Sampling Device Harnesses Powerful Molecular Interactions, Overcomes Barriers in Detecting Volatile Contaminants

A NIEHS Superfund Research Program (SRP)-funded study showed how unique microsensors that harness powerful molecular interactions can selectively detect trace amounts of aromatic volatile organic compounds (VOCs) in the environment.

Aromatic VOCs are a subgroup of ring-shaped compounds found in the atmosphere. This group includes benzene, toluene, ethylbenzene, and xylenes, sometimes referred to as BTEX, which are often found at Superfund sites. They have been linked to adverse health effects like cancer, even at low concentrations. Measuring the pollutants at low concentrations is challenging because existing tools lack required sensitivity, are not selective for specific VOC compounds, and do not perform well with mixtures of VOCs.

To overcome these limitations, the research team, from the University of Louisville SRP Center, took advantage of strong interactions between molecules with positive and negative electrical charges to develop a highly sensitive VOC sensor.

First, the team created functionalized gold nanoparticle cores surrounded by a layer of thiols that attach tightly to positively charged metal atoms. Then, the sensing material was integrated into an electrical circuit to create a sensor that responds to interactions between the positively charged metals and the electron-rich rings of specific BTEX compounds.

Next, they evaluated which metals – lithium, sodium, or potassium – performed best in the sensor, in terms of sensitivity and selectivity, for aromatic VOCs.

Then, they measured the electrical response to individual VOCs — benzene, toluene, ethylbenzene, xylene, nitrobenzene, cyclohexane, ethanol, and acetone — across a range of concentrations from 5 parts per million to 100 parts per billion.

Finally, they sought to clarify the specific molecular interactions underlying the sensor’s performance and whether environmental conditions, such as humidity, altered the results.

The team reported that the sensors showed rapid high sensitivity and selectivity toward electron-rich aromatic VOCs, in particular benzene, toluene, ethylbenzene, and xylene. They explained that the characteristics of these compounds point to a particular type of strong molecular interaction driving sensor performance. Cation-pi interactions are strong attractive forces between a positively charged cation, such as the metals, and an electron-rich, negatively charged system, such as the rings of the BTEX compounds.

Among the different metals tested, the researchers reported the highest responses for the sensors with sodium or potassium. The team also calculated the sensors' limit of detection and found that sensors using sodium and potassium can detect BTEX compounds at concentrations as low as 0.1 to 3 ppb.

While humidity lessened the effectiveness of the sensors, the authors offered potential alternatives, such as using a sorbent tube to remove water, that could be explored in future studies to expand their applicability to diverse environmental conditions. They also tested the long-term stability of the sensors, reporting that new sensors could be prepared by removing the previous sensing film and adding a new layer of the sensing material.

According to the authors, the robust responses to electron-rich aromatic VOCs suggest their nanoparticle-based sensors could enhance the ability to rapidly detect these compounds at low concentrations, which may better clarify what VOCs people are exposed to and their potential health risks.

If you'd like to learn more about this research, visit the Superfund Research Program website at niehs.nih.gov/srp. From there, click on the Research Brief title under the banner, and refer to the additional information listed under the research brief. If you have any questions or comments about this month's podcast, send an email to srpinfo@niehs.nih.gov.

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