Acenaphthenequinone, naphthalimide, and naphthalic anhydride analogs

Using Photochromes to "Gate" PICT

- **Proposed mechanism for "PICT gate"**
  - PICT is not initiated upon irradiation of SW film with visible light.
  - Irradiation with UV light causes isomerization to long-wavelength (LW) form.
  - PICT is initiated upon irradiation of LW film with visible light.
  - LW form and/or photochromes revert to SW form.

Computational Methodology

1. Structures used for calculations.
2. Calculated using Gaussian09 and/or Gaussian16 on HBM-funded Cluster at Hope College, with one or two 3.5 GHz Intel Xeon X55 processors per job.
3. Theoretical Density Functional Theory (DFT) with B3LYP exchange-correlation functional.
4. Basis sets vary between: 6-31G(d), 6-31G(d,p), and 6-311G(d,p).
6. Basic computations consider a single molecule in the gas phase in vacuum.
7. Solvent stabilization plays an important role in condensed phase energetics, particularly for charged species.
8. Solvent is represented implicitly by a continuous electric field with permittivity ε specific to the solvent.
9. Calculations using CPCM were faster, easier to converge, and provided slightly more accurate gas-phase energies using the conductor-like polarizable continuum model (CPCM).

Future Work

- Investigate slight differences between MDI and 6-31G(d) geometries, particularly for photochromes.
- Study the effect of using UAH vs. UAD for CPCM calculations necessary for molecules with intramolecular hydrogen bonding.
- Continue application of these computations to other structures and problems, including more conformationally flexible molecules.
- Continue synthesis and evaluation of potential photochromic materials for thin-film photovoltaic and photonic applications.
- Obtain detailed calculations on UV photolysis schemes in (S,D) versus (S,s) configurations, which were not considered previously in thin-film calculations of (S,D) and (S,s) photoisomers.
- Input energies for triple photolysis (T) and input energies for triple photolysis (T).

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References and Notes

2. Carley Craine (U. Minnesota)
3. Computational tools used:
   - Carley Craine (U. Minnesota)
   - Gaussian09 and Gaussian16

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