Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supplementary Information (ESI)

Light-driven modulation of fluorescence color from azobenzene derivatives containing electron-donating and electron-withdrawing groups

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Contents:

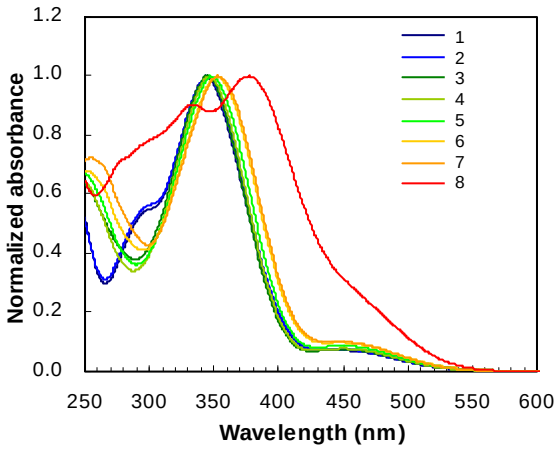


Figure S1 UV-vis absorption spectra of as-prepared **1-8** in dichloromethane solution.

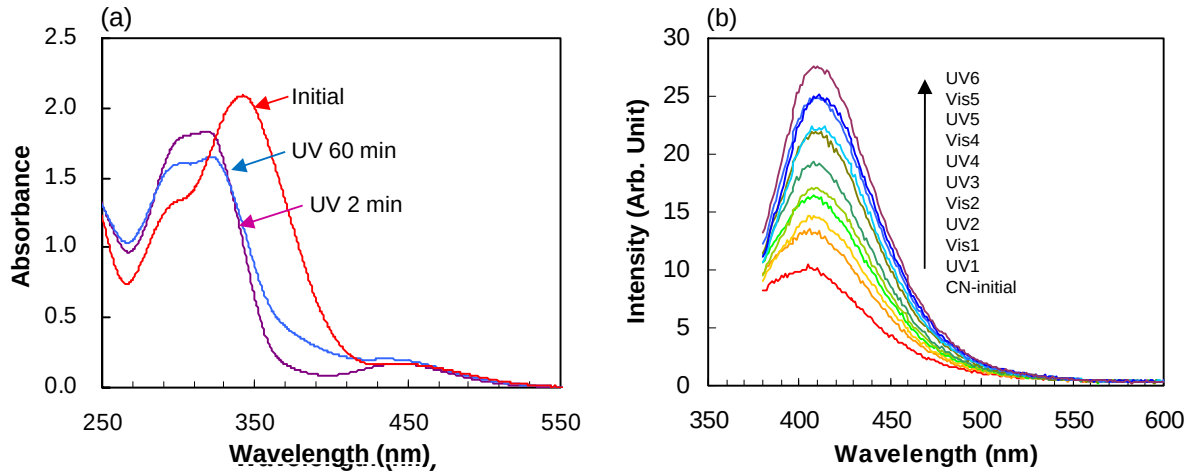


Figure S2 (a) Absorption spectral changes of **1** in dichloromethane solution. (b) Fluorescence spectral changes of **1** in dichloromethane solution upon alternating UV and visible light irradiation (λ_{max} = 330 nm).

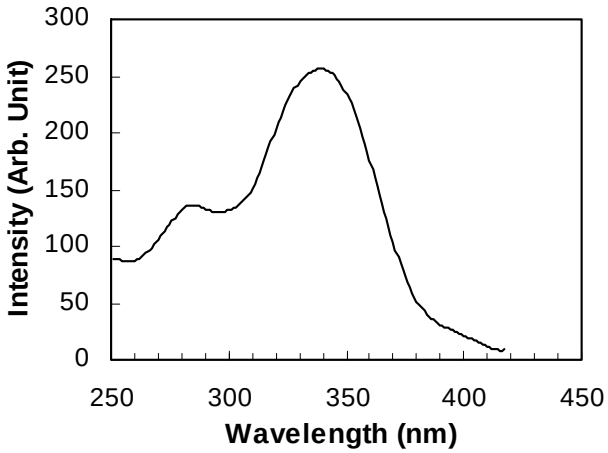


Figure S3 Uncorrected excitation spectrum of UV-exposed **1** solution (monitored at 420 nm).

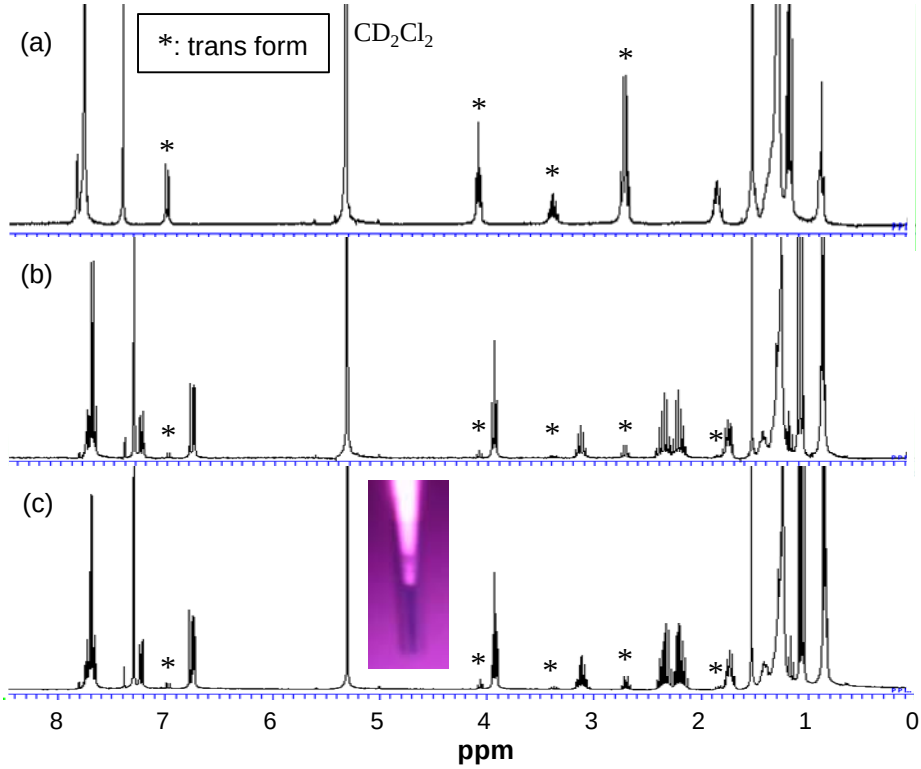


Figure S4 ^{1}H NMR spectra of **1** in CD_2Cl_2. (a) Initial. (b) After irradiation with UV light for 20 min. (c) After prolonged irradiation with UV light. Photographic image showing weak blue fluorescence (λ_{ex} = 365 nm).

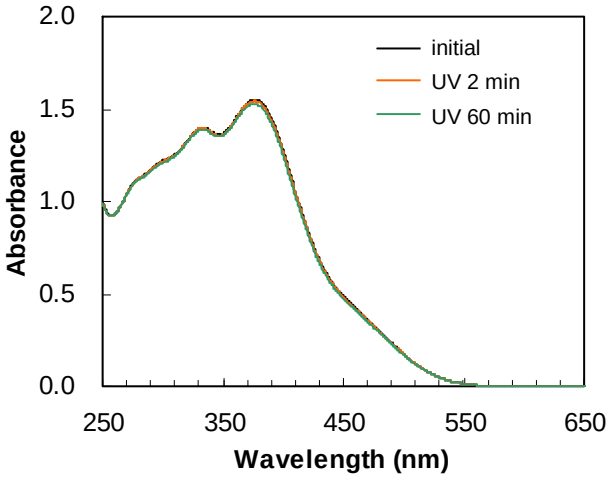
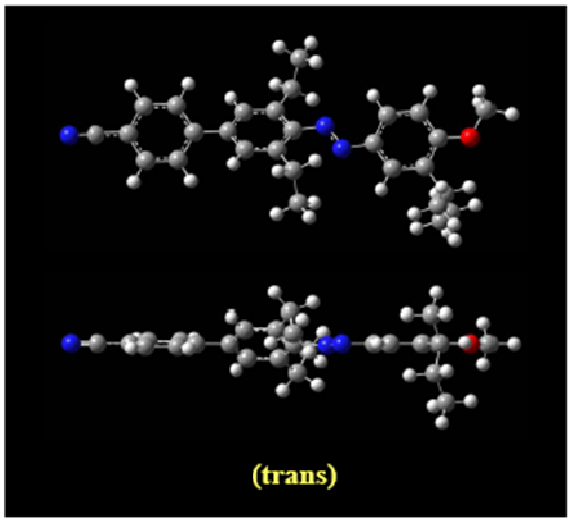
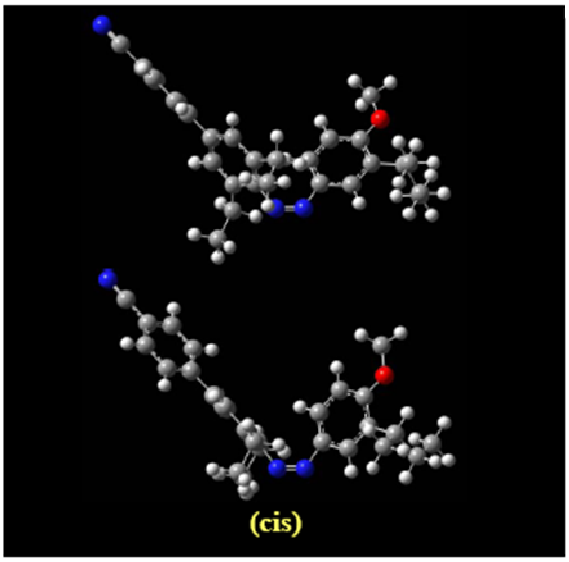


Figure S5 UV-vis absorption spectra of **8** in dichloromethane solution.

6. Calculation results

Optimized structures of trans and cis isomers of **1** by B3LYP/6-31G(d,p) level.





Dipole moment : 8.1918 Debye

C-N=N-C: -178.08°

C-C-N=N: -155.52°

Ph-Ph: -36.39°

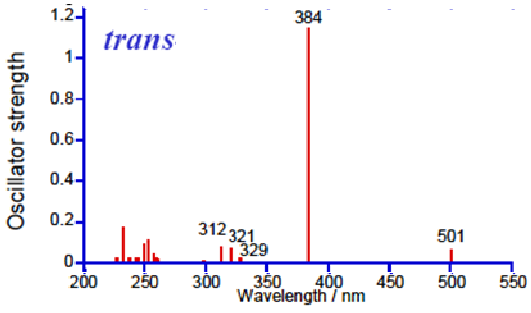
Dipole moment : 5.7297 Debye

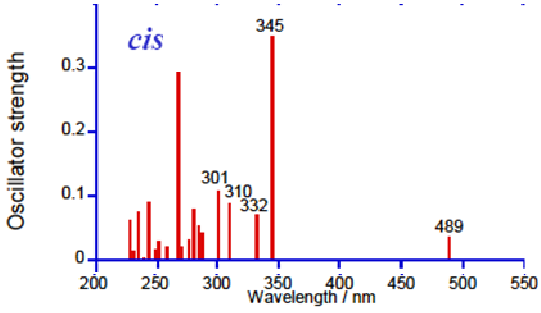
C-N=N-C: -4.70°

C-C-N=N: -78.06°

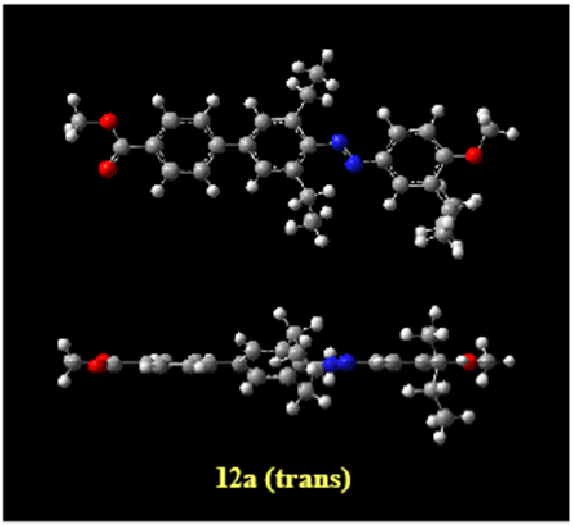
Ph-Ph: -35.88°

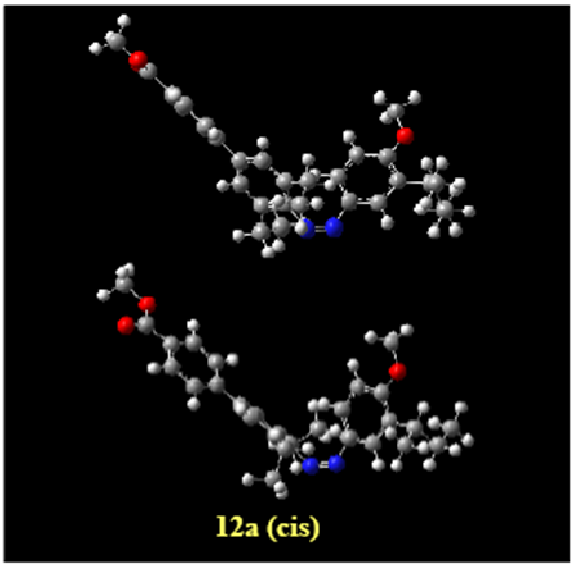
ΔE(cis-trans) = 12.6878 kcal / mol
12.4818 kcal / mol (w/ZPE)





Optimized structures of trans and cis isomers of 2 by B3LYP/6-31G(d,p) level.





Dipole moment : 4.6105 Debye

C-N=N-C: -178.01°

C-C-N=N: -156.11°

Ph-Ph: -35.81°

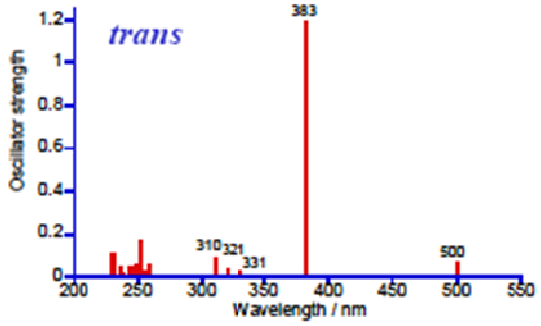
Dipole moment : 4.9195 Debye

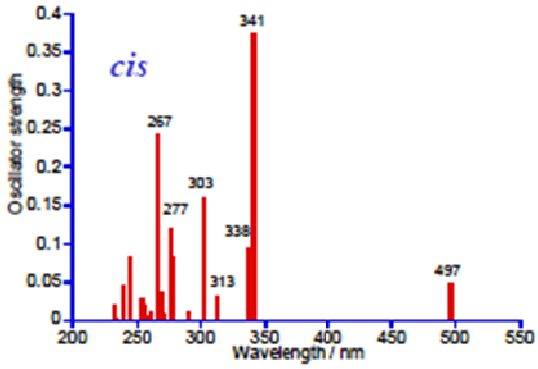
C-N=N-C: -5.38°

C-C-N=N: -73.18°

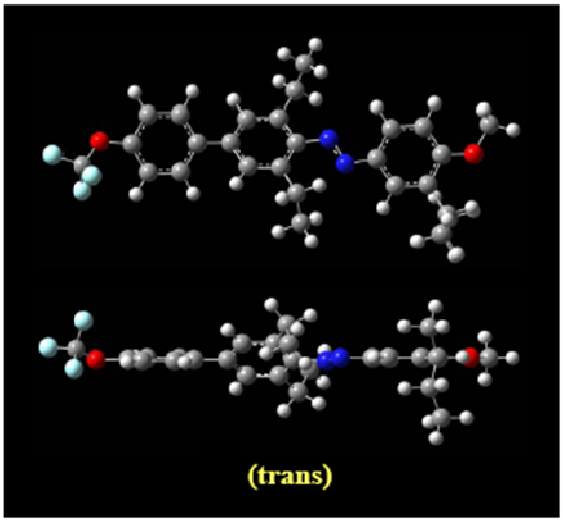
Ph-Ph: -36.16°

ΔE(cis-trans) = 12.9304 kcal / mol
12.6770 kcal / mol (w/ZPE)





Optimized structures of trans and cis isomers of **3** by B3LYP/6-31G(d,p) level.

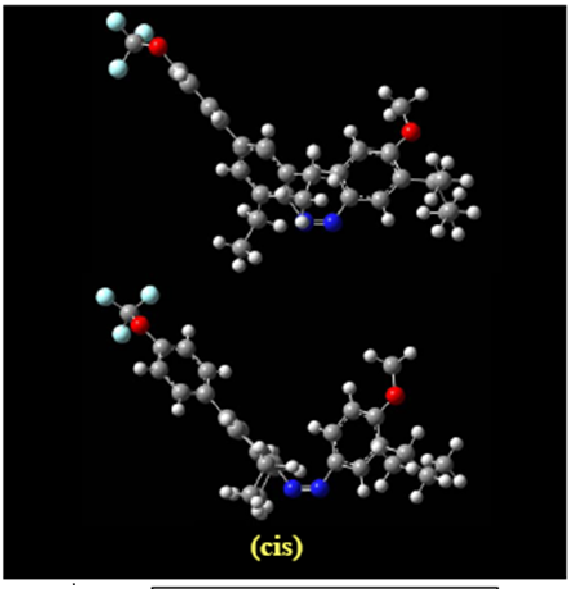


Dipole moment : 4.7494 Debye

C-N=N-C: -177.87°

C-C-N=N: -155.27°

Ph-Ph: -36.46°



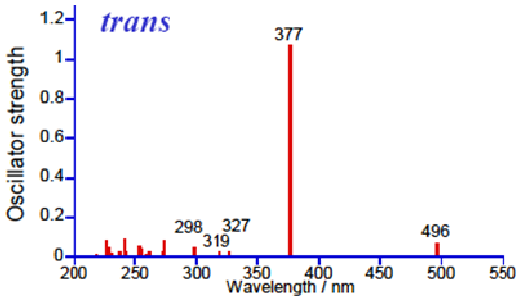
Dipole moment : 4.0130 Debye

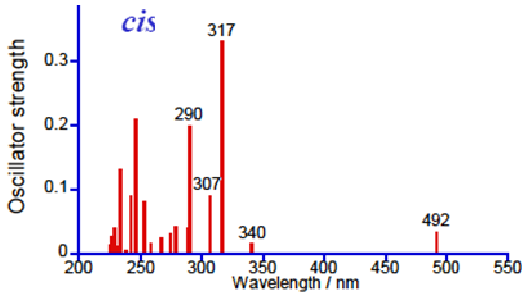
C-N=N-C: -4.81°

C-C-N=N: -77.21°

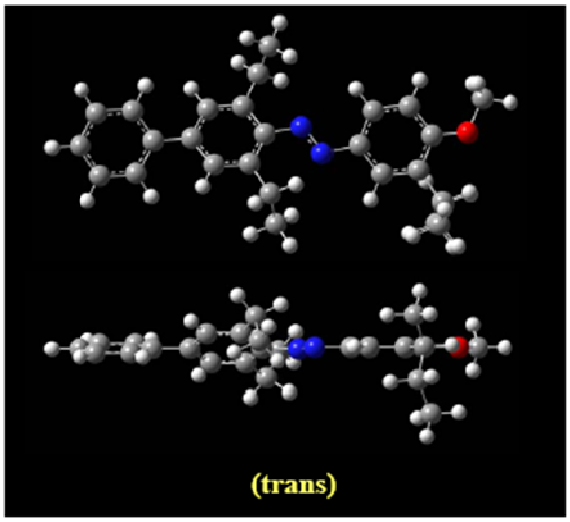
Ph-Ph: -36.77°

ΔE(cis-trans) = 12.9265 kcal / mol
12.7422 kcal / mol (w/ZPE)





Optimized structures of trans and cis isomers of **4** by B3LYP/6-31G(d,p) level.

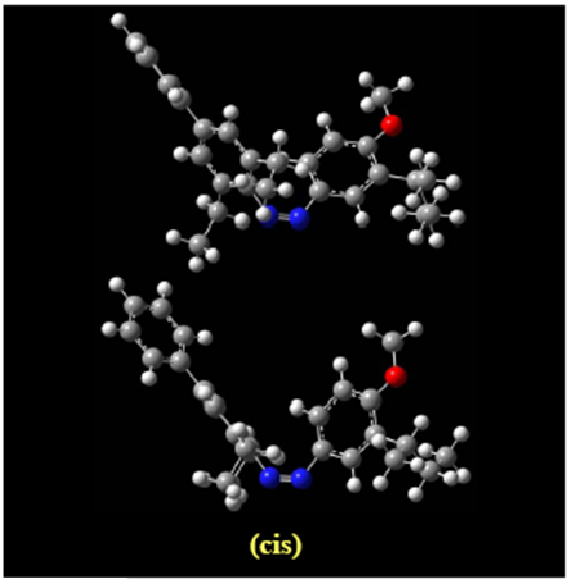


Dipole moment : 2.2937 Debye

C-N=N-C: -178.33°

C-C-N=N: -158.28°

Ph-Ph: -37.03°



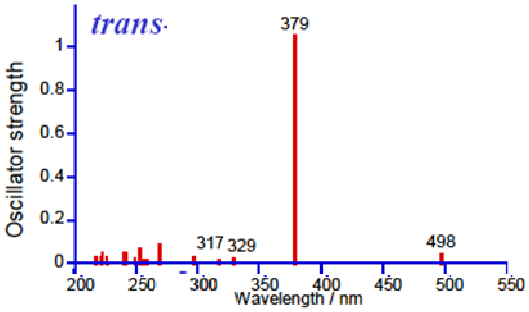
Dipole moment : 4.2949 Debye

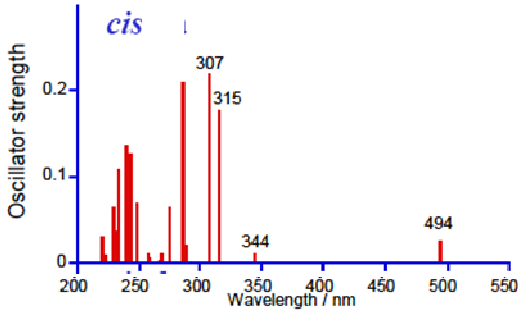
C-N=N-C: -4.19°

C-C-N=N: -78.77°

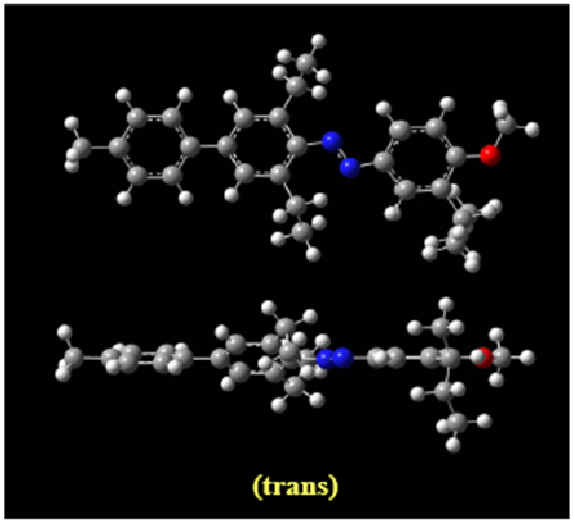
Ph-Ph: -37.46°

ΔE(cis-trans) = 12.9265 kcal / mol
12.7422 kcal / mol (w/ZPE)





Optimized structures of trans and cis isomers of **5** by B3LYP/6-31G(d,p) level.

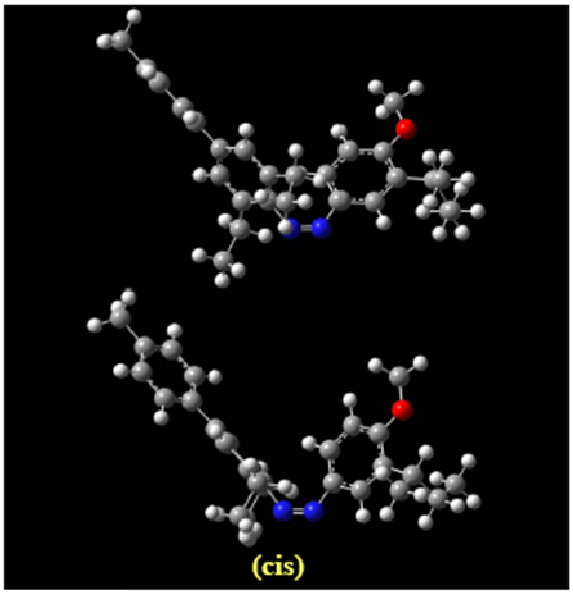


Dipole moment : 1.8138 Debye

C-N=N-C: -178.24°

C-C-N=N: -158.36°

Ph-Ph: -36.40°



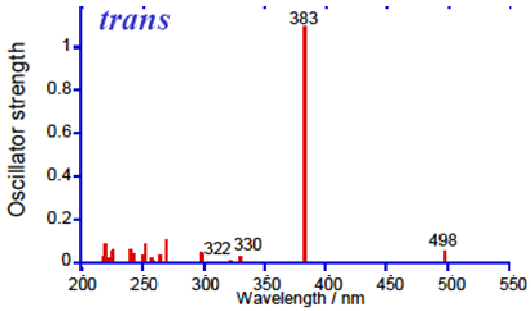
Dipole moment : 4.5057 Debye

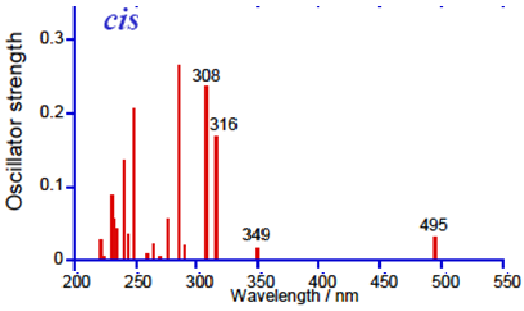
C-N=N-C: -4.61°

C-C-N=N: -77.25°

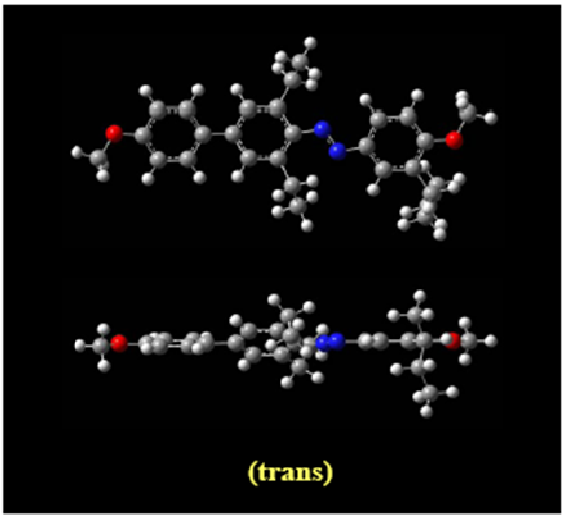
Ph-Ph: -36.83°

ΔE(cis-trans) = 12.9510 kcal / mol
12.7780 kcal / mol (w/ZPE)





Optimized structures of trans and cis isomers of **6** by B3LYP/6-31G(d,p) level.

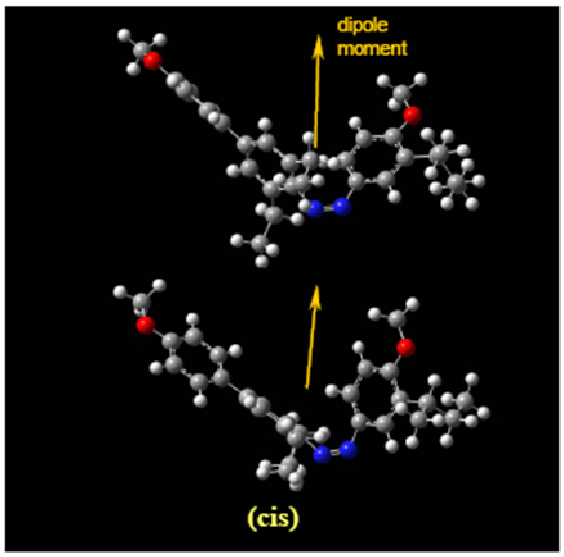


Dipole moment : 0.7701 Debye

C-N=N-C: -178.13°

C-C-N=N: -158.92°

Ph-Ph: -35.16°



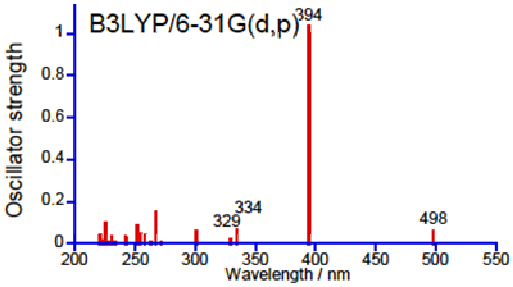
Dipole moment : 5.2331 Debye

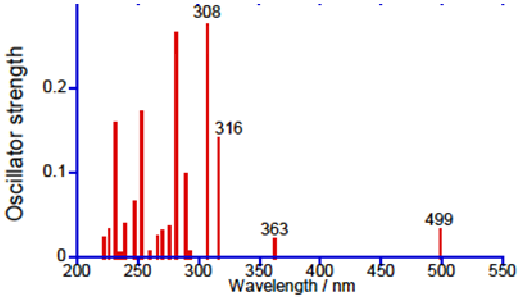
C-N=N-C: -4.91°

C-C-N=N: -77.00°

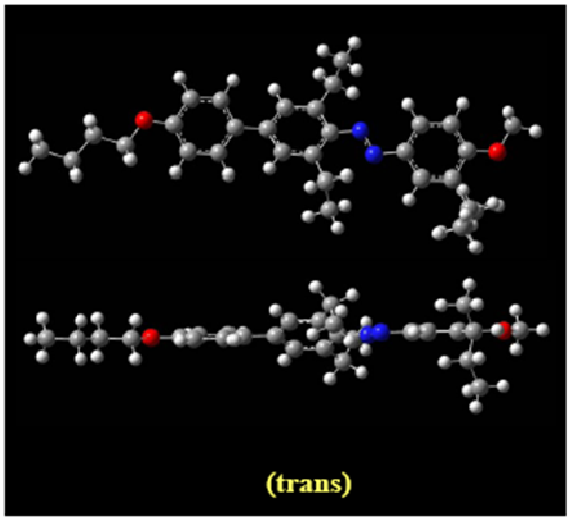
Ph-Ph: -36.81°

ΔE(cis-trans) = 13.0671 kcal / mol
12.8803 kcal / mol (w/ZPE)





Optimized structures of trans and cis isomers of **7** by B3LYP/6-31G(d,p) level.

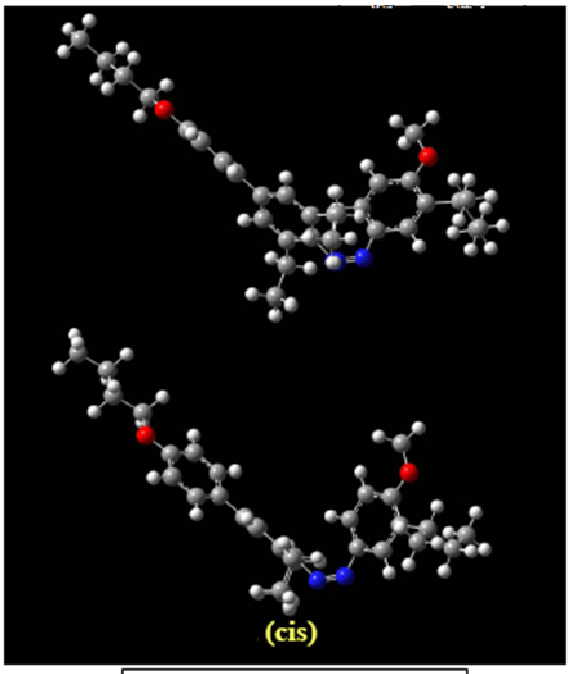


Dipole moment : 0.3728 Debye

C-N=N-C: -178.02°

C-C-N=N: -157.35°

Ph-Ph: -34.61°



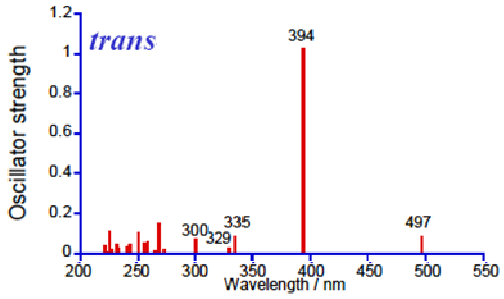
Dipole moment : 5.4209 Debye

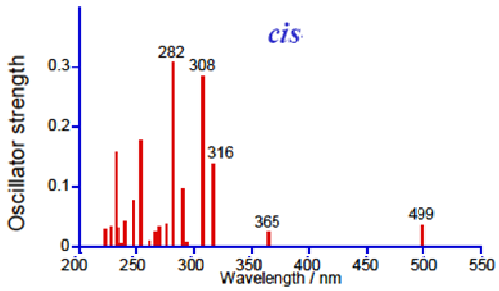
C-N=N-C: -4.86°

C-C-N=N: -76.70°

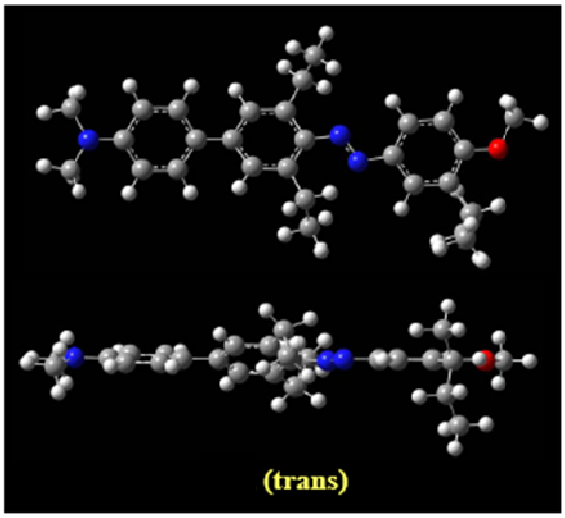
Ph-Ph: -36.32°

ΔE(cis-trans) = 13.1313 kcal / mol
12.7774 kcal / mol (w/ZPE)





Optimized structures of trans and cis isomers of **8** by B3LYP/6-31G(d,p) level.

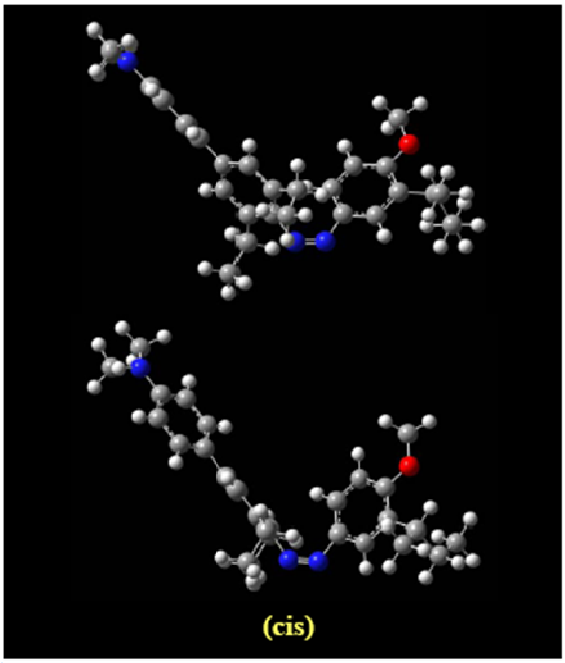


Dipole moment : 2.0326 Debye

C-N=N-C: -178.27°

C-C-N=N: -160.59°

Ph-Ph: -33.71°



Dipole moment : 5.7468 Debye

C-N=N-C: -4.81°

C-C-N=N: -76.78°

Ph-Ph: -35.38°

ΔE(cis-trans) = 13.2580 kcal / mol
13.0089 kcal / mol (w/ZPE)