Progress in Structure Determination, Reaction and Classification of Organic Compounds

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Abstract. In recent years, with the continuous development of synthetic organic chemistry, a large number of new compounds are synthesized every year. Many of these compounds not only have novel structures, but also have complex structures. The traditional four spectral analysis methods are difficult to understand its spatial structure clearly and comprehensively. At the same time, with the understanding of the spatial structure of related compounds, it is possible to further explore the relationship between the structure and properties of compounds. This paper analyzes different kinds of organic compounds, including nitrogen-containing organic compounds, polycyclic aromatic hydrocarbons and volatile organic compounds. The detection methods of volatile organic compounds and derivatization chromatography were discussed. Through VOC test, the results show that the average concentration of each substance decreases with time.

Keywords: Organic Compounds, Structure Determination, Reaction, Classification.

1. Introduction
In the past two decades, the research interest of organic chemistry has gradually developed from the synthesis of new compounds to the study of the reaction and catalytic properties of these compounds. This is mainly because organic compounds have many unique reaction properties. The study of its reactivity can reveal some new reactions and promote the development of the application of organic compounds in organic synthesis and catalytic polymerization.

With the continuous development of science and technology, many experts have studied organic compounds. For example, Bai x, Guo h, Chen D reported nocv, a unique cytochrome P450 protein found in noc-i biosynthesis pathway, which is responsible for establishing intramolecular ether bonds through two oxidation steps. This observation is due to the heterologous overexpression of nocv gene in the engineering Streptomyces strain producing bicyclic NOS intermediate nos1260, and the isolation and structural characterization of two subsequent functional products [1]. Li Y, Tang s, yusova reported a molecular structure determination method, which relies on the multifunctional guanidine organic sulfonate hydrogen bond main framework toolkit. The framework forms crystal inclusion complexes with target molecules in one-step crystallization, which complements the crystal sponge method, which relies on diffusing the target into the cage of metal organic framework [2]. Gomes L R, Silva e, Souza m studied the ability of fluorine to contact closely with various atoms in organic compounds, and reported the crystal structure, Hirshfeld surface analysis (HSA) and pixel energy
calculation of trifluoromethylquinoline derivatives [3]. Although there are many research results on the structure of organic compounds, there are still deficiencies in the structure determination, reaction and classification of organic compounds.

In order to study the structure determination, reaction and classification of organic compounds, the analytical model and monitoring method were established through the study of the structure determination of organic compounds. The results show that derivative chromatography is beneficial to the reaction and classification of organic compounds.

2. Method

2.1 Organic Compounds

2.1.1. Polycyclic aromatic hydrocarbons. The electrons in PAHs are delocalized in the whole system, which can provide a large number of electron carriers, so they have good charge transfer ability. At the same time, polycyclic aromatic hydrocarbons have a strong planar conjugate structure, which can increase the role of intermolecular π-π accumulation and intermolecular force, and can also make polycyclic aromatic hydrocarbons self assemble into tightly ordered disk crystals, further improving the charge transfer ability of polycyclic aromatic hydrocarbons [4]. At present, polycyclic aromatic hydrocarbons with various structures have been widely used in various organic electronic fields, such as organic light-emitting diodes, field-effect transistors and so on.

2.1.2. Volatile organic compounds. Volatile organic compounds (VOCs) are a common indoor air pollutant. These substances exist in the indoor air of buildings and will cause various negative effects on human body [5]. For example, exposure to low concentration formaldehyde will cause sensory stimulation, while exposure to high concentration formaldehyde will cause sensory stimulation, vomiting, spasm and even death. Long term exposure to low concentration benzene can have adverse effects on hematopoietic cells and increase the incidence rate of anemia and leukemia. Short term exposure to high concentrations of benzene can damage the central nervous system, resulting in drowsiness, dizziness, headache, shortness of breath and loss of consciousness. Exposure to limonene by people sensitive to limonene may cause respiratory diseases and damage the liver, kidney and nervous system [6].

2.1.3. Nitrogenous organic compounds. Quinoxaline is an important nitrogen-containing heterocyclic compound, which is widely used in biological and industrial fields. Many quinoxaline derivatives are used as many favorable intermediates in organic synthesis, and various substituted active quinoxaline compounds are also used as basic materials for the preparation of organic semiconductors. The quinoxaline unit contains two symmetrical and unsaturated nitrogen atoms, which can improve the electron affinity and electron absorption factor [7]. The basic skeleton of quinoxaline is a bicyclic structure, which has two types of rings: benzene and pyrazine. Because there are two benzene rings, it is also called benzopyrazine. In ring structures, compounds besides carbon that contain at least one or more different atoms are called heteroloops. In many synthetic laboratories, functional quinoxoline were prepared by iodine catalyzing condensation of different substituted phthaldiamine and monodecarboxyl compounds.

2.2 Structural Determination

2.2.1. Detection method of volatile organic compounds. Compared with the traditional complex analysis methods, the gas sensor has the advantages of small volume and simple operation, and has great advantages in the detection of volatile organic compounds. At present, more mature electrochemical sensors take electrolyte as the main element and take the linear change of current intensity generated by the oxidation-reduction reaction of target gas on the electrode as the output
signal. The types of electrolyte mainly include acid-base electrolyte, ionic liquid electrolyte, organic solvent, etc. With the deepening of the research on semiconductor materials, semiconductor sensors have become the main type of gas sensors. Conductive semiconductor sensors are more common. The main principle is to detect the gas through the resistance difference of semiconductor materials in the atmosphere of different volatile organic compounds. In addition, by loading precious metals on semiconductor materials, people use their strong catalytic activity to improve the performance of sensors [8]. However, because most semiconductor sensors work at high temperature, semiconductor sensors still have the disadvantages of poor selectivity, poor stability and high power consumption. Carbon nano material is a new type of gas sensing material with large specific surface area. After carbon nanomaterials adsorb volatile organic compounds, the resistivity or mass change. It can capture the mass change of carbon nano materials through the change of electrochemical signal output by the sensor, or use micro cantilever technology to detect VOCs. At present, the processing cost of carbon nano materials is still very high, the material properties are uneven, and the surface is easy to be polluted.

2.2. Derivatization chromatography. Derivatization chromatography is to use chemical reaction to derivatize the components to be tested into products that meet the requirements of chromatographic analysis and analyze them. Through this treatment, a specific functional group is added to the original material, or part of its functional group is replaced with another functional group, so as to carry out directional separation and detection by chromatography. The properties of derivatives are different from raw materials, such as obtaining higher stability. These functional groups can be esters, halogen and ethers, which need to be selected according to the specific properties of the components to be tested. Derivatizers must be stable, excessive and easy to separate from products and by-products [9]. If it is unstable, the reproducibility is poor, but the quantitative reaction is incomplete, resulting in inaccurate detection.

2.3 Analysis Model and Monitoring Method
Install CO2 sensors in densely populated areas and regularly collect indoor CO2 concentration at specific time steps. According to the indoor CO2 concentration value and the calculation formula between indoor CO2 concentration and indoor TVOC concentration, the indoor TVOC concentration value is estimated: the indoor gas pollutants and the gas pollutants released by indoor personnel meet the following mass conservation equation, as shown in formula (1):

\[ V \frac{dc_{in}}{dt} = C_{out}Q + F \]

When the indoor population is stable, the indoor pollutant concentration reaches a stable state per unit time [10]. Therefore, it can be concluded that indoor CO2 and indoor TVOC per unit time meet the following mass conservation equation, as shown in formula (2-3):

\[ C_{out}co_{2}Q + F_{co_{2}} = C_{in}co_{2}Q \]

\[ C_{out}TVOCQ + F_{TVOC} = C_{in}TVOCQ \]

Where: \( C_{IN} \), CO2 is indoor CO2 concentration, \( \mu \ g / m^3 \); \( C_{IN} \) and TVOC are indoor TVOC concentration, \( \mu \ g / m^3 \). Amount of CO2 in FCO2 room, \( \mu \ g / h \) [11].

3. Experience

3.1 Object Extraction
The sample is taken from the indoor central area of the autonomous breathing area, 1.5-1.8m away from the ground and close to human breathing (more than 0.5m away from the wall). Samples were taken at 8 a.m. and 8 p.m. at each location [12]. Collect the air sample in triplicate into a 20ml vial, put
it into a clean sealed bag and transport it to the laboratory. All air samples collected on the same day shall be analyzed using SPME fibers. Delete outliers with RSD greater than 30%. Before air sampling, wash 1L gas sampling bag with distilled water and dry it at 80 °C for 4H. Use the air pump to continuously deliver air to increase air exchange, then let it open for 3 minutes, fill it with air, seal tightly, install it and take it back to the laboratory for determination. Saw the wood floor sample to 15cm × After 30cm, it is crushed into powder with particle size less than 0.5cm, sealed with plastic and refrigerated in the refrigerator. Weigh 5.00g wood flour into the sample bottle, add 0.50g anhydrous sodium bisulfate, stir evenly with a glass rod, add 15ml methanol, shake well, ultrasonic adsorption for 20min, take out the supernatant and analyze according to the following steps.

3.2 Experimental Analysis

HS-SPME operation process: take 1.0ml of sample solution to be analyzed, place it in a 20ml headspace bottle, cover and seal it, insert the needle with SPME fiber into the upper part of the solution in the headspace bottle, extract it at 40 °C for 20min, and then desorb it at 260 °C at the gas chromatography injection port for 2min. All chemical reaction processes were tracked and monitored by gf254 thin layer chromatography silica gel plate (TLC), and silica gel H (200-300 mesh) was used for column chromatography. Each part of the device is connected together through a tee, one end of the tee is connected with a capillary, and the other end of the capillary is connected with a syringe containing reaction liquid. The other end of the three connecting rod is connected with the metal spray needle, and is clamped on the spray needle with the copper clip, and the upper potential is applied to make the spray needle generate charged spray. The third joint of the tee is connected with the capillary, which is used to add nitrogen to the reaction liquid to improve the atomization efficiency. The reaction products were confirmed by lcqfleet mass spectrometer (thermosficher scientific). The droplet sprayer is placed directly from the capillary of 8mm at the entrance of the mass spectrometer, and the high pressure is applied to the metal spray needle. Due to the high sensitivity of mass spectrometry, the reaction was carried out using 0.1 mmol · L−1 reactants (diamine and diketone). The mass spectrometer operates in positive mode, and the parameters are as follows: the capillary temperature is 350 °C. Capillary voltage is 10V. The tube lens is 90V. By adjusting the distance between spray source and mass spectrometer, spray voltage and solution speed, the abundance of product ions is the largest.

4. Discussion

4.1 VOC Test Results

The formaldehyde concentration released by the building materials tested in this experiment is high. Almost all formaldehyde concentrations have reached the threshold of chronic exposure reference concentration, and 20% of the concentration has reached the threshold of acute exposure reference concentration, indicating that the use of these building materials may lead to excessive formaldehyde concentration in indoor air and serious health risks. After eliminating the ultra-high concentration data of 6 VOCs, compare the average value, as shown in Table 1. Each substance corresponds to three columns. From left to right are the concentration data of 1H point, 24h point and 48h point.

| Substance       | Concentration (ug/m³) |
|-----------------|-----------------------|
| formaldehyde    | 23                    |
| acetic acid     | 34                    |
| toluene         | 17                    |
| ethylbenzene    | 28                    |
| Benzaldehyde    | 15                    |
| Isoxacinol      | 21                    |
It can be seen from the above that the concentration of acetic acid is 23 ug/m³, the concentration of toluene is 34 ug/m³, the concentration of ethylbenzene is 17 ug/m³, the concentration of benzene is 28 ug/m³, the concentration of benzaldehyde is 15 ug/m³, and the concentration of isochorol is 21 ug/m³. The specific results are shown in Figure 1.

![Figure 1. Average concentration of each substance at each time point (excluding ultra-high value)](image)

It can be seen from the above figure that the highest average concentration is toluene and the lowest is benzaldehyde. It can be seen that except formaldehyde, the average concentration difference of the other five substances is very small. In general, the average concentration of each substance decreases over time.

4.2 $N, N$-double ($\beta$-Raw Material Ratio of Methyl Propionate) Substituted Amine (3)

In order to determine the best ratio of raw materials for addition reaction, we selected the amount of substituted amine (benzylamine as an example) and methyl acrylate of different substances for experiments. The results are shown in Table 2.

| N (benzylamine LA): n (methyl acrylate) molar ratio | Addition reaction yield |
|-----------------------------------------------|------------------------|
| 1:2.0                                         | 34.4                   |
| 1:2.2                                         | 56.6                   |
| 1:2.5                                         | 56.8                   |
| 1:3.0                                         | 76.6                   |
| 1:3.2                                         | 78.6                   |
| 1:3.5                                         | 87.6                   |

It can be seen from the above that when the ratio (molar ratio) of benzylamine and methyl acrylate is 1:2.0, the yield of addition reaction is 34.4%. When the molar ratio of benzylamine to methyl acrylate was 1:2.2, the yield of addition reaction was 56.6%. When the molar ratio of benzylamine to methyl acrylate was 1:2.5, the yield of addition reaction was 56.8%. When the molar ratio of benzylamine to methyl acrylate was 1:3.0, the yield of addition reaction was 76.6%. When the molar ratio of benzylamine to methyl acrylate was 1:3.2, the yield of addition reaction was 78.6%. When the ratio (molar ratio) of benzylamine and methyl acrylate was 1:3.5, the yield of addition reaction was 87.6%, and the specific results are shown in Figure 2.
As can be seen from Figure 2, before the molar ratio (molar ratio) of benzylamine to methyl acrylate is greater than 1:3.0, with the increase of molar ratio. The yield of the addition product was also improved. When the ratio is greater than 1:3.0, the yield change is not obvious and increases slightly. This is because reducing the amount of methyl acrylate will increase the formation of secondary amine by-products in the reaction, thereby reducing the yield of compound (3). The excess of methyl acrylate has little effect on the increase of (3) yield. Therefore, the output of product (3) and the saving of raw materials are comprehensive.

5. Conclusion
The separation of difficult to separate organics such as alkanes / aromatics is of great significance in the production of petrochemical products. At present, although most separation processes have been highly optimized, there are still some problems, such as low solvent selectivity, volatile, complex separation process equipment, high energy consumption, large environmental pollution and so on. There is an urgent need to find a greener and more efficient separation process. In this paper, N, n-double (β) - The results showed that the ratio of benzylamine to methyl acrylate increased with the increase of the ratio. The previous ratio (molar ratio) of benzylamine to methyl acrylate was greater than 1:3.0, and the yield of the addition product also increased. When the ratio was greater than 1:3.0, the yield did not change significantly and increased slightly.

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