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Study on the Self-Organization System of Nicotine Molecular Imprinted Polymer

HUI-MIN BI[1,*], JUN-PING HU[1], YAN LIU[1], XING-QUAN CHAI[1], QIANG CHEN[1] and CHUN-HUA DONG[1,2]

[1]Handan Key Laboratory of Organic Small Molecule Materials, Handan College, Hebei 056002, Handan Province, P.R. China
[2]Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P.R. China

*Corresponding author: E-mail: binbi99@163.com

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The geometry optimization, energy and binding energy (ΔE) of imprinted molecule with functional monomer was studied by Gaussian 03. The template molecule is nicotine and α-methacrylic acid, acrylamide and trifluoromethyl acrylic acid as functional monomer, respectively. The order of the binding energy of cotinine with the above monomers was discussed and the lowest binding energy is methacrylic acid, because of that, there are a hydrogen bonding and a electrostatic interaction in the molecular imprinted polymer by nicotine and α-methacrylic acid and it can be speculated that the best molecular recognition ability is by the molecular imprinted polymer of nicotine and α-methacrylic acid. It is helpful to interpret experiment phenomena and found functional monomer selectivity.

Keywords: Nicotine, Molecularly imprinted polymer, Computer simulation, Functional monomer.

INTRODUCTION

Nicotine (NIC) is an alkaloid in tobacco. The most characteristic, pharmacological effects of it is the substances motivation to induced and enhancement of smoking addiction in the human central nervous system[1-4]. The studies of nicotine have been extensive attention of the biomedical, environmental science, tobacco and health research. The cotinine is the main decomposition products from nicotine, the concentration of cotinine in body fluids was the measurable standard to distinguish between smokers and non-smokers, non-smokers by the flue gas hazards commonly[5,6]. Molecular imprinting technique could synthesized molecularly imprinted polymers, it has high selectivity and identification. Therefore, molecular imprinting technique has been applied in the detection of nicotine contents.

Molecularly imprinted polymer is a synthetic new functional polymer material have the ability to identify the template molecule specifically. The molecularly imprinted polymer have lots of advantages, such as simple and low cost to preparation, so the molecularly imprinted polymer has been widely used in the fields of environment, medicine, food and military[7-9].

The nicotine is template in this study and we chose α-methacrylic acid (MAA), acrylamide (AM) and trifluoromethyl acrylic acid (TFMAA) as different functional monomers to form polymers with template respectively. Furthermore the interaction energy of the various components between the template molecules in the assembly process-functional monomer complex was calculated. It could predicted the ability to identify these types of monomers for the nicotine from the theoretically and explained some experimental phenomena what have been found, to provide a basis for experiment and could reduce unnecessary consumption of the experiment.

EXPERIMENTAL

The geometries of all compounds were optimized using the PM3 method. Harmonic vibrational frequencies calculated at the same level were used for characterization of stationary points as a minimum. All quantum calculations were performed with the Gaussian 03 program. Hydrogen bonding and electrostatic interaction are the main consideration to form the molecularly imprinted polymer in the pre-assembled system. The binding energy reflected the interaction between nicotine and different monomer, it was calculated according to the following formula:

ΔE = E (molecularly imprinted polymer) - ΣE (Each components of the molecularly imprinted polymer)

The E is the single energy of components, in order to select the functional monomer, all the possible complexes formed the monomer and template molecules were calculated in the study and the comparison of the strength of the interaction between the template molecule and the functional monomer[10].

RESULTS AND DISCUSSION

Stability configurations of the molecularly imprinted polymer: The geometry parameters of the template molecule and the functional monomer are shown in Fig. 1.

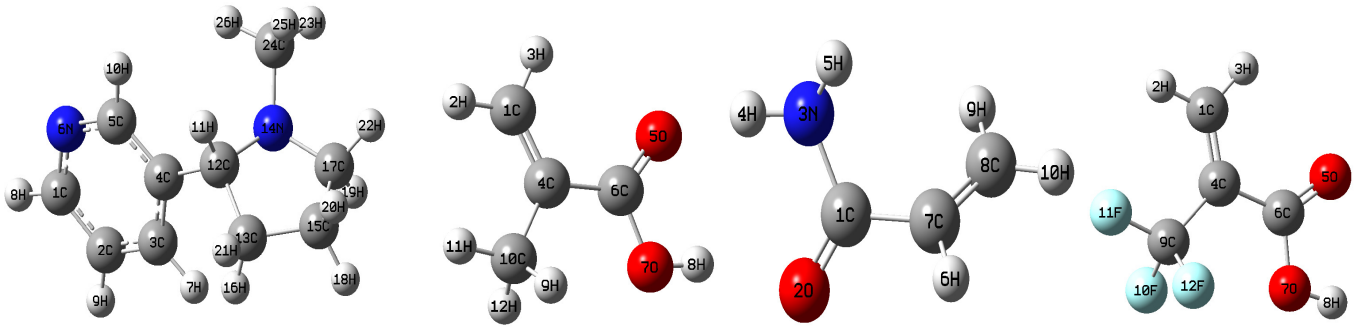

Fig. 1. Conformation of nicotine (NIC), α-methacrylic acid (MAA), acrylamide (AM) and trifluoromethyl acrylic acid (TFMAA)

Electrostatic interaction may exist between the nicotine and methacrylic acid, to form the nicotine positive ion and α-methacrylic acid anion, the optimized configuration of the ions are shown in Fig. 2.

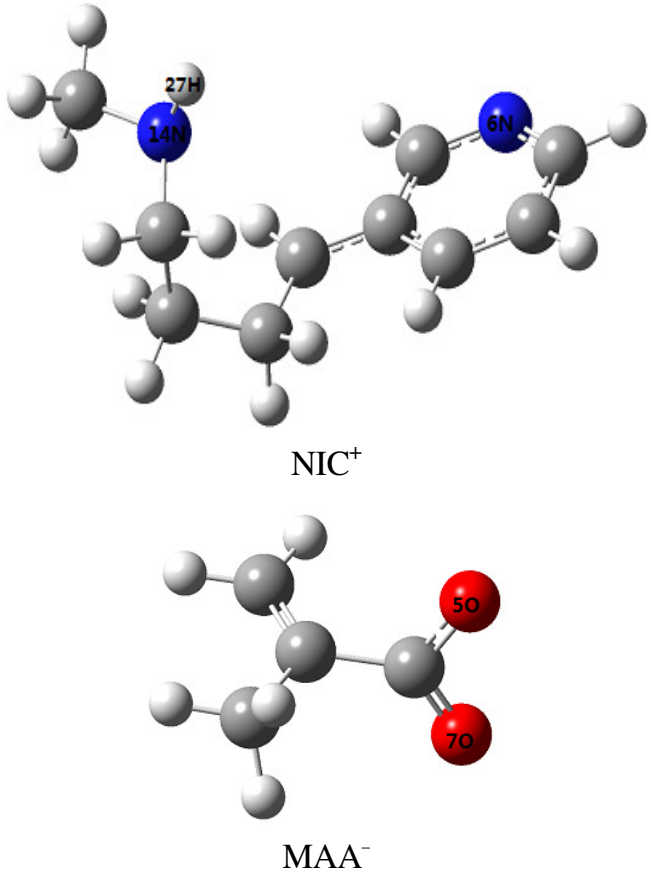

Fig. 2. Conformation of nicotine^{+} and α-methacrylic acid^{-}

Stability configurations of the molecularly imprinted polymer: The molecularly imprinted polymer of nicotine and different functional monomer were build and the principle is the lowest of binding energy. The geometry parameters are shown in Fig. 3.

Binding energy between the template molecule and different functional monomer: The energies of the template molecule, different functional monomer , the precomplex and their binding energies (ΔE) were listed in Table-1.

TABLE-1
ENERGIES (E) OF THE TEMPLATE MOLECULE, FUNCTIONAL MONOMERS AND THE PRECOMPLEX AND THEIR BINDING ENERGIES (ΔE)

Conformation	E (au)	ΔE (au)	ΔE (KJ mol^{-1})
NIC	0.253277		
NIC^{+}	0.278858		
MAA	-0.038133		
MAA^{-}	0.031336		
AM	0.039099		
TFMAA	-0.292660		
Complex(a)	0.207581	-0.06448	-169.3633163
Complex(b)	0.328825	-0.00265	-6.960496095
Complex(c)	-0.342878	-0.010835	-28.45923592

Complex(a):MAA+NIC^{+}+MAA^{-}, Complex(b):AM +NIC+ AM, Complex(c):TFMAA + NIC +TFMAA

We prepolymerized of the template molecule and functional monomers by all possible forms and calculated their binding energies (ΔE), The lower of value of ΔE, the more stable of complexes that were pre-polymerization by the template molecule and functional monomer and the functional monomer imprinting effect is stronger for the same template molecule. Therefore, computer simulations predict the order of ΔE by different functional monomers with a template molecule, it could screening functional monomer which has better imprint effectively and reducing the time of the experiment and consumption greatly.

It can be concluded that ΔE complex (a) < ΔE complex (c) < ΔE complex (b) by Table-1, so the ΔE between nicotinamide and α-methacrylic acid is the strongest, Therefore, the stability of the complexes is best by them. The order of the recognition ability can be speculated by the order of ΔE of three monomer with nicotine synthesized molecularly imprinted polymer respectively, it is MAA > TFMAA > AM.

There are a hydrogen bonding and a electrostatic interaction in the molecularly imprinted polymer by nicotine and methacrylic acid, the ΔE of the molecularly imprinted polymer is the highest and the stability of them is the best. There are two hydrogen bonding in the molecularly imprinted polymer by nicotine and trifluoromethyl acrylic acid, nicotine and acrylamide respectively and the stability of the molecularly imprinted polymer by nicotine and trifluoromethyl acrylic acid is better than the molecularly imprinted polymer by nicotine and acrylamide, so the stability is the worst of the molecularly imprinted polymer by nicotine and acrylamide.

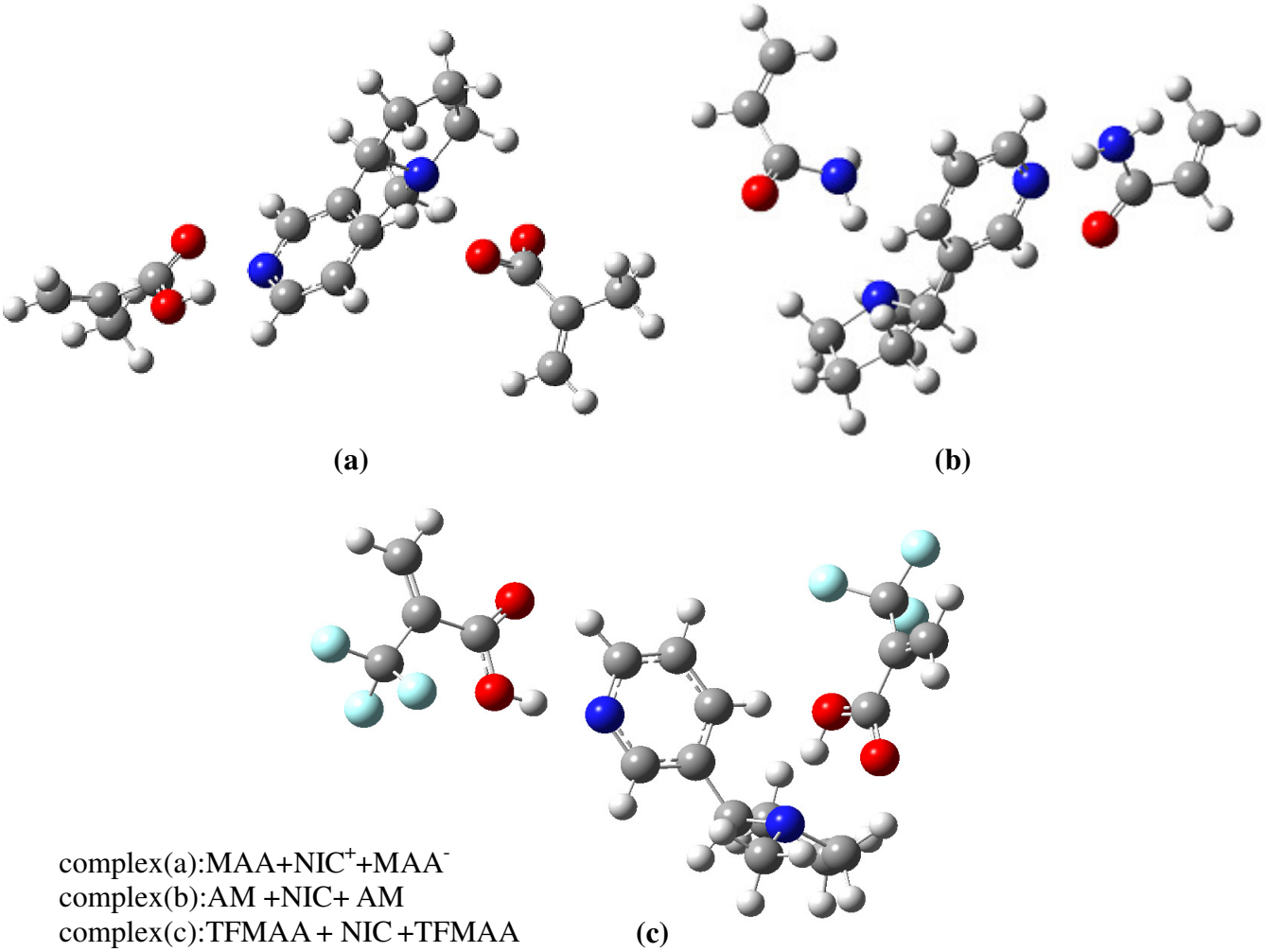

Fig. 3. Complex formed between nicotine with functional monomer

Conclusion

The template molecule is nicotine and methacrylic acid, acrylamide and trifluoromethyl acrylic acid as functional monomer, respectively. The molecularly imprinted polymers are simulated between nicotine and different functional monomer, the binding energies (ΔE) were calculated and be compared, the lowest binding energy is methacrylic acid, it can be speculated that the best molecular recognition ability is by the molecularly imprinted polymer of nicotine and methacrylic acid. It is helpful to interpret experiment phenomena and found functional monomer selectivity.

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