)-3-(phenyl)-1,4-dihydro-1,2,4-benzotriazin-4-yl: A Tricky "Structure-to-Magnetism" Correlation Aided by DFT Calculations

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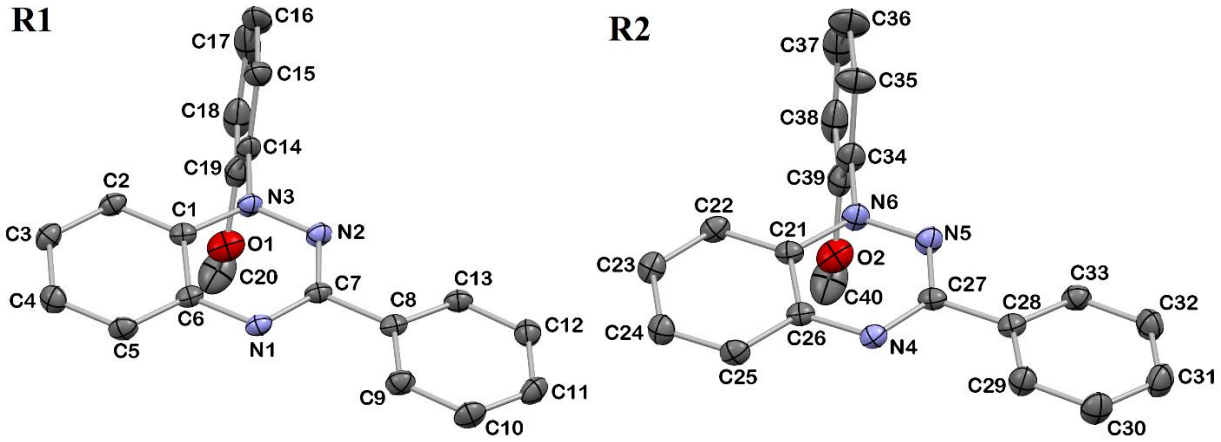
Supporting Information

Table T1 Comparison of selected experimental and computational UB3LYP/6-311+G(d,p) intramolecular geometrical parameters for the 1-(2-Methoxyphenyl)-3-(phenyl)-1,4-dihydro-1,2,4-benzotriazin-4-yl.



XRD (R1)	XRD (R2)	DFT
Bond Lengths (Å)		
N3-N2 = 1.374(2)	N6-N5 = 1.368(2)	N-N = 1.360(3)
N2-C7 = 1.335(3)	N5-C27 = 1.334(3)	N-C = 1.337(0)
C7-N1 = 1.333(3)	C27-N4 = 1.334(3)	C-N = 1.335(0)
N1-C6 = 1.379(2)	N4-C26 = 1.378(2)	N-C = 1.368(5)
C6-C1 = 1.412(3)	C26-C21 = 1.404(3)	C-C = 1.421(4)
C1-N3 = 1.380(3)	C21-N6 = 1.385(3)	C-N = 1.390(0)
Bond Angles (º)		
N3-N2-C7 = 115.0(2)	N6-N5-C27 = 115.1(2)	N-N-C = 116.4(6)
N2-C7-N1 = 127.5(2)	N5-C27-N4 = 127.5(2)	N-C-N = 126.7(2)
C7-N1-C6 = 116.4(2)	C27-N4-C26 = 116.3(2)	C-N-C = 116.5(6)
N1-C6-C1 = 121.2(2)	N4-C26-C21 = 121.4(2)	N-C-C = 121.4(7)
C6-C1-N3 = 116.1(2)	C26-C21-N6 = 116.1(2)	C-C-N = 115.9(3)
C1-N3-N2 = 123.7(2)	C21-N6-N5 = 123.5(2)	C-N-N = 122.6(8)
Dihedral Angles (º)		
C1-N3-C14-C19 = 79.6(3)	C21-N6-C34-C35 = 79.1(3)	C-N-C-C = 71.9(2)
C19-C14-N3-N2 = 89.5(2)	C39-C34-N6-N5 = 86.4(3)	C-C-N-N = 110.5(3)
N1-C7-C8-C9 = 6.1(3)	N4-C27-C28-C29 = 7.6(3)	N-C-C-C = 2.3(6)
N2-C7-C8-C13 = 5.4(3)	N5-C27-C28-C33 = 7.7(3)	N-C-C-C = 2.1(7)

Fig. S1 Mean distance between the centroids of 1,2,4-triazinyl and N-(2-anisole) rings in dimer I (left) and dimer II (right).

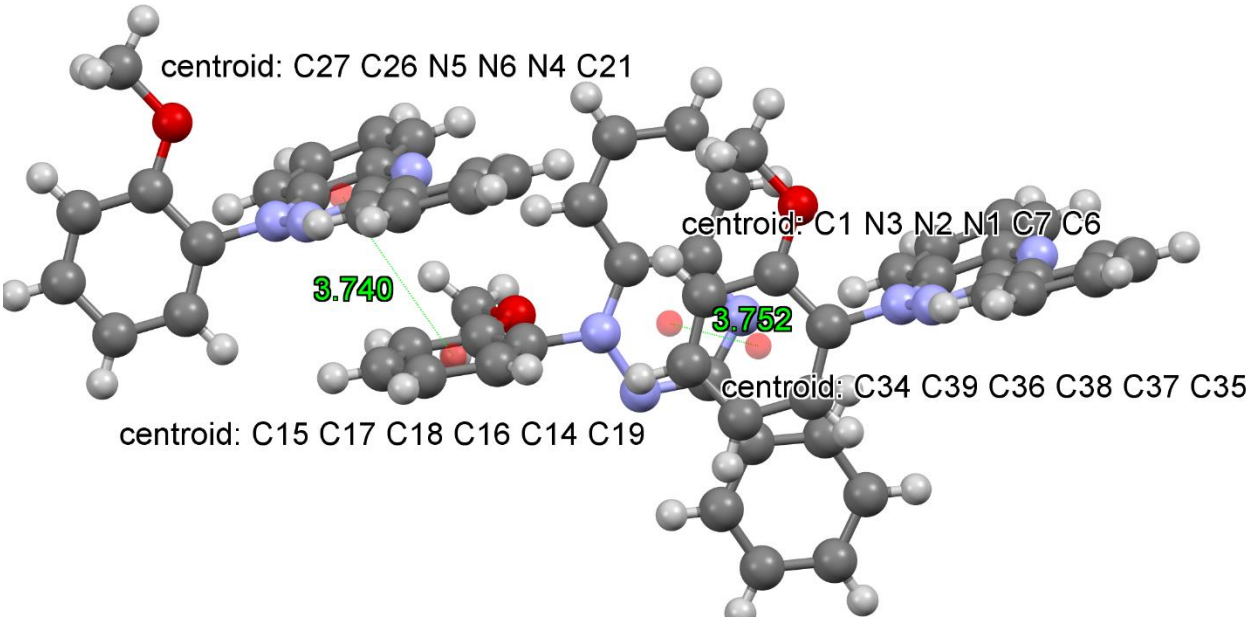


Fig. S2 Dihedral angles of alternating radicals forming the herringbone pattern of chain C2.

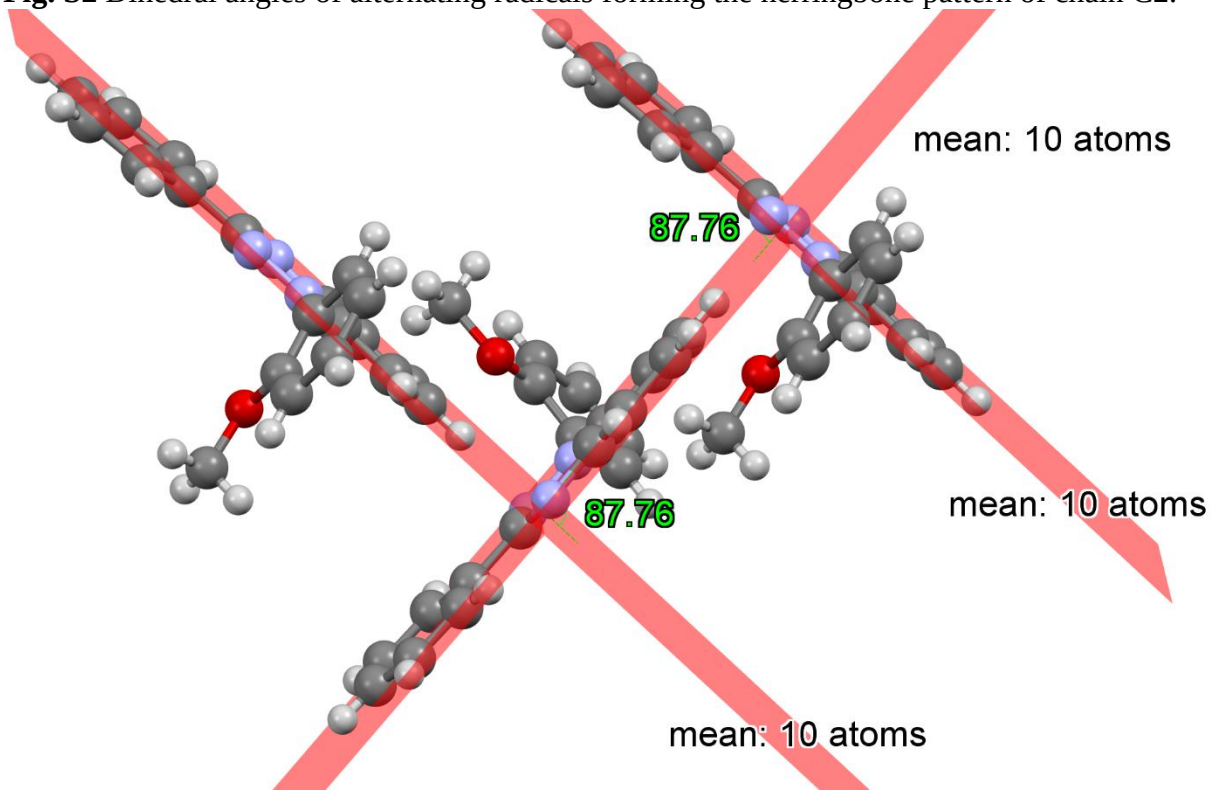
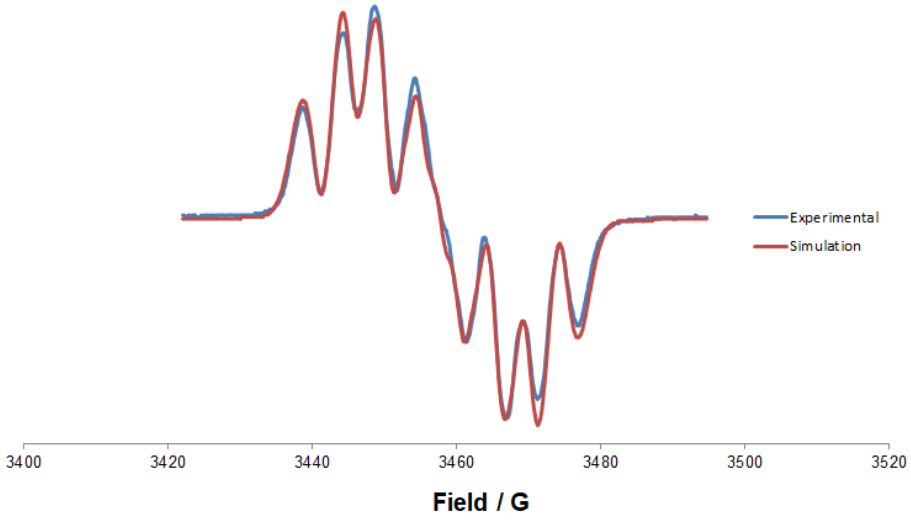


Fig. S3 Experimental (CH_2Cl_2, 25°C) and simulated EPR for 1-(2-Methoxyphenyl)-3-(phenyl)-1,4-dihydro-1,2,4-benzotriazin-4-yl.



Fitting parameters: g = 2.003685, $a_N(1)$ = 7.55 G, $a_N(2)$ = 4.70 G, $a_N(4)$ = 5.04 G (Lineshape: ΔH_{pp} = 2.01 G, 15% Lorentzian, 85% Gaussian).

Fig. S4 Powder X-ray diffraction patterns for radical **2** (top) collected at 300 K (red line) and calculated from the single crystal X-ray structure at 100 K (blue line).