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Accessory Publication

X-ray-Triggered Thermoluminescence and DFT Characterization of *gem*-Diphenyltrimethylenemethane Biradical

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(1) The Computational Results for ^{3}4¨ and 5˙.

Table S1. The Cartesian Coordinates (in Å) of the ground state biradical ^{3}**4¨** optimized with UB3LYP/cc-pVDZ. (The sum of electronic and zero-point energy is –617.824395 Hartree.)

	X	Y	Z
C1	0.648037	1.025857	2.886032
C2	0.000000	0.000000	2.173349
C3	0.000000	0.000000	0.705664
C4	-0.648037	-1.025857	2.886032
C5	0.000000	1.268405	-0.033457
C6	0.000000	-1.268405	-0.033457
C7	0.709630	-2.399630	0.438122
C8	-0.706327	-1.407842	-1.252865
C9	-0.710019	-2.612189	-1.953470
C10	0.711112	-3.599391	-0.270133
C11	-0.000483	-3.716228	-1.468984
C12	-0.709630	2.399630	0.438122
C13	0.706327	1.407842	-1.252865
C14	0.710019	2.612189	-1.953470
C15	-0.711112	3.599391	-0.270133
C16	0.000483	3.716228	-1.468984
H17	1.205290	1.812521	2.379777
H18	0.620661	1.036630	3.977046
H19	-0.620661	-1.036630	3.977046
H20	-1.205290	-1.812521	2.379777
H21	-1.276379	-0.560714	-1.636135
H22	-1.277417	-2.692160	-2.883202
H23	1.283416	-2.319579	1.362027
H24	1.279759	-4.449522	0.112884
H25	-0.000835	-4.658091	-2.020901
H26	1.276379	0.560714	-1.636135
H27	1.277417	2.692160	-2.883202
H28	-1.283416	2.319579	1.362027
H29	-1.279759	4.449522	0.112884
H30	0.000835	4.658091	-2.020901

Table S2. The Cartesian Coordinates (in Å) of **5˙** optimized with UB3LYP/cc-pVDZ. (The sum of electronic and zero-point energy is –541.105699 Hartree.)

	X	Y	Z
C1	-0.039265	2.525077	0.131180
C2	-0.012781	1.021310	0.033884
C3	1.278134	0.334838	0.034349
C4	-1.275768	0.311077	-0.011769
C5	-2.485608	0.943019	0.388806
C6	-1.388008	-1.014040	-0.518496
C7	-2.615655	-1.663266	-0.591302
C8	-3.709503	0.284169	0.320189
C9	-3.787879	-1.025582	-0.166114
C10	2.416114	0.903375	-0.592113
C11	1.465398	-0.904820	0.698421
C12	2.707123	-1.535095	0.724725
C13	3.653125	0.263780	-0.574053
C14	3.810464	-0.960191	0.084730
H15	0.959955	2.963829	0.022042
H16	-0.705539	2.980891	-0.620481
H17	-0.414361	2.849386	1.120694
H18	-0.497887	-1.518910	-0.892626
H19	-2.662420	-2.676190	-0.997237
H20	-2.459530	1.959695	0.780356
H21	-4.614510	0.798249	0.651358
H22	-4.749457	-1.538891	-0.222133
H23	0.627180	-1.353404	1.232109
H24	2.817782	-2.480145	1.260960
H25	2.318236	1.847204	-1.130331
H26	4.503082	0.723486	-1.083051
H27	4.782116	-1.457100	0.103715

(End)