SUPPLEMENTARY MATERIALS

Spin Catalysis in Photochemical Reactions and Its Applications to Quantum Information Nanotechnology

Boris F. Minaev
Uppsala University, Institute of Physics and Astronomy, Uppsala, Sweden
(Author's e-mail: bfmin43@ukr.net)

List of Content

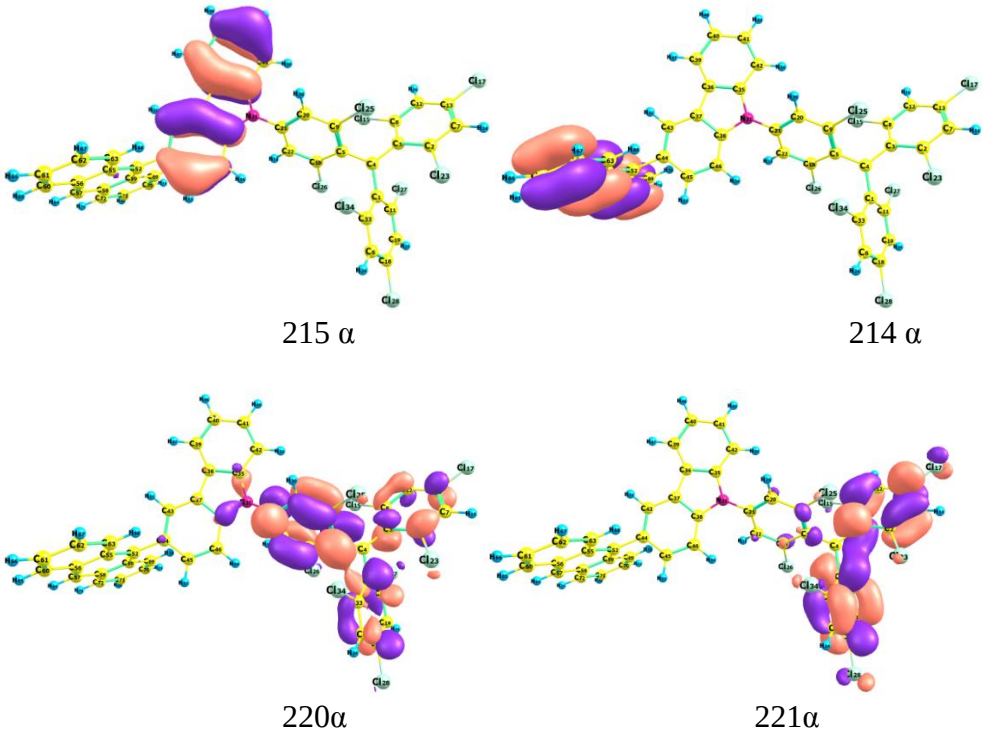
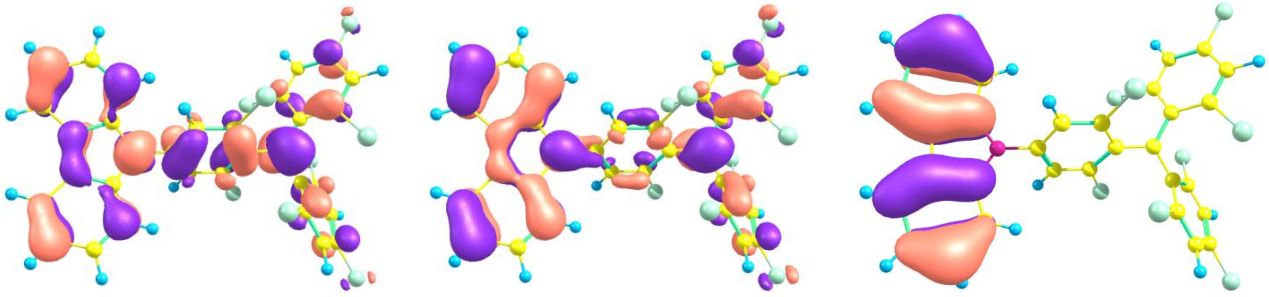


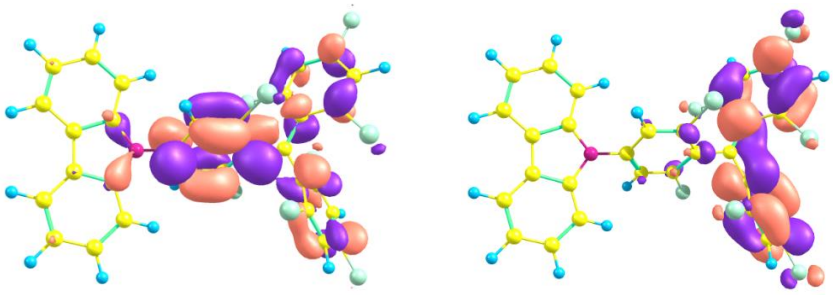
Figure S1. Additional molecular orbitals for α spins of the radical TTM-Cz-Anthracene depicted in Figure 1B. MO 215 β and 215 α are almost identical

Table S1. TD DFT calculation of the electronic absorption spectrum of the TTM-Cz radical

State	E(eV)	λ (nm)	*f*	Configuration state function	S^2
D_1	1.875	661.2	0.0935	0.98(171β -172β)	0.826
D_2	2.253	550.4	0	0.99(170β -172β)	0.821
D_3	2.661	465.8	0.0169	0.79(169β -172β)+ 0.37(168β -172β)	0.997
D_4	2.765	448.4	0	0.80(167β -172β)	1.00
D_5	2.892	428.8	0.0034	0.72(166β -172β)	0.872
D_6	2.951	420.0	0.0017	0.74(164β -172β)+ +0.53(167β -172β)	0.922
D_7	2.951	419.9	0.0040	0.79(165β -172β)	0.864
D_8	3.117	397.7	0.0987	0.51(172α -173α)+ 0.60(163β -172β)	1.39
D_9	3.171	391.0	0	0.57(170β -176β)- 0.57(170α -178α)	2.63
D_{10}	3.274	378.6	0.1715	0.57(163β -172β)- 0.57(172α -173α)	1.11

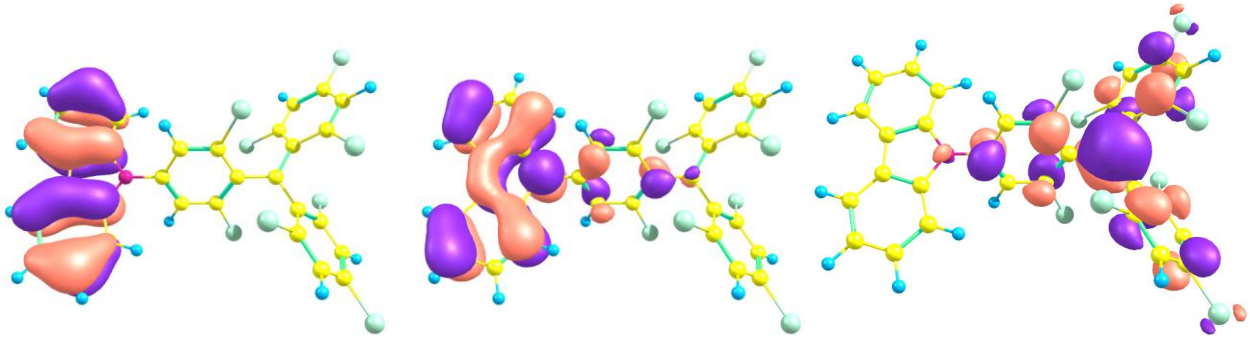


172α 171α 170α

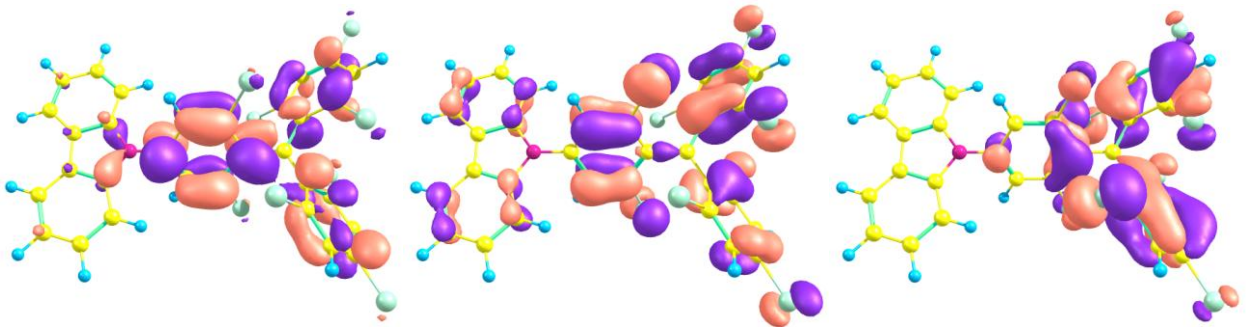


173α 174α

Figure S2A. Molecular orbitals for the α spin of the TTM-Cz radical



170β 171β 172β



173β 169β 167β

Figure S2B. Molecular orbitals for the β spin of the TTM-Cz radical

We have optimized the quartet state of the B radical presented in Figure 1B by the UB3LYP method (Figure S3) and analyzed its atomic spin density (by Mulliken) and EPR parameters: isotropic hyperfine coupling (HFC) constants of magnetic isotope nuclei ^{13}C, ^{35}Cl, ^{14}N and ^{1}H and anisotropic HFC tensor (Table S2).

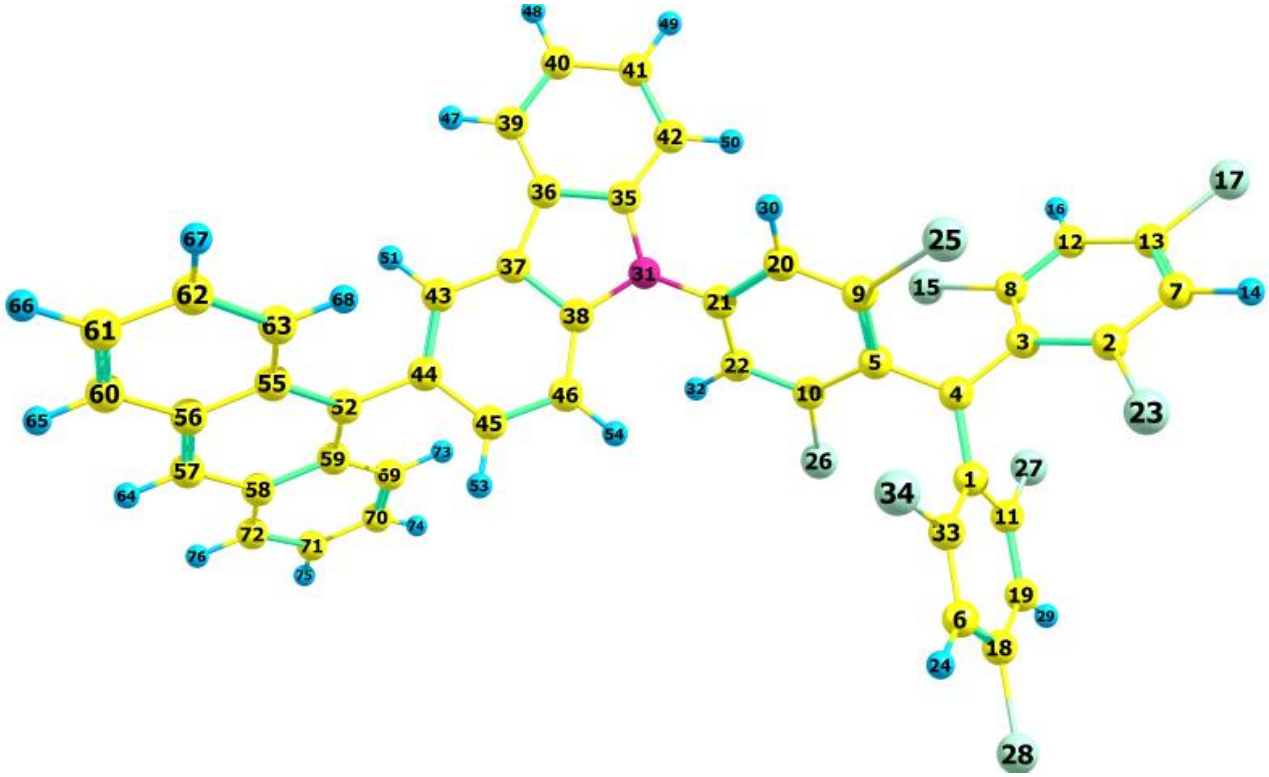


Figure S3. Optimized quartet state and numeration of atoms in the B radical (TTM-Cz-An)

Table S2. Spin density, atomic charge (according to Mulliken) and EPR parameters of the quartet state of the B radical (TTM-Cz-An). Long axis *a*, short axis *b*, and *c* is perpendicular axis to the carbazole moiety

Atomic numbers of isotope (A)	Spin density	Isortopic a_A HFC (MHz) constant	Anisotropic B_{aa} (MHz)	HFC tensor B_{bb} (MHz)	Components B_{cc} (MHz)	Atomic charge (a.u.)
1 ^{13}C	-0.120	-10.98	-9.96	3.92	6.04	0.133
2 ^{13}C	0.093	10.39	-7.14	-5.34	12.48	-0.122
3 ^{13}C	-0.121	-10.99	-10.01	3.91	6.10	0.134
4 ^{13}C	0.760	33.76	-55.24	-55.18	110.42	-0.122
5 ^{13}C	-0.121	-11.12	-10.48	4.09	6.39	0.140
6 ^{13}C	-0.047	-2.26	-5.65	2.30	3.35	0.089

7 ^{13}C	-0.047	-2.30	-5.69	2.31	3.38	0.089
8 ^{13}C	0.094	10.37	-7.12	-5.34	12.46	-0.121
9 ^{13}C	0.096	10.96	-7.25	-5.56	12.81	-0.143
10 ^{13}C	0.097	10.89	-7.34	-5.56	12.90	-0.143
11 ^{13}C	0.094	10.38	-7.11	-5.34	12.45	-0.121
12 ^{13}C	-0.047	-2.87	-5.69	2.30	3.39	0.088
13 ^{13}C	0.084	4.00	-6.69	-5.79	12.48	-0.088
14 ^{1}H	-0.002	1,37	-1.20	-0.35	1.55	0.138
15 ^{35}Cl	0.003	0.06	-2.11	-0.32	2.43	0.021
16 ^{1}H	0.002	1.39	-1.21	-0.39	1.60	0.138
17 ^{35}Cl	0.007	0.29	-2.81	-1.63	4.44	0.012
18 ^{13}C	0.086	3.98	-6.66	-5.70	12.45	-0.089
19 ^{13}C	-0.047	-2.29	-5.66	2.31	3.35	-0.049
20 ^{13}C	-0.046	-1.76	-5.71	2.41	3,30	-0.073
21 ^{13}C	0086	3.51	-6.80	-5.90	12.70	0.268
22 ^{13}C	-0.048	-1.85	-5.74	2.40	3.34	-0.074
23 ^{35}Cl	0.003	0.08	-2.16	-0.33	2.49	0.023
24 ^{1}H	0.002	1.39	-1.10	-0.40	1.50	0.138
25 ^{35}Cl	0.003	0.05	-2.16	-0.40	2.56	0.018
26 ^{13}Cl	0.004	0.0	-2.21	-0.38	2.59	0.018
27 ^{35}Cl	0.003	0.08	-2.15	-0.34	2.49	0.022
28 ^{35}Cl	0.007	0.29	-2.81	-1.62	4.44	0.012
29 ^{1}H	0.002	1.37	-1.17	-0.30	1.47	0.138
30 ^{1}H	0.002	1.35	-1.37	-0.40	1.77	0.136
31 ^{14}N	0.008	-0.02	-0.78	-0.66	1.44	;
32 ^{1}H	0.002	1.36	-1.47	-0.57	2.04	0.135
33 ^{13}C	0.093	10.35	-7.10	-3.35	12.45	-0.121
34 ^{35}Cl	0.003	0.06	-2.10	-0.32	2.42	0.021
35 ^{13}C	-0.003	0.38	-0.93	0.19	0.74	0.292
36 ^{13}C	0.008	0.57	-0.87	-0.31	0.87	0.040
37 ^{13}C	-0.010	-0.07	-1.44	0.07	1.36	0.051
38 ^{13}C	0.025	1.46	-2.25	-0.81	3.06	0.296
39 ^{13}C	-0.004	-0.21	-0.65	0.19	0.46	-0.131
40 ^{13}C	0.006	0.28	-0.43	-0.29	0.72	-0.099
41 ^{13}C	-0.004	-0.29	-0.59	0.27	0.32	-0.098
42 ^{13}C	0.006	0.23	-0.34	-0.25	0.60	-0.110
43 ^{13}C	0.024	7.26	-3.78	-2.11	5.89	-0.164
44 ^{13}C	-0.062	-6.74	-3.88	0.63	2.25	-0,003
45 ^{13}C	0.034	6.61	-3.15	-1.51	4.66	-0.120
46 ^{13}C	-0.011	-0.09	-1.82	0.18	1.63	-0.111
47 ^{1}H	0.000	0.01	-0.67	-0.43	1.10	0.093
48 ^{1}H	0.000	-0.14	-0.31	-0.21	0.52	0.087
49 ^{1}H	0.000	0.09	-0.34	0.03	0.31	0.090
50 ^{1}H	-0.000	-0.145	-0.72	0.26	0.46	0.101
51 ^{1}H	-0.002	-0.98	-2.97	-0.64	3.61	0.100
52 ^{13}C	0.629	25.88	-44.01	-43.79	87.80	-0.079
53 ^{1}H	-0.002	-0.78	-3.04	-1.00	4.04	0.103
54 ^{1}H	0.001	0.64	-2.97	-0.64	3.61	0.100
55 ^{13}C	-0.086	-6.97	-4.98	1.19	3.79	0.120
56 ^{13}C	-0.104	-7.59	-7.91	2.68	5.23	0.120
57 ^{13}C	0.616	24.57	-42.88	-42.05	84.93	-0.202

58 ^{13}C	-0.104	-7.61	-7.96	2.70	5.26	0.120
59 ^{13}C	-0.086	-6.94	-4.96	1.18	3.78	0.119
60 ^{13}C	0.228	8.34	-16.52	-15.55	32.07	-0.153
61 ^{13}C	0.066	0.70	-6.35	-5.76	12.11	-0.085
62 ^{13}C	0.101	2.21	-8.48	-7.98	16.46	-0085
63 ^{13}C	0.206	7.16	-14.93	-13.82	28.75	-0.168
64 ^{1}H	-0.026	-13.17	-20.54	-2.82	23.36	0.082
65 ^{1}H	-0.010	-5.29	-6.04	-3.02	9.06	0.083
66 ^{1}H	-0.004	-2.70	-4.06	-2.31	6.37	0.085
67 ^{1}H	-0.006	-2.9	-5.05	-2.17	7.25	0.085
68 ^{13}H	-0.009	-4.85	-5.40	-3.16	8.56	0.097
69 ^{1}C	0.206	7.11	-14.87	-13.76	28.63	-0.167
70 ^{13}C	0.102	2.24	-8.52	-8.04	16.56	-0.085
71 ^{13}C	0.067	0.66	-6.30	-5.70	12.00	-0.085
72 ^{13}C	0.228	8.36	-16.55	-15.58	32.12	-0.153
73 ^{13}C	-0.009	-4.83	-5.41	-3.08	8.49	0.095
74 ^{13}C	-0.006	-3.00	-5.11	-2.10	7.21	0.085
75 ^{13}C	-0.004	-2.18	-4.20	-2.30	6.32	0.085
76 ^{13}C	-0.010	-5.30	-6.08	-3.00	9.08	0.083

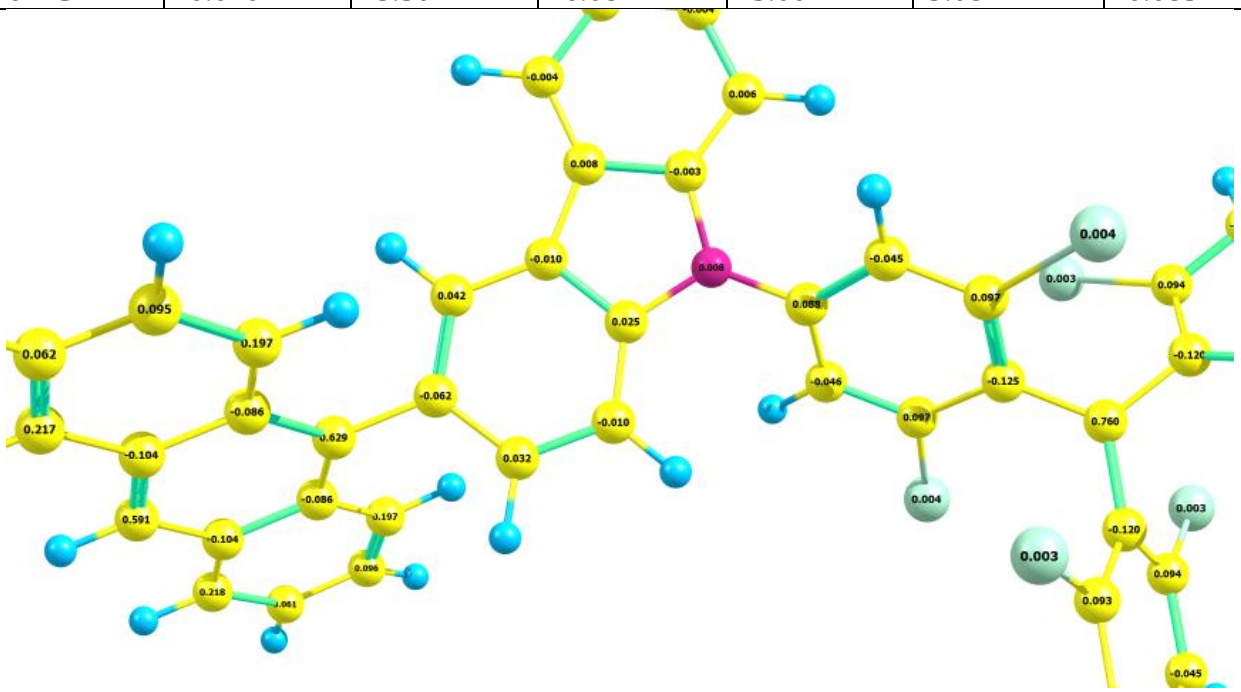


Figure S4. Atomic spin density of the TTM-Cz-An radical in the DFT optimized quartet state

Spin density of the most important atoms in the chemically relevant part of the TTM-Cz-An radical in the quartet state is shown in Figure 4S. Spin density at protons is added to the neighboring carbon atoms. It is fully presented in Table S2. Figure S4 clearly shows that 3 spins are distributed mostly on the C4 atom of the TTM radical (0.76) and close lying C1, C3, C5 atoms bear negative spin polarization (-0,126 on each atom). The carbazole moiety has negligible spin density and only benzene ring linked to anthracene shows some small spin polarization. About two non-paired spins are sitting in the anthracene moiety (mostly on 52 and 57 atoms); this corresponds to the triplet excited state of anthracene.

Strong electric polarization in TTM-Cz moiety is seen in Table S2; one can note large negative charge at N atom (-0.743e) and polarization around C4 atom. Essential negative charges at C57, C60, C63, C69 and C72 atoms correspond to the triplet-excited anthracene.