Detection of Ketones using Ion Mobility Spectrometry

Introduction

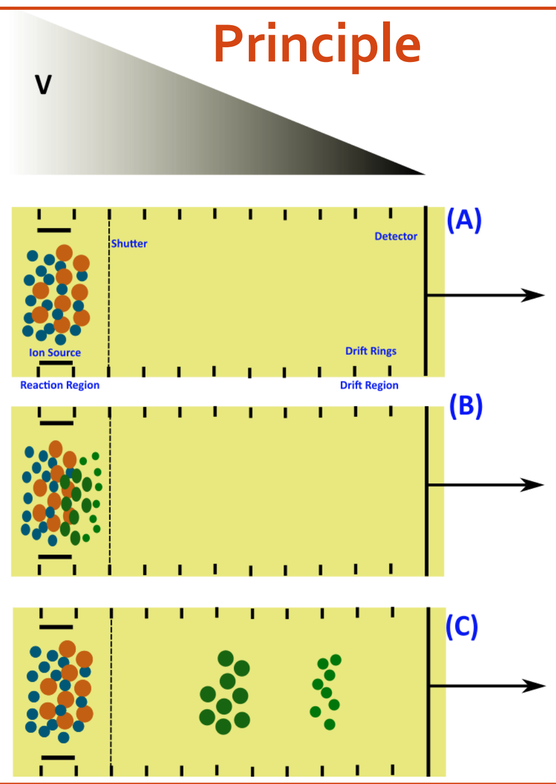
- Volatile organic compound (VOC) detection is increasingly important for **monitoring environmental quality, ensuring workplace safety, and supporting medical diagnostics.**
- This study focuses on how varying temperatures affect ketone detection using ion mobility spectrometry (IMS) equipped with corona discharge ionization (CDI) in positive mode.

Ion-Molecule Reactions

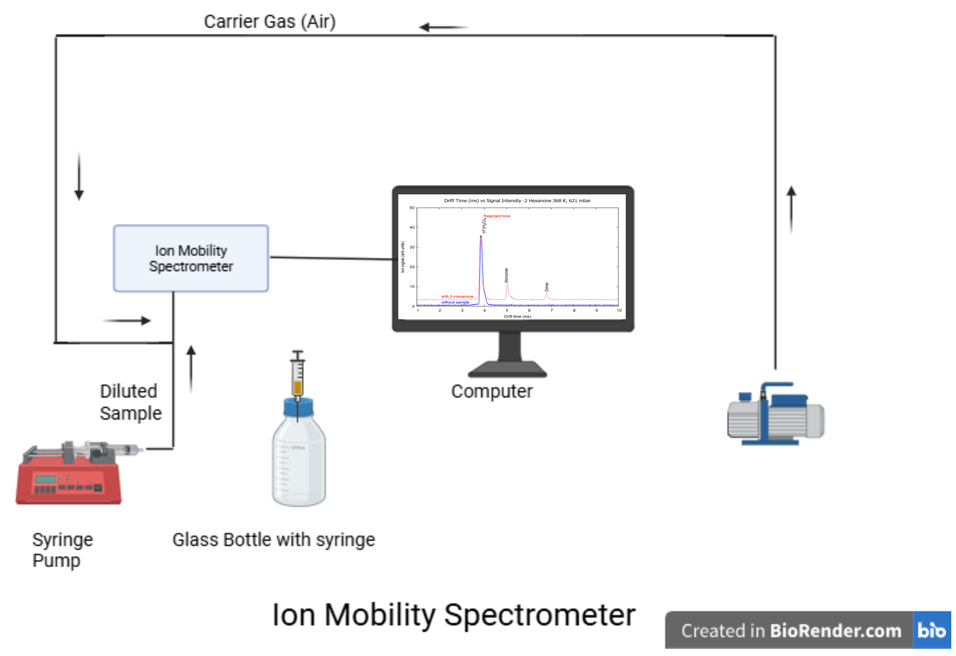
Ketones have a higher proton affinity, so they readily accept a proton

$$H^+ \cdot (H_2O)_n + A \rightleftharpoons A \cdot H^+ \cdot (H_2O)_m + (n-m)H_2O$$

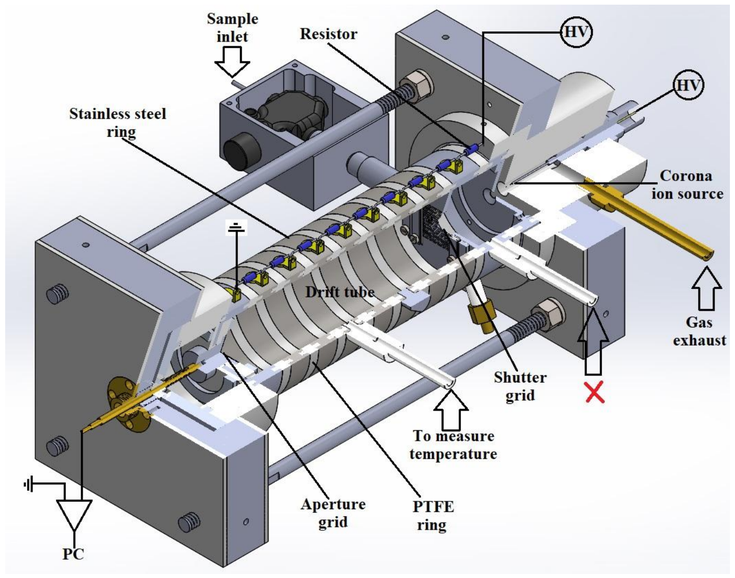
Principle



Experimental Setup



Ion Mobility Spectrometry

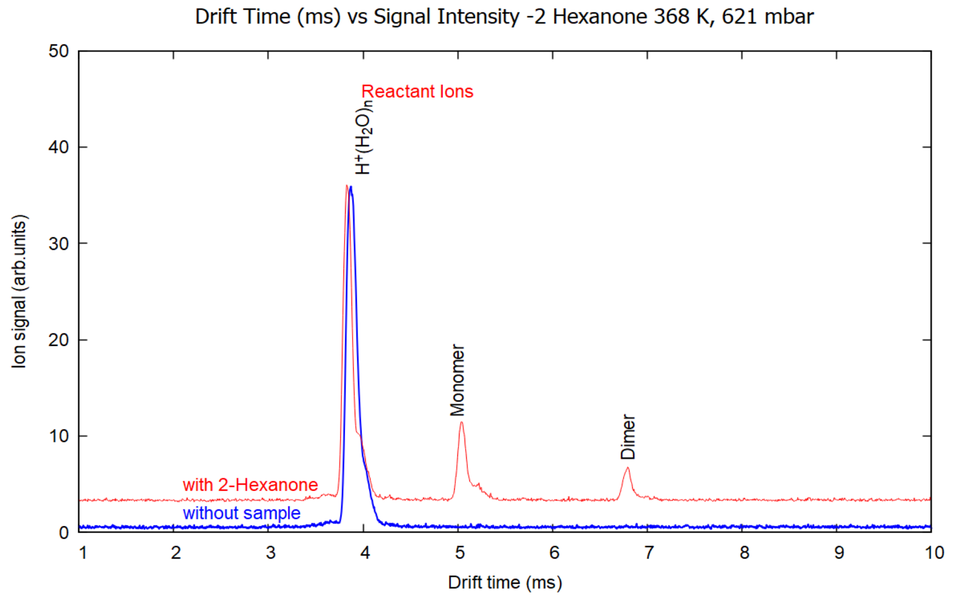


Moravský et al., 2021, Rapid Commun Mass Spectrom. 2021;35(17):e9145

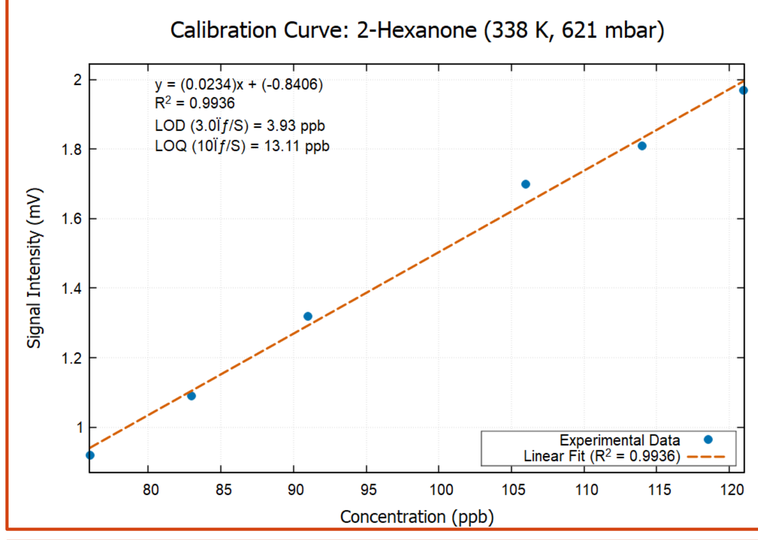
Parameters

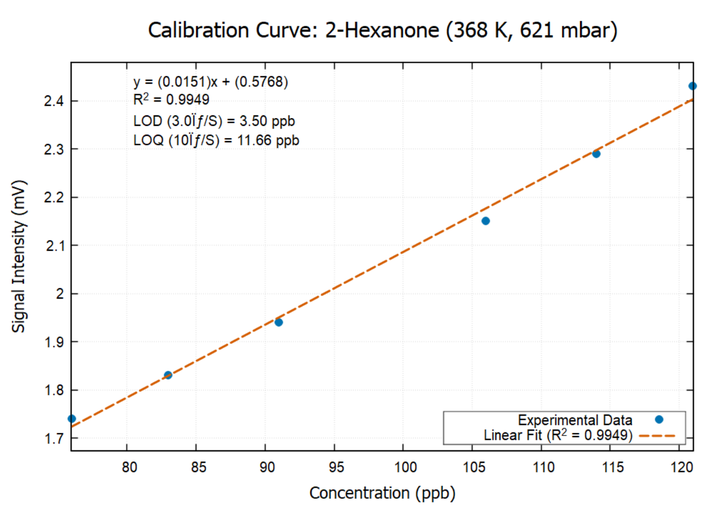
Operating parameter	Unit
IMS drift tube length	11.93 cm
Electric field intensity	670.6 V.cm^{-1}
IMS operating pressure	621 mbar
IMS operating temperature	370 K
Drift gas flow	600 mL.min^{-1}
CD current	10 µA
Shutter grid pulse width	80 µs
Shutter grid frequency	16 Hz
Carrier Gas Flow rate	100 ml/min

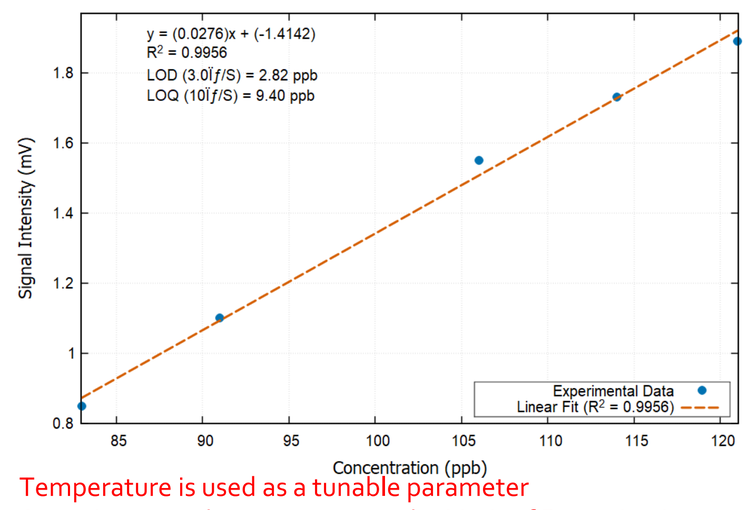
Detector Response vs Drift Time



Calibration Curve







- Temperature is used as a tunable parameter
- As we increase the temperature, the Limit of Detection improves.

References:

[1] Michalczuk, B., Moravský, L., Hrdá, J., & Matejčík, Š. (2020). Atmospheric Pressure Chemical Ionisation study of selected Volatile Organic Compounds (VOCs) by Ion Mobility Spectrometry coupled with orthogonal acceleration Time Of Flight Mass Spectrometry. International Journal of Mass Spectrometry, 449. https://doi.org/10.1016/j.ijms.2019.116275

[2] An, X., Eiceman, G. A., Räsänen, R.-M., Rodriguez, J. E., & Stone, J. A. (2013). Dissociation of Proton Bound Ketone Dimers in Asymmetric Electric Fields with Differential Mobility Spectrometry and in Uniform Electric Fields with Linear Ion Mobility Spectrometry. The Journal of Physical Chemistry A, 117(30), 6389–6401. https://doi.org/10.1021/jp401640t

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FAKULTA MATEMATIKY, FYZIKY A INFORMATIKY
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