

Fragmentation of fulminic acid, HCNO, following core excitation and ionization

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Motivation

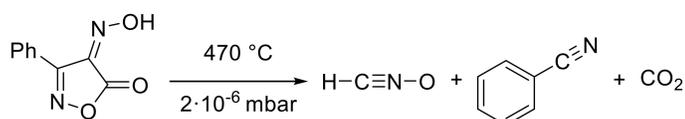
- HCNO has been detected in the interstellar medium
- a prebiotic role has been suggested for the CHNO isomers
- interaction with soft X-ray radiation leads to ionization or resonant excitation of C, N or O 1s electrons
- core ionized and core excited states decay via Auger-Meitner processes
- Auger electron-photoion coincidence spectroscopy allows investigation of different fragmentation channels and ionization site-dependent fragmentation tendencies after Auger-Meitner decay

N. Marcelino, J. Cernicharo, B. Tercero, E. Roueff, *Astrophys. J.* **2008**, 690, L27-L30.

Experimental details

Synthesis of HCNO

Pyrolysis of 3-phenyl-4-oximino-isoxazol-5(4H)-one:



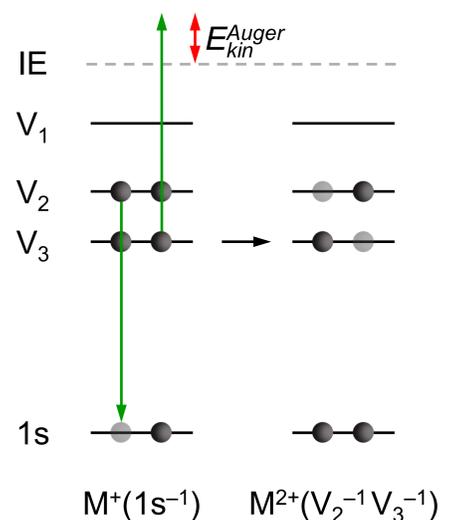
C. Wentrup, B. Gerecht, H. Briehl, *Angew. Chem. Int. Ed.* **1979**, 18, 467–468.

EPICEA setup at the PLEIADES beamline at SOLEIL SYNCHROTRON

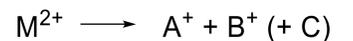
- 35 – 1000 eV light produced by Apple II HU80 undulator
- photon beam crosses gaseous sample
- Auger electrons and (fragment) ions are detected in coincidence
- ionic fragments are analyzed by TOF-MS
- electron kinetic energy is analyzed by a double toroidal electron analyzer

Auger-Meitner process

Auger electron emission after 1s-ionization with soft X-ray radiation

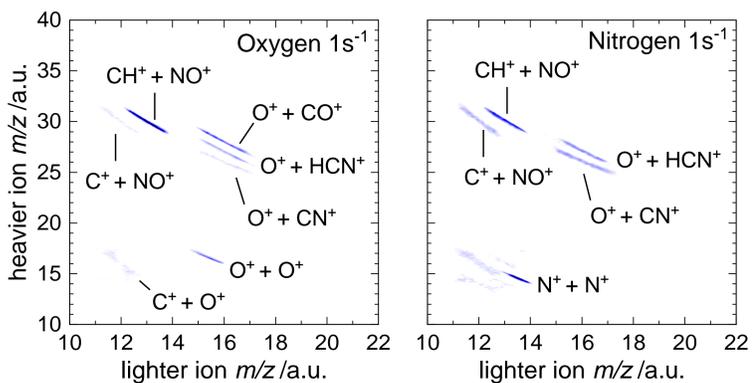


Fragmentation after Auger-Meitner decay:



Fragmentation after 1s ionization

Ion-ion-coincidence maps

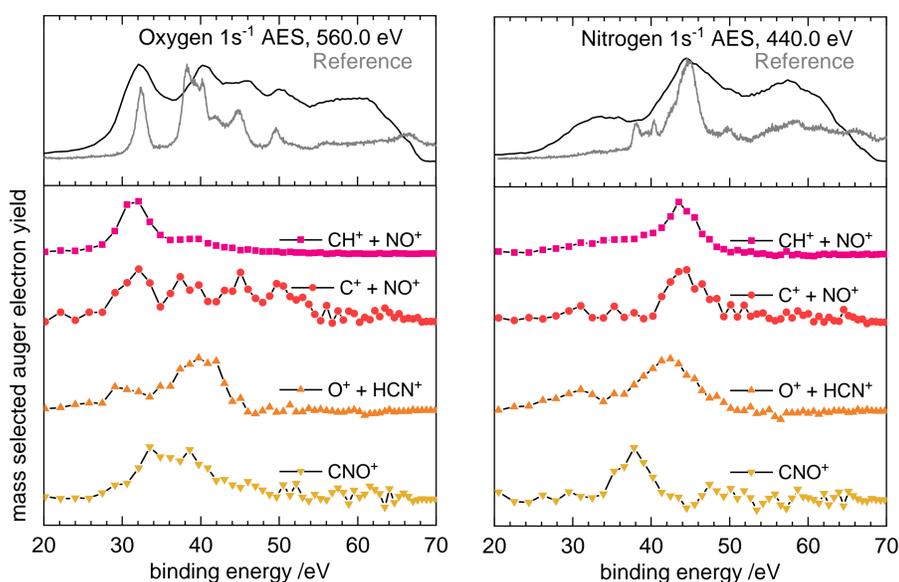


branching ratios

| Channel | C 1s ⁻¹ /% | N 1s ⁻¹ /% | O 1s ⁻¹ /% |
|-----------------------------------|-----------------------|-----------------------|-----------------------|
| CH ⁺ + NO ⁺ | 66 | 37 | 72 |
| C ⁺ + NO ⁺ | 12 | 18 | 6 |
| O ⁺ + HCN ⁺ | 5 | 21 | 14 |
| O ⁺ + CN ⁺ | 17 | 23 | 7 |
| CNO ⁺ + H ⁺ | – | 1 | 1 |
| Sum | 100 | 100 | 100 |

branching ratios show different fragmentation patterns for different ionization sites

Ion pair selected Auger electron spectra



Reference spectra taken from: M. Gerlach et al., *Phys. Chem. Chem. Phys.* **2022**, 24, 15217.

Conclusion

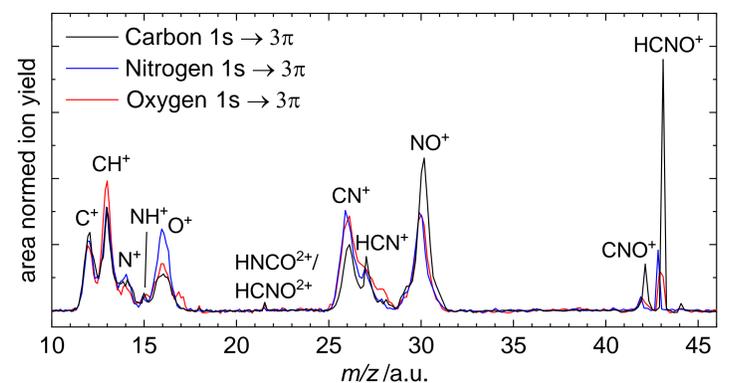
- identification of fragmentation pathways after normal and resonant Auger-Meitner decay of HCNO by Auger electron-photoion coincidence spectroscopy
- fragmentation is mainly governed by the Auger final state distribution, which depends on the ionization/excitation site
- in some cases certain final states may produce specific ion pairs

Acknowledgements

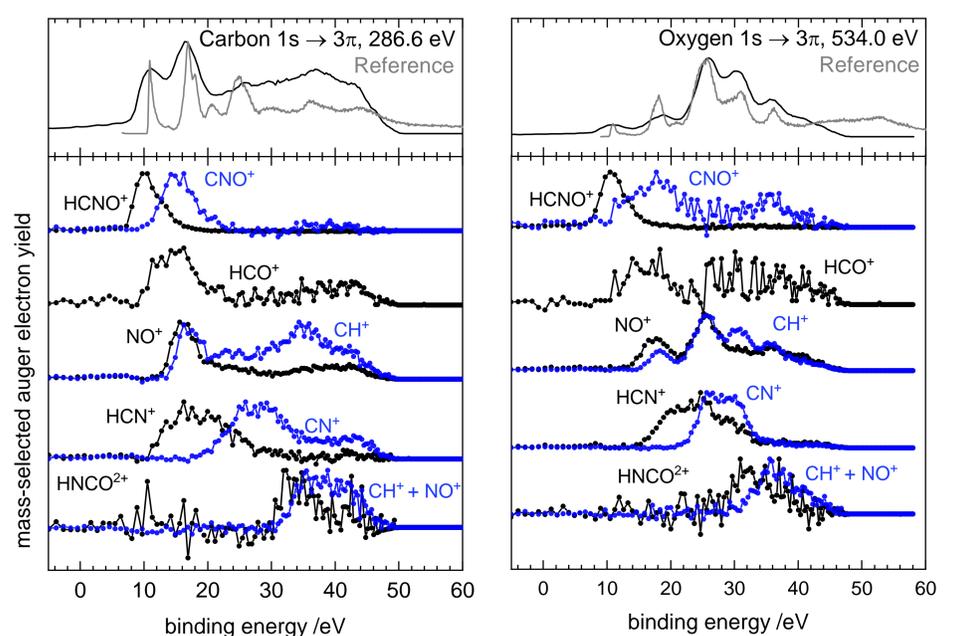


Fragmentation after 1s excitation

TOF mass spectra after resonant core excitation



Mass selected Auger electron spectra



Reference spectra taken from: M. Gerlach et al., *Phys. Chem. Chem. Phys.* **2022**, 24, 15217.