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Diaminotriazine-substituted nitronyl nitroxide: A novel building block for organic magnets possessing multiple hydrogen bonding substituents as structure-determining supramolecular synthons

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Table 1S. Atomic spin densities ρ and hyperfine coupling constants (hfcc's) A of the radical **1**.[a,b,e]

atom	spin density ρ		hfcc A/ MHz	
	geometry I[d]	geometry II[e]	geometry I[d]	geometry II[e]
O1	0.340682	0.314039		
N1	0.272163	0.251849	23.7269	21.4761
C1	-0.181159	-0.185800		
N2	0.272163	0.281367	23.7268	23.5639
O2	0.340682	0.361546		
C2	-0.012135	-0.011041		
C3	-0.012135	-0.014620		
C4	0.016337	0.005449		
C5	0.003902	0.012988		
C6	0.003903	0.015333		
C7	0.016336	0.005241		
H9	-0.001256	-0.000201	-1.8323	-0.5006
H10	-0.000299	-0.001083	0.9250	-1.0303
H11	-0.000631	-0.000484	-1.0797	-1.0990
H12	0.000357	-0.000015	-0.6218	-0.5641
H13	-0.000989	-0.000346	-0.9172	-0.0985
H14	-0.000962	-0.000556	-1.0366	-1.1082
H15	0.000357	0.000147	-0.6221	-0.5469
H16	-0.000989	-0.000487	-0.9169	-0.5936
H17	-0.000961	-0.000872	-1.0364	-1.1715
H18	-0.001256	-0.000294	-1.8322	-0.7933
H19	-0.000298	-0.001097	0.9251	-0.4887
H20	-0.000631	-0.000357	-1.0797	-0.9222
C8	0.036216	0.028026		
C9	-0.042783	-0.028363		
C10	0.022394	0.014858		
C11	-0.039873	-0.026753		

atom	spin density ρ		hfcc A/ MHz	
	geometry I[d]	geometry II[e]	geometry I[d]	geometry II[e]
C12	0.022395	0.014410		
C13	-0.042783	-0.029691		
H5	-0.001255	-0.000896	-1.4489	-1.0549
H6	0.001427	0.001651	3.5317	1.9678
H7	-0.001256	-0.000862	-1.4489	-0.9757
H8	0.001427	0.001936	3.5320	2.0174
N3	-0.005682	-0.003032	-0.3573	-0.2332
N4	-0.004328	-0.002244	-0.2839	-0.1464
N5	-0.005681	-0.003046	-0.3573	-0.2306
C14	0.003539	0.001835		
C15	0.001301	0.000614		
C16	0.001301	0.000645		
N6	0.000223	0.000081	0.0321	0.0113
H1	0.000007	0.000004	-0.0042	0.0008
H3	0.000000	0.000003	-0.0160	-0.0044
N7	0.000223	0.000116	0.0321	0.0140
H2	0.000007	0.000003	-0.0042	-0.0037
H4	0.000000	0.000000	-0.0160	-0.0082

[a]The convergence criteria was 1×10^{-8} hartree. The expectation values $<S^2>$ before and after the spin-projection, *i.e.*, the annihilation of higher spin multiplicity components, are 0.8098 and 0.7506, respectively.

[b]The atom numbering scheme is given in Scheme 1S.

[c]The molecular geometry I was taken from the X-ray crystal structure.

[d]The geometry optimization at the UB3LYP/3-21G level gave the molecular geometry II.

[e]The spin density and the hfcc values were calculated at the UB3LYP/DZVP level.

Scheme 1S. Atom numbering scheme of the radical **1**, corresponding to the DFT-calculated spin density distribution in Table 1S.