A DFT Study on Pyruvic acid radical, monomer and dimer.

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Introduction
Trouble!!!

come from

Molecule.
PA monomers

First Character: **Trans and Cis**

Torsion angle

- 180 °C
- 0 °C
Cis

Trans
Second Character: **trans and cis**

Torsion angle

- 180 °C
- 0 °C
Third Character: *eclipsed and staggered*
Possible conformers:  \(2 \times 2 \times 2 = 8\)

Example: Eclipsed PA s
Stability vs. Total Energy (<< 0)

Stability vs. Vibrational Frequencies

Imaginary Frequencies
• Energy (Staggered Structures) >> E (eclipsed structure)

• All Staggered Structures have imaginary frequencies.
PA dimers
Questions:

- geometries
- Stability
- Imaginary Freq.
- Hydrogen Bond length
- Binding energy
- BSSE
BE: Binding Energy

Uncorrected BE:
\[ E \text{ (dimer)} - E \text{ (m1)} - E \text{ (m2)} \]

Basis Set Superposition Error (BSSE):
\[(E \text{ (m1 with m2 basis set)} + E \text{ (m2 with m1 basis set)}) - ((E\text{(fix geometry m1 without m2 basis set)}) - E\text{(fix geometry m2)})\]

(using “Massage” command, fix the geometry of each single part in the dimer)
1. Both have similar total energy
2. Both have not imaginary frequencies
3. Hydrogen bond length: 1.6 A
4. Bond have a high binding energy (~60 kJ/mol)
5. BSSE is very small to be negotiable

Both have similar geometry and vibrational frequencies, thus it is difficult to be identified.
PA radical
Planar Structure
Stability?

~130 kJ/mol

12 kJ/mol
Conclusions

- 3 stable pyruvic acid monomer conformers
- 2 stable pyruvic acid dimer conformers
- 1 pyruvic acid radical
- Radical is not thermodynamic and kinetic stable but could exist on the metal surface
Thank You!!!