

Vapor Phase Detection and identification of Nerve Agent Simulants using the D3 Klarite® SERS technology

SUMMARY

In the event of accidental or malicious exposure to a hazardous airborne chemical agent, it is necessary to detect and positively identify the compound(s) in the vapor phase at significantly less than the lethal dose, so that the appropriate action can be taken.



Figure 1 – The D3 Technologies Klarite SERS substrates

Surface Enhanced Raman Spectroscopy (SERS) has been shown to provide highly sensitive detection (sub ppb level) of analytes in solution. The recently developed Klarite® SERS substrates were used in this study to collect SERS data for the detection and identification of nerve agent simulants in the vapor phase.

EXPERIMENTAL

SERS and bulk Raman spectra were measured using a low power density Raman system with a 785 nm laser (250 mW, 130 μm diameter illumination), and an automated XYZ stage and camera to allow easy alignment and visualization of the sample (see Figure 1).

Diethyl methylphosphonate (DEMP) and Dimethyl methylphosphonate (DMMP; a precursor for the nerve agent Sarin) were sourced from Sigma-Aldrich (catalogue numbers 62461 and D169102; 97 % purity). Vapor phase measurements were made using a low volume, sealed chamber system incorporating a Klarite substrate as the sensing surface. Microlitre volumes of simulant material were pipetted into reservoirs in close proximity to, but not in direct contact with, the Klarite surface.

Measurements were taken at the indicated time points directly after the system was sealed (from 5 min to 24 hr). All measurements were made at ambient temperature.

RESULTS

The SERS spectra of DMMP and DEMP from vapor are shown in figures 2 and 3 respectively along with a bulk Raman spectrum (Reference).

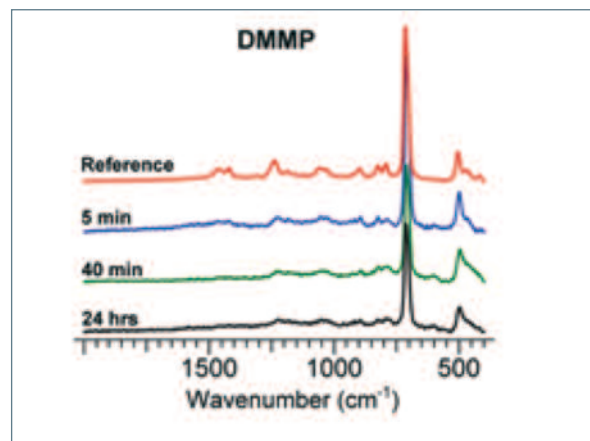


Figure 2 – Bulk Raman spectrum of pure DMMP liquid (Reference) and SERS spectra of DMMP vapor in the sealed system at timepoints of 5 min, 40 min and 24 hr after deposition into the reservoir

Application
Note



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The SERS spectra of both simulants show a series of unique, high intensity peaks which give a fingerprint of the molecular structure of the test substance. This feature of SERS allows the identification of unknown compounds in addition to their detection at low concentrations. Furthermore, the band positions and relative intensities of the SERS spectra match closely to the bulk Raman signal, indicating that the Klarite surface does not significantly affect the vibrational properties of the groups comprising the molecular structure. Finally, spectra measured from outside the enhancing region of the Klarite are devoid of features, indicating that the unique architecture of the Klarite surface is required for the enhancing effect (see Figure 4).

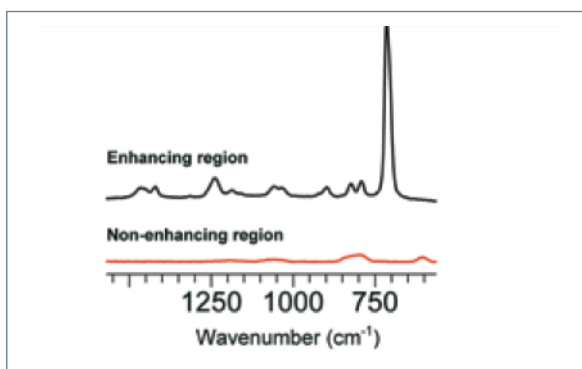


Figure 4 – SERS Spectra of DMMP vapor in the enhancing and nonenhancing regions of Klarite

CONCLUSION

We have demonstrated the feasibility of using the D3 Technologies SERS substrates to detect and identify nerve agent simulants in the vapor phase. With further development and refinement, the D3 Technologies SERS platform has the potential to provide an early warning system for airborne chemical threats.

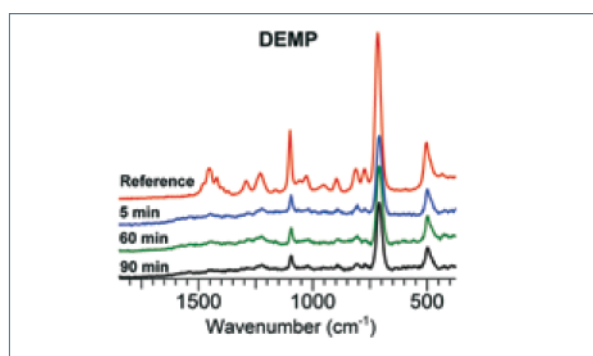


Figure 3 – Bulk Raman spectrum of pure DEMP liquid (Reference) and SERS spectra of DEMP vapor in the sealed system at timepoints of 5, 60 and 90 min after deposition into the reservoir

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