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# Decontamination of water by selective formation of chlordecone and β-hexachlorocyclohexane molecular inclusion complexes with natural cyclodextrins: Theoretical Study.


Queiroz Portorreal[1,2], A Anthuan Ferino-Pérez[3], et al.

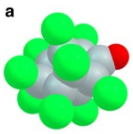
[1]*Instituto Tecnológico de Santo Domingo (INTEC), República Dominicana*

[2]*Ministerio de Energía y Minas (MEM), República Dominicana*

[3]*Instituto Superior de Tecnologías y Ciencias Aplicadas (InSTEC), Universidad de La Habana, La Habana, CP 10600, Cuba*


## Introduction: Molecular Inclusion Complexes for Water Treatment of POP's

Persistent organic pollutant (POPs) are toxic substances that present a very serious threat to the environment and human health.



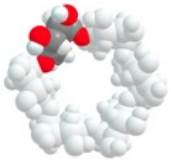
CLD

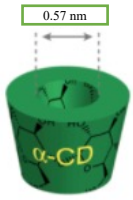
β-HCH

Two of them, chlordecone (a) CLD, $C_{10}Cl_{10}O$ and (b) β-hexachlorocyclohexane, β-HCH, $C_6H_6Cl_6$ had been the focus of several investigations due to their presence in polluted areas of various islands of the Caribbean.

These pollutants have a marked tendency to bioaccumulate and biomagnificate through different environmental compartments. Both molecules, CLD and β-HCH, are generally detected in surface waters of the south of Guadeloupe, where banana plantations are generally located.

Molecular inclusion complexes are a type of supramolecular structures that have gained popularity due to their application in several areas. Among the most popular host molecules are the natural occurring cyclodextrins (CDs), a family of cyclic oligosaccharides formed from 6-8 α-D-glucopyranose units (α-CD, β-CD, and γ-CD respectively) linked by (1 to 4) glycosidic bonds


α-CD

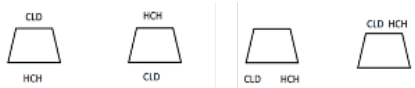



The particular tridimensional structure of CDs makes them very attractive as host molecules thanks to the combination of a capacity to encapsulate lipophilic molecules of a certain size inside their cavities and their solubility in water.

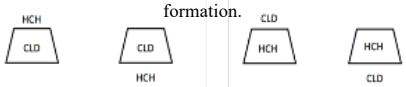
The aim of this work is to theoretically evaluate the competitive formation of host guest complexes pesticides@CDs, in a mixture containing both CLD and HCH.

## Methods:

For the study of the competitive formation of molecular inclusion complexes of CLD and β-HCH with CD, initial positions of the molecules involved were taken as depicted in the following manner:




Initial positions for the calculation of competitive formation.

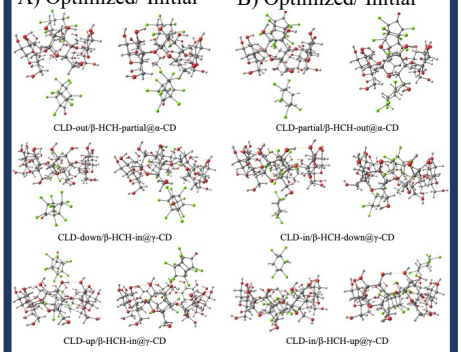



The four initial positions, in the first line, were chosen to evaluate the simultaneous interaction of both pesticides with the host molecule in the cases where each pesticide interacts from different sides of the cavity and when both pesticides interact by the same side of the CD. In the second line, were evaluated to explore the interaction of one of the pesticides when a complex is already formed with the other pesticide. Geometries of the formed complexes in the case of partial occlusion of the pollutants were obtained from the works of Gamboa-Carballo et al. and Ferino-Pérez et al.

Representative structures were optimized using Density Functional Theory (DFT). M06-2X functionality describes correctly the interactions found in the non-covalent dimers in the case of the Van der Waals interactions present.

## Results DFT

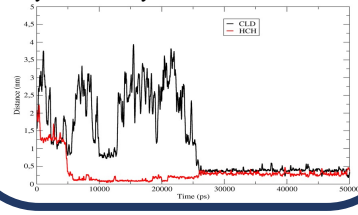
A) Optimized/ Initial B) Optimized/ Initial




Geometries obtained for the interaction of the pesticides with formed complexes. In (A) interactions of CLD with β-HCH@CD complexes and in (B) interactions of β-HCH with CLD@CD complexes.

## Results MD

In the Molecular Dynamic simulation, the smaller β-HCH molecule gets closer to the cavity of γ-CD and forms the complex within the first 5 ns of simulation time, while the bigger CLD molecule enters the cavity after 25 ns of simulation time. When CLD molecule occupies the cavity, a rearrangement of the already formed β-HCH@γ-CD complex occurs. The β-HCH molecule get further from the center of mass of γ-CD therefore allowing the second molecule to be accommodated inside the cavity of its cavity.




## Conclusions:

- DFT studies showed that interactions of both pesticides with CDs is by steric factors and guided by a maximization of the hydrophobic interactions with the other pesticide or with the inner atoms of CD cavity*.
- MD results corroborate the formation of stable complexes of both pesticides with the studied CDs.
- α-CD only form inclusion complexes with β-HCH.
- γ-CD as host molecule is capable of accommodate both pesticides inside its cavity.
- Selective separation of the pesticide is possible, introducing first α-CD to trap β-HCH and then CDs (β or γ) to trap CLD.

*Preferred


## Acknowledgment

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## References


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