

## Schriftliche Prüfung Moderne MS Summer 2013

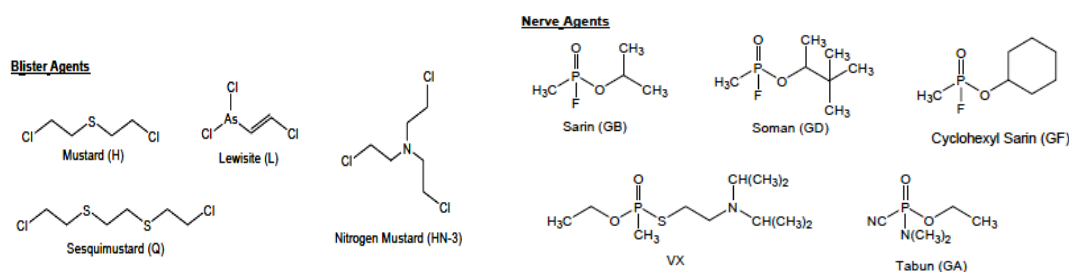
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Vorname: \_\_\_\_\_ Name: \_\_\_\_\_

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- Zeit: 60 Min. Teilen Sie sich Ihre Zeit gut ein.  
*Time: 60 min, organize your time carefully.*
- Sie können auf Englisch oder Deutsch antworten  
*Answers are accepted in German or English.*
- Es sind alle Hilfsmittel mit Ausnahme von Computern und Telekommunikation erlaubt.  
*It is allowed to use all resources except for computers and communication devices.*
- Unleserliche Texte, unklare Formulierungen oder unsaubere Skizzen können nicht bewertet werden. Bitte bemühen Sie sich um eine saubere Darstellung.  
*Unreadable text, unclear formulations or graphs are not graded. Please try to use clear illustrations and descriptions*
- Schreiben Sie jedes abzugebende Blatt einzeln mit Ihrem Namen und Vornamen an.  
*Label every page with name and surname.*
- Dieses Deckblatt ist ausgefüllt abzugeben. Die Aufgabenstellung ist ebenfalls einzureichen.  
*Please fill in the first page. Hand in all pages including cover page and questions.*
- Wir bitten Sie um Fairness und wünschen Ihnen viel Erfolg!  
*We ask you for fairness and wish you good luck!*

Recently, a highly sensitive mass spectrometric detection method was described to analyze chemical warfare agents (CWAs) and so-called "CWA simulants", based on ion-molecule reactions. The structures of some well-known CWAs are pictured below. Limits of detection were in the low ppb range, well below reported exposure limits for CWAs.



The method (A.M. Graichen and R.W. Vachet, *J. Am. Soc. Mass Spectrom.*, 24 (2013) 917-925) works by producing ions of Ni(II) unsaturated complexes with an ESI source and letting these react with vapors of the CWA simulants that are drawn through a membrane inlet tube whose outside is exposed to the vacuum of the mass spectrometer. One ... two neutral sample molecules are found to add to the Ni(II) complex ions.

**Answer the following questions:**

- Starting with Ni(bpy)<sup>2+</sup> at m/z = 185, what signals (m/z values) would you expect in the mass spectrum recorded from reacting with Mustard gas, Sarin, and VX?
- Assume that you would have no exact knowledge of the CWA that reacted with Ni(bpy)<sup>2+</sup>. How could you unambiguously determine from the mass spectrum that the product ions are also doubly charged?
- What kind of mass analyzer is ideally suited to allow the kind of "reactive ionization" described above? Sketch a workflow for the analysis of a gaseous CWA sample.
- How would you determine the limit of detection for a CWA simulant experimentally? Describe the procedure explicitly, in particular how to prepare a low concentration (≈ ppb level) vapor sample.
- Imagine a miniaturized, MS-based analytical system working with the principle described above, which can be applied in the battlefield. Which type of mass spectrometer would you employ, and where would you pay most attention during the engineering to save space and weight?