Supporting Information

QM/MM investigation on 1,3-dipolar cycloadditions of phthalazinium dicyanomethanide with three different dipolarophiles on water and in solutions

Xin Yang, Ying Xue*

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Sichuan University, Chengdu 610064,
People’s Republic of China
Table S1. Computed and experimental densities of water-acetonitrile mixture solvents at 25 °C (g.cm⁻³).

Figure S1. Illustration of the 0.619-mixture solvent box.

Figure S2. Illustration of the 0.9-mixture solvent box.

Figure S3. (A) Side and (B) overhead illustration of “on water” 1,3-dipolar cycloadditions with MVK transition structure from the QM/MM/MC calculations.

Figure S4. (A) Side and (B) overhead illustration of “on water” 1,3-dipolar cycloadditions with MAC transition structure from the QM/MM/MC calculations.

Figure S5. (A) Side and (B) overhead illustration of “on water” 1,3-dipolar cycloadditions with MVK transition structure from the QM/MM/MC calculations.

Figure S6. Solute-solvent energy pair distribution for the transition structure (solid) and reactant (solid) of the 1,3-dipolar cycloadditions of 1,3-dipolar 1 and MAC at CH₃CN, in water, and on water. The ordinate records the number of solvent molecules that interact with the solutes with their interaction energy on the abscissa. Units for the ordinate are number of molecules per kcal/mol.

Figure S7. Solute-solvent energy pair distribution for the transition structure (solid) and reactant (solid) of the 1,3-dipolar cycloadditions of 1,3-dipolar 1 and STY at CH₃CN, in water, and on water. The ordinate records the number of solvent molecules that interact with the solutes with their interaction energy on the abscissa. Units for the ordinate are number of molecules per kcal/mol.

Condensed-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MVK optimizations in PCM.

Condensed-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MAC optimizations in PCM.

Condensed-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and STY optimizations in PCM.

Gas-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MVK optimizations.

Gas-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MAC optimizations.

Gas-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and STY optimizations.
Table S1. Computed and experimental densities of water-acetonitrile mixture solvents at 25 °C (g.cm\(^{-3}\))

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<th>(X_{\text{H}_2\text{O}})</th>
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\(^a\) Based on values at 20 °C, \(X_{\text{H}_2\text{O}}=0.957\)

References:

Figure S1. Illustration of the 0.619-mixture solvent box
Figure S2. Illustration of the 0.9-mixture solvent box
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Condensed-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MVK optimizations in PCM:

Water transition structure

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IR Inten

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Sum of electronic and thermal Free Energies= -872.993605

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C      | -2.70553100        | -0.46119500        | 1.59965200         |
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C      | 0.11626400         | -0.46040300        | 0.23997400         |
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### CH$_3$CN transition structure

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Condensed-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MAC optimizations in PCM:

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CH$_3$CN transition structure

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Condensed-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and STY optimizations in PCM:

Water transition structure

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Sum of electronic and thermal Free Energies = -951.377064
### CH₃CN transition structure

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### Gas-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MVK optimizations:

**transition structure**

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**Sum of electronic and zero-point Energies**

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**Sum of electronic and thermal Energies**

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**Gas-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and MAC optimizations:**

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Sum of electronic and zero-point Energies= -948.176536
Sum of electronic and thermal Energies= -948.158068
Sum of electronic and thermal Enthalpies= -948.157124
Sum of electronic and thermal Free Energies= -948.223895

Gas-phase B3LYP/6-311+G(2d,p) 1,3-dipolar 1 and STY optimizations:

transition structure
### Frequencies

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### Sum of electronic and zero-point Energies

\[-951.306254\]

### Sum of electronic and thermal Energies

\[-951.287575\]

### Sum of electronic and thermal Enthalpies

\[-951.286631\]

### Sum of electronic and thermal Free Energies

\[-951.354427\]
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