

UV Fourier transform absorption cross sections of benzene, toluene, ortho-, meta-, and para-xylene

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SUMMARY

- WHAT? Temperature and pressure effects on the absorption cross sections of BTX in the 35000-42000 cm⁻¹ (286-238 nm) range
- HOW? A Fourier transform spectrometer coupled to a 10 cm cell → Pure BTX & BTX+air mixtures spectra @ 253, 263, 273, 283, and 293 K.

What's the problem ?

- Large disagreements exist between published cross sections
- Literature cross sections were recorded at low resolutions

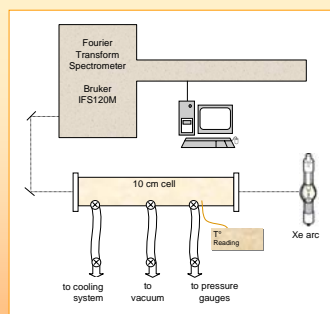
What this work aims at ?

Produce new (higher resolutions) laboratory measurements, and study the temperature and pressure effects on the BTX cross sections to support astrophysics and atmospheric (urban) measurements

EXPERIMENTAL

Experimental conditions

Spectral range	30000-42000 cm ⁻¹
Resolution	1.0 cm ⁻¹
Absorption path length	10 cm
Temperature	253, 263, 273, 283, 293 K
BTX pressure	0.5 - 5 hPa
Dry air pressure	5 - 55 hPa
Lamp & detector	Xe & UV diode
Co-added scans	10 x 64



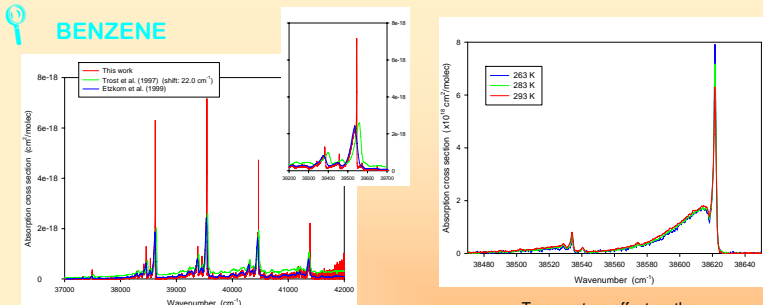
Data processing

- Blanks recorded before and after BTX measurement
- Spectra of pure BTX at each temperature with different pressures
- Spectra of mixtures of BTX with dry air at different total pressures at each temperature
- Cross sections calculated using

$$\sigma(\nu) = \frac{1}{n_{\text{BTX}} d} \times \ln \left(\frac{B I_{\text{obs}}(\nu) + B I_{\text{obs}}(\nu) / 2}{I(\nu)} \right)$$

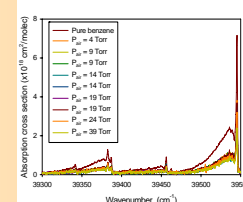


BENZENE



Comparison of benzene absorption cross section at 293K with values from the literature

- Effect of the higher resolution clearly visible
- Wavenumber shifts (not constant) in literature data
- Factor of 2 between this work and Trost et al. (1997)



Temperature effect on the benzene absorption cross section

- Small temperature effect affecting mainly the peak intensity

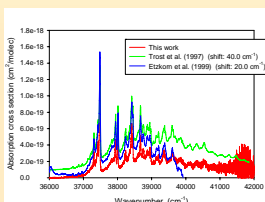
Pressure effect on the benzene absorption cross section

- Similar decrease in XS for all pressures of buffer gas
- Important for atmospheric measurements

TOLUENE

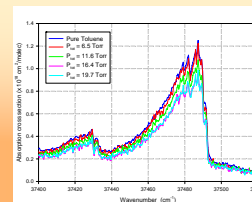
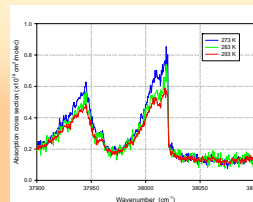
Comparison of toluene absorption cross section at 293 K with values from the literature

- Large differences with literature data



Temperature effect on the toluene absorption cross section

- As expected, when T increases, intensity of peaks decrease



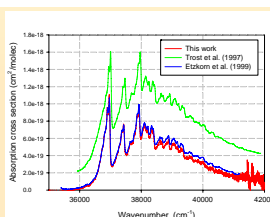
Pressure effect on the toluene absorption cross section

- Visible pressure effect with respect to buffer gas pressures

XYLENES

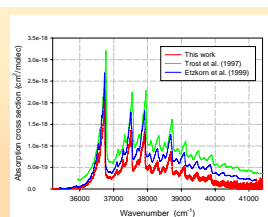
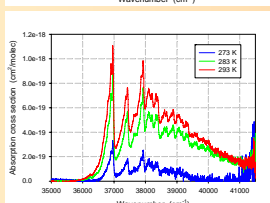
Comparison of m-xylene absorption cross section at 293 K with values from the literature

- Large differences with Trost et al.
- Good agreement with Etzkom et al.



Temperature effect on the m-xylene absorption cross section

- Reverse temperature effect than expected
- But bad S/N due to very low pressure at low T

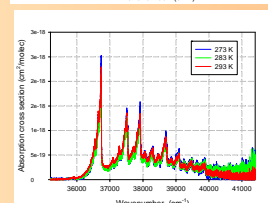


Comparison of p-xylene absorption cross section at 293K with values from the literature

- Large differences with Trost et al. and with Etzkom et al.

Temperature effect on the p-xylene absorption cross section

- No temperature effect observed.

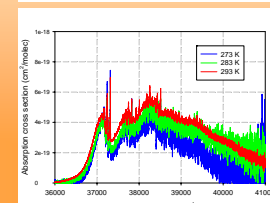
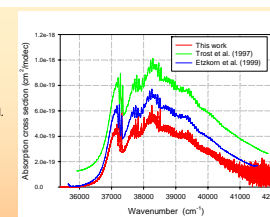


Comparison of o-xylene absorption cross section at 293K with values from the literature

- Large differences with Trost et al. and with Etzkom et al.

Temperature effect on the o-xylene absorption cross section

- S/N too low to infer any temperature effect.



CONCLUSIONS

- High resolution absorption cross sections of BTX
- Temperature and pressure effect different for each species
- Large differences with literature data