Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Relationship Between the Structural Characteristics of Retinal and Its Visual Function—A Theoretical Study

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**Keywords:** retinal, terminal group, conjugation length, saturated group, theoretical study

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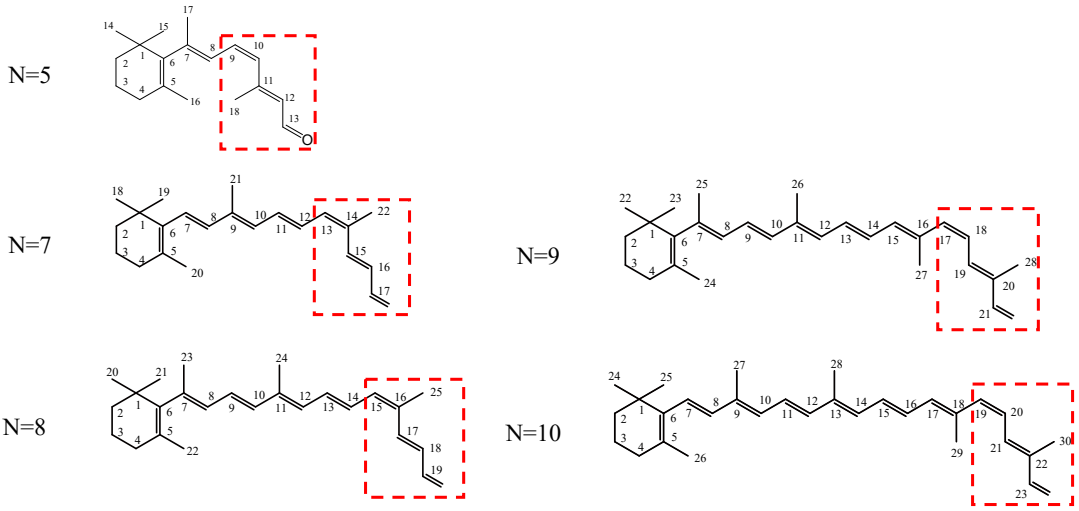


Fig. S1 Structures for 11-cis retinal derivatives with N=5 and 7-10, where the conjugated skeleton in the red box is the same as retinal, while the position of -$CH_3$ is arranged according to the arrangement rule in carotenoids.

Fig. S2 The closed-shell and double radical form of retinal.

| Retinal Derivatives | HOMO (eV) | LUMO (eV) | Gap (eV) |
|---|---|---|---|
| C=O | -5.37 | -2.34 | 3.03 |
| C=C | -4.82 | -1.70 | 3.12 |
| C=N | -5.09 | -1.97 | 3.12 |

Table S1 The energies of frontier orbitals for retinal with C=O, C=N and C=C.

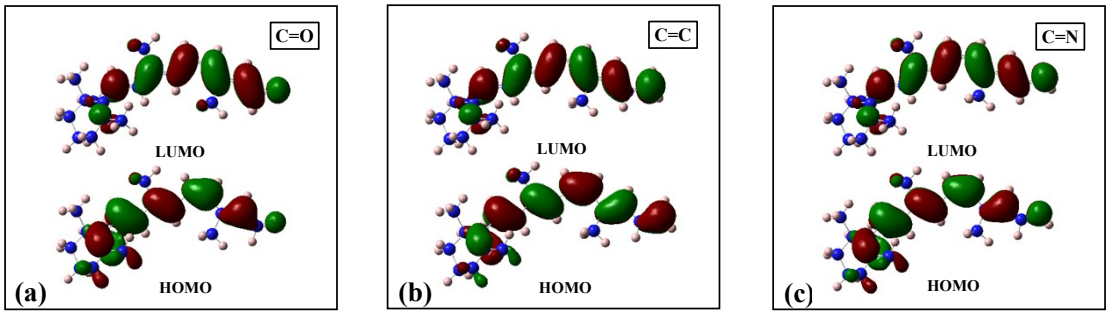


Fig. S3 The orbital distribution for 11-*cis* retinal and derivatives with terminal group C=C and C=N.

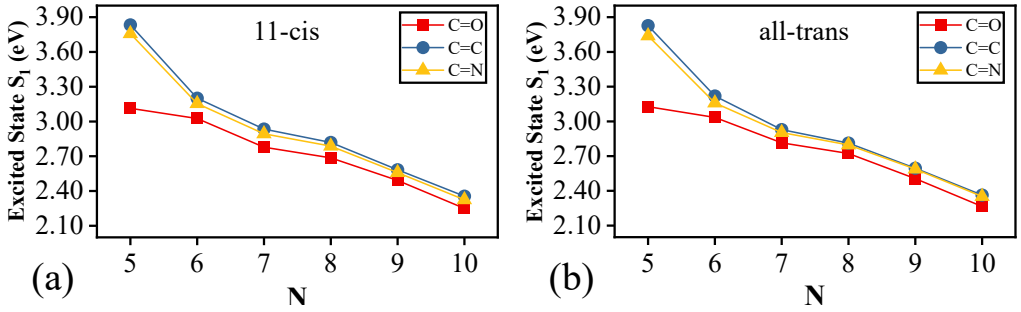


Fig. S4 The values of excited state $S_1$ for retinal derivatives with N=5 and 7-10 in 11-cis and all-trans configurations by b3lyp mothed.

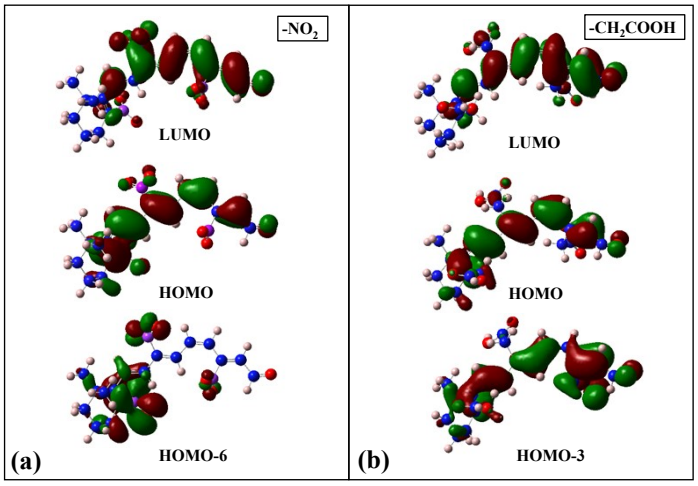


Fig. S5 Molecular orbitals for retinal with R=$NO_2$ (left) and R=$CH_2COOH$ (right). C, O, N and H atoms are shown in blue, red, purple and pink, respectively.

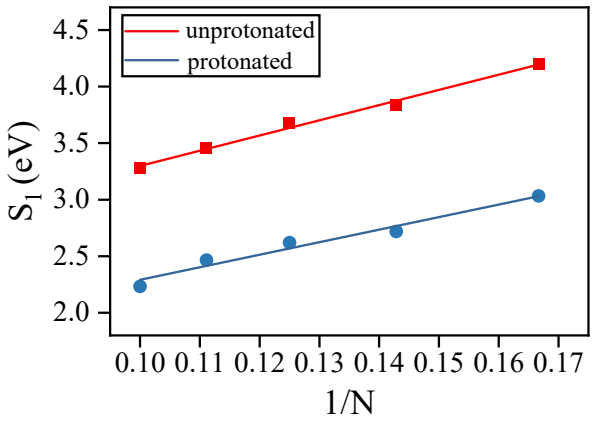


Fig. S6 The energy of $S_1$ for all-*trans* retinal and its derivatives with N=6-10.