Abstract

While a lot of attention has been placed on how the methyl groups, charge distribution and protein environment influence the photo transduction process of retinal few reports the influence of the conformation of β-ionone ring during the retinal change from meta I to meta II. In this research, we try to find coordinates between the conformation and the retinal photo transduction process. Few conformational studies have been conducted to determine the influence of the pKa value. HF, B3LYP and MP2 gas phase calculation methods are conducted in order to compare the accuracy of these methods. After the MP2 level scanning was done for each dihedral for both protonated and deprotonated retinal.

Method

Coordinates Search is done using Harvest-Plane, B3LYP and MPS 2.0 programs are done for each dihedral. Geometry optimization is completed in vacuum at DFT/B3LYP/6-31G* and DFT/B3LYP/6-31G**/6-31+G*/6 level. Geometry is refined by performing CASPT2/6-311G**/6-311G*/6 calculation. pKa values are calculated using B3LYP/6-31G**/6-31G* and MP2/6-31G**/6-311G*/6-311G**/6 level. Proton affinity measures the basicity of gas phase retinal, and it is also a primary parameter. Different methods used to scan all of dihedrals to obtain highly accurate energy barrier data. Reparametrization was done by adjusting the dihedral potential to fit the energy difference between MD and QM calculation.

Conclusion

Unlike most of previous research, we take the β-ionone ring of retinaxa consideration during our research. The influence of it creates 54 degrees C6-C7 dihedral of the lowest rotational barrier instead of cis or trans in the deprotonated retinal. According to MP2 coordinates search, the delocalization of the positive charge is protonated retinal's internal π system of C6-C7 which has double bond character. This may be used to set up new parameters for CHARMM. Difference G0_G0 methods don't influence pKa value very much. However, the pKa value is affected a great deal by HF, B3LYP and MP2 gas phase energy calculation methods ranging from -3 to +3. MP2 at level 17 to 20 seems to be the better choice. According to previous research, pKa give at the most reactive protonable sites. The pKa value of retinal suggests that the reparametrization is necessary for retinal. Therefore, the value of pKa for retinal can be adjusted by adjusting the dihedral potential to fit the energy difference between MD and QM energy calculation.

The pKa of Retinal Depends On the Conformation of the β-Ionone Ring and the Reparametrization of CHARMM Force Field For Retinal

Shengshuang Zhu, Scott Feller

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