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The electronic structure of photosensitizing psoralens has been investigated by the *ab initio* calculations. The photocycloaddition reaction of 8-methoxypsoralen with thymine is studied as a model for the photosensitizing reaction of psoralen with DNA bases. The photocycloadduct was inferred to be a C⁴-cycloaddition product with the stereochemistry of *Syn, H-H, Syn, H-T* formed through [2+2] addition reaction between the 3,4 double bonds of 8-methoxypsoralen and 5,6 double bond of thymine base.

Key-words : Ab initio, C⁴-cycloaddition, 8-methoxypsoralen