ECSOC-28
2024
Conference

The 28th Intl. Electronic Conference on Synthetic Organic Chemistry

15–30 November 2024 | Online

MDPI

Investigating the Molecular Interactions of Thymol and Menthol as Green Solvents Using DFT Methods

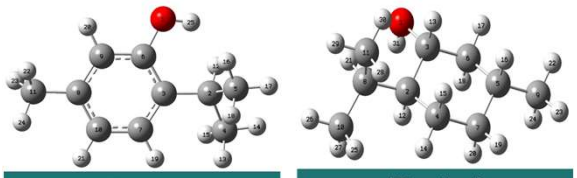
•M. Hammar[1,2] , N. Benbrahim[1] & A. Negadi[2],

•[1] *Laboratory of Advanced Materials and Physicochemistry for Environment and Health, Djillali Liabes University, Sidi Bel Abbes, Algeria.*

•[2] *Laboratory of Thermodynamics and Molecular Modeling, Abou Bekr Belkaid University, Tlemcen, Algeria.*

INTRODUCTION & AIM

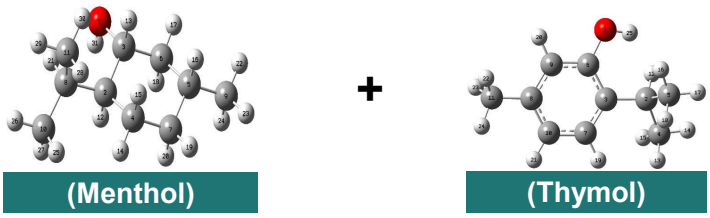
This work investigates Thymol and Menthol mixtures' conformational stability and interaction energies to improve our knowledge of green solvents.



METHOD

Gaussian 09 Software

Density **F**unctional **T**heory (**DFT**):
B3LYP/6-31G(d,p)



Geometry Optimization

Thym_Ment_2 ⟷ Thym_Ment_3

Thym_Ment_1

Interaction Energy Calculations + NBO

RESULTS

RESULTS & DISCUSSION

Figure 1: Thymol-menthol 1:1 Calculated Dimers.

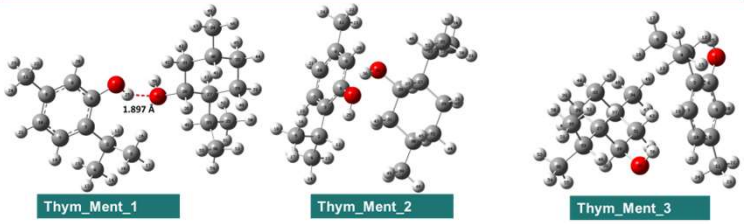


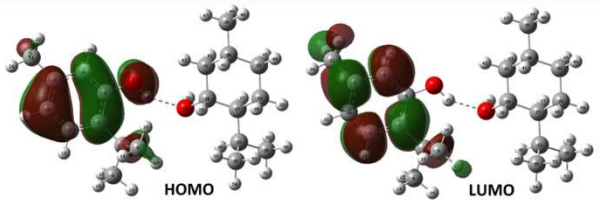
Table 1: Electronic Properties Of Thymol-menthol 1:1 Calculated Dimers.

Dimer	Relative Energy (kcal/mol)	Corrected Complexation Energy (kcal/mol)	Gap (eV)
Thym_Ment_1	0.0	-10.4	5.840
Thym_Ment_2	5.0	-7.4	5.944
Thym_Ment_3	8.5	-7.3	5.963

Table 2: Electric Properties Of Thymol-menthol 1:1 Dimers.

Dimer	Dipole moment (Debye)	Polarizability (α) (kcal/mol)
Thym_Ment_1	3.23	138853.4
Thym_Ment_2	2.79	134284.5
Thym_Ment_3	2.64	134151.5

Figure 2: The HOMO and LUMO of the Thym_Ment_1 dimer.



CONCLUSION

- **Thym_Ment_1, featuring a strong O-H...O-H hydrogen bond, exhibited the highest stability, with the lowest electronic and complexation energies, as well as a higher chemical reactivity.**
- **The dimeric form 1:1 Thymol:Menthol probably exists under the form Thym_Ment_1. It remains to be confirmed by calculations in solution and/or liquid form.**