Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

The Involvement of Triplet State in the Isomerization of Retinaloids

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1. Vertical Excitation Energies

1.1. TD-CAM-B3LYP excitation energies

The figure below depicts the vertical excitation energies at the TD-CAM-B3LYP/cc-pVDZ level of theory at the optimized ground state. The numeric values of the corresponding VEE listed in the following table.

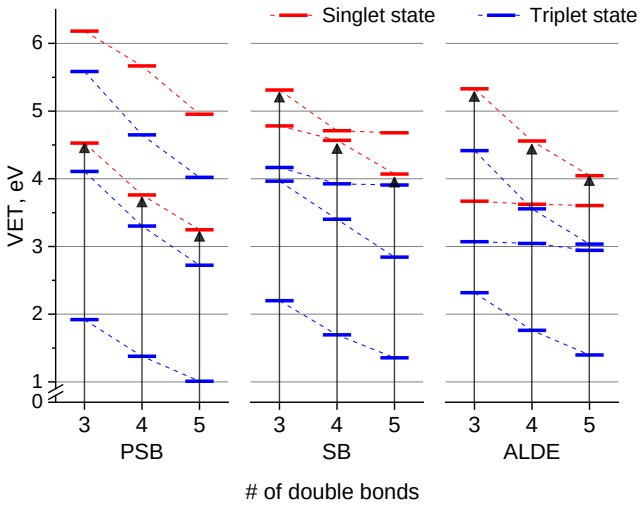

Fig S1. Graphical representation of the CAM-B3LYP vertical excitation energies.

Table 1. CAM-B3LYP vertical excitation energies in units of eV.

	PSB			SB			RAL		
	3	4	5	3	4	5	3	4	5
S_1	4.53	3.76	3.25	4.78	4.57	4.07	3.67	3.62	3.60
S_2	6.18	5.67	4.95	5.31	4.71	4.68	5.33	4.56	4.05
T_1	1.92	1.38	1.01	2.20	1.69	1.36	2.32	1.76	1.40
T_2	4.11	3.30	2.72	3.96	3.40	2.84	3.07	3.05	2.94
T_3	5.59	4.65	4.02	4.17	3.93	3.91	4.42	3.56	3.04

1.2. CC2 excitation energies

The figure below depicts the vertical excitation energies at the CC2/cc-pVDZ level of theory at the optimized ground state. The numeric values of the corresponding VEE listed in the following table.

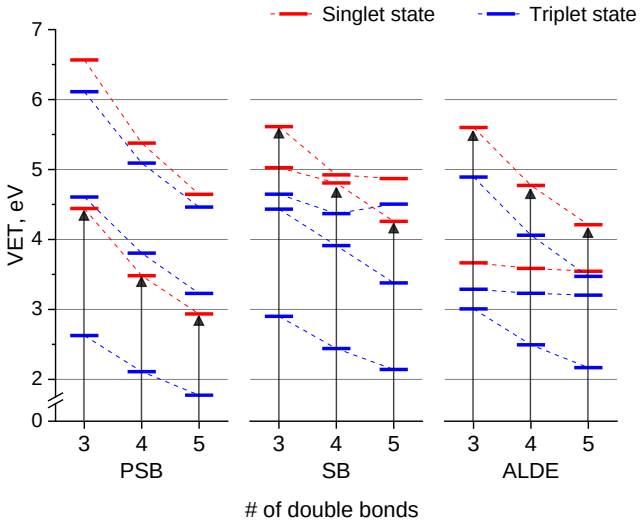

Fig S2. Graphical representation of the CC2 vertical excitation energies.

Table 2. CC2 vertical excitation energies in units of eV.

	PSB			SB			RAL		
	3	4	5	3	4	5	3	4	5
S_1	4.44	3.48	2.94	5.03	4.81	4.26	3.67	3.59	3.55
S_2	6.57	5.38	4.65	5.61	4.92	4.87	5.60	4.77	4.21
T_1	2.63	2.11	1.77	2.90	2.44	2.14	3.01	2.49	2.17
T_2	4.61	3.80	3.23	4.43	3.91	3.38	3.29	3.23	3.20
T_3	6.11	5.09	4.46	4.65	4.37	4.51	4.89	4.06	3.47

1.3 XMS-CASPT2 excitation energies

The figure that depicts the vertical excitation energies at the XMS-CASPT2/cc-pVDZ level of theory is placed in the manuscript as Figure 4. The numeric values of the corresponding VEE listed in the following table.

Table 3. XMS-CASPT2 vertical excitation energies in units of eV.

	PSB			SB			RAL		
	3	4	5	3	4	5	3	4	5
S_1	4.12	3.34	2.83	4.73	4.45	4.01	3.55	3.44	3.36
S_2	5.32	4.24	3.55	5.14	4.56	4.08	5.18	4.50	4.03
T_1	2.47	1.82	1.52	2.80	2.33	2.07	2.96	2.46	2.14
T_2	4.42	3.45	2.92	4.28	3.78	3.28	3.23	3.19	3.14
T_3	6.07	4.68	4.01	4.53	4.17	4.10	4.81	3.99	3.43