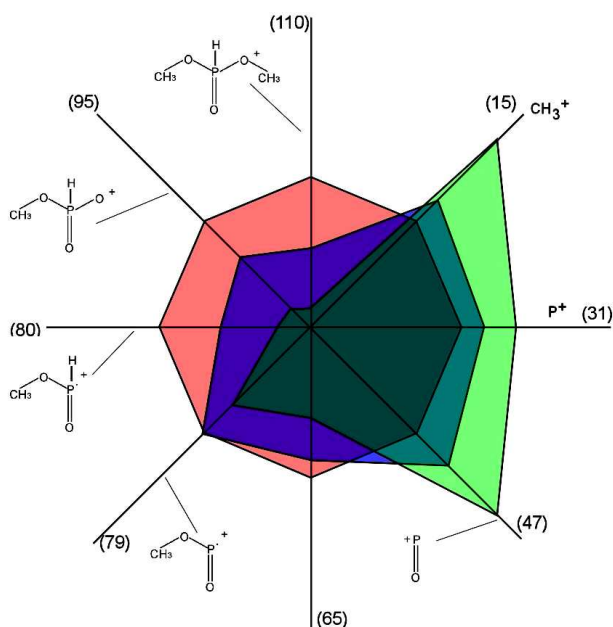


## MIIPS™ application notes What can you do with MIIPS™?

### Multidimensional identification of chemical warfare agents using shaped femtosecond pulses

Phase shaped femtosecond laser pulses and mass spectrometry are implemented as a tool for improving molecular identification. We have demonstrated that the fragmentation pattern in the mass spectra of several chemical warfare simulants is sensitive to the phase characteristics of the incident laser field. The changes in the relative yield of fragment ions observed upon pulse shaping (enhancement or suppression) contributes a new dimension for mass spectrometry that improves molecular identification. This performance enhancement allows the quantitative analysis of mixtures of isomers, something that cannot be done with conventional mass spectrometry methods.



Spider plot representation of changes in the mass spectrum of dimethyl phosphite for differently shaped pulses (intensities of MS lines). Results for TL pulses (orange) and two different binary phase shaped pulses (green and purple).

As a result of the nonlinear dependence of ionization and fragmentation following the laser-molecule interactions, the integrated intensity of the mass spectrum decreases from a maximum obtained for TL pulses to lower values obtained with phase modulated pulses. By normalizing the mass spectrum obtained for each shaped laser pulse, it is possible to determine the relative yield of each fragment ion given a particular shaped pulse. The recorded deviation of the

average relative yield from the value observed for transform limited pulses for each compound is used for identification. Molecular identification, typically based on the position and intensity of the traditional MS, can now be aided by a new dimension given by this average deviation.

Possible applications include the detection of chemical warfare agents and explosives in public spaces, and in containers.

| Chemical                     | value       | Safe | Caution | Danger |
|------------------------------|-------------|------|---------|--------|
| Meta Nitrotoluene            | 1.004       | ●    | ●       | ●      |
| Ortho Nitrotoluene           | 0.9957      | ●    | ●       | ●      |
| Para Nitrotoluene            | 0.9953      | ●    | ●       | ●      |
| Benzene                      | 0           | ●    | ●       | ●      |
| Pyridine                     | 0.149       | ●    | ●       | ●      |
| 4 Chloro Benzonitrile        | 0           | ●    | ●       | ●      |
| 1 Nitropyrazole              | 0           | ●    | ●       | ●      |
| Dimethyl phosphite           | 0           | ●    | ●       | ●      |
| 2 Chloro ethyl ethyl sulfide | 0           | ●    | ●       | ●      |
| Safe level is below          | 0.1         |      |         |        |
| Caution level is between     | 0.1 and 0.5 |      |         |        |
| Danger level is above        | 0.5         |      |         |        |

| Chemical                     | value       | Safe | Caution | Danger |
|------------------------------|-------------|------|---------|--------|
| Meta Nitrotoluene            | 0           | ●    | ●       | ●      |
| Ortho Nitrotoluene           | 0.9957      | ●    | ●       | ●      |
| Para Nitrotoluene            | 0.9953      | ●    | ●       | ●      |
| Benzene                      | 0.9939      | ●    | ●       | ●      |
| Pyridine                     | 1.557       | ●    | ●       | ●      |
| 4 Chloro Benzonitrile        | 1           | ●    | ●       | ●      |
| 1 Nitropyrazole              | 0.9926      | ●    | ●       | ●      |
| Dimethyl phosphite           | 1.002       | ●    | ●       | ●      |
| 2 Chloro ethyl ethyl sulfide | 1           | ●    | ●       | ●      |
| Safe level is below          | 0.1         |      |         |        |
| Caution level is between     | 0.1 and 0.5 |      |         |        |
| Danger level is above        | 0.5         |      |         |        |

User interface in the beta-level software used for identification of chemical agents in the laboratory conditions.

#### References:

Pastirk, I., Kangas, M., Dantus, M. J. Phys. Chem. A, 109, 2413 (2005)  
J. M. Dela Cruz, V. V. Lozovoy, M. Dantus, J. Mol. Spectr. 42, 178-186 (2006).

For R&D applications please consider the Silhouette™ from Coherent, Inc., a pulse shaper with MIIPS™ technology and the support from Coherent Inc. For industrial applications contact BioPhotonic Solutions, Inc.

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