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OF CATALYSIS

Effect of Cu(I) additive on sorption by imidazole based ionic liquids studied by in situ ATR-FTIR spectroscopy

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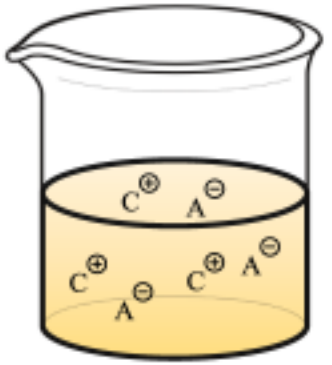
Ionic liquids

Ionic liquids (ILs) are a special type of functional materials with unique physical and chemical properties.

IL is a liquid completely consisting of ions. As a rule, ILs are assumed as the molten salts with a melting point below 100 °C.



Thermal and chemical stability

Good solubility

Tuning

Conductivity

Non-volatility

Main fields of IL possible applications

- Synthesis
- Analytical methods
- **Separation processes**
- Storage and transportation of gases
- Catalysis
- Electrochemistry

Reversible chemical complexation

The Cu(I) ion possesses a unique orbital structure that allows for complexation with a carbon–carbon double bond

The weak chemical interaction is reversed by displacement by another species, by temperature swings, and/or by pressure swings

The Cu(I)-ethylene complex alone is unstable and labile, and thus, additional ligands are used to increase stability

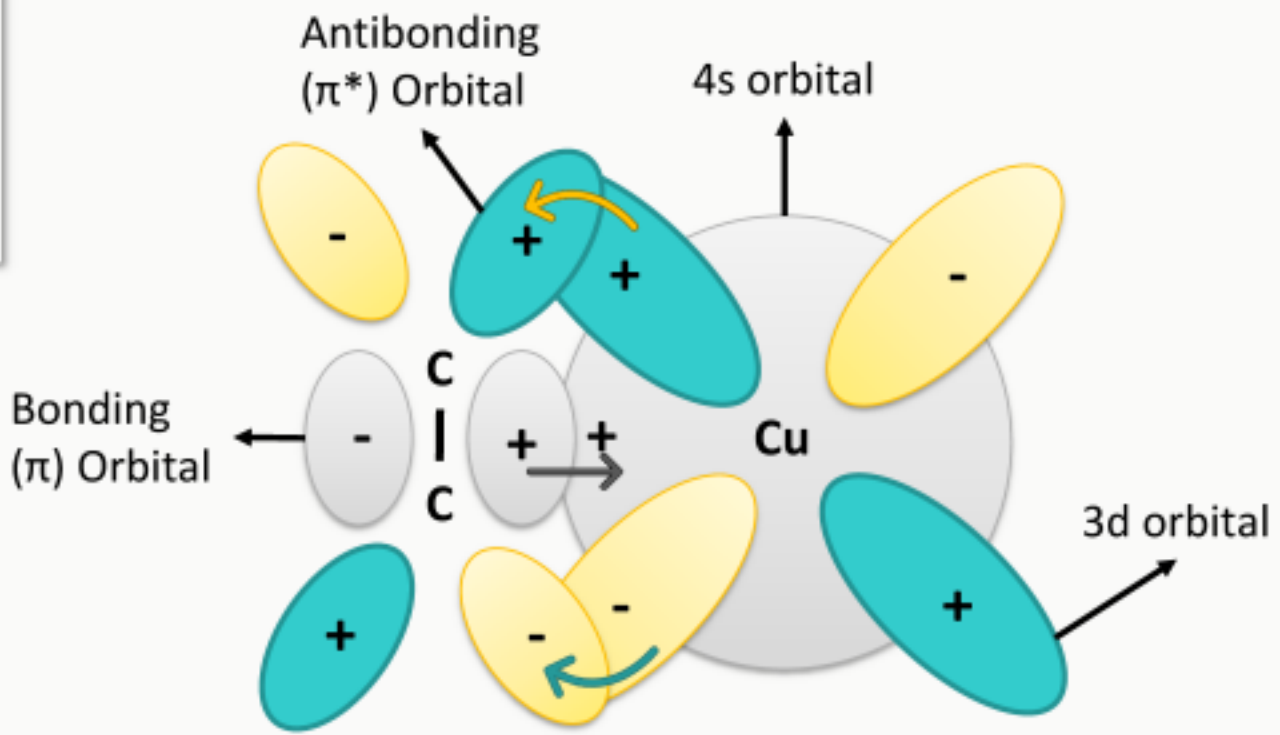
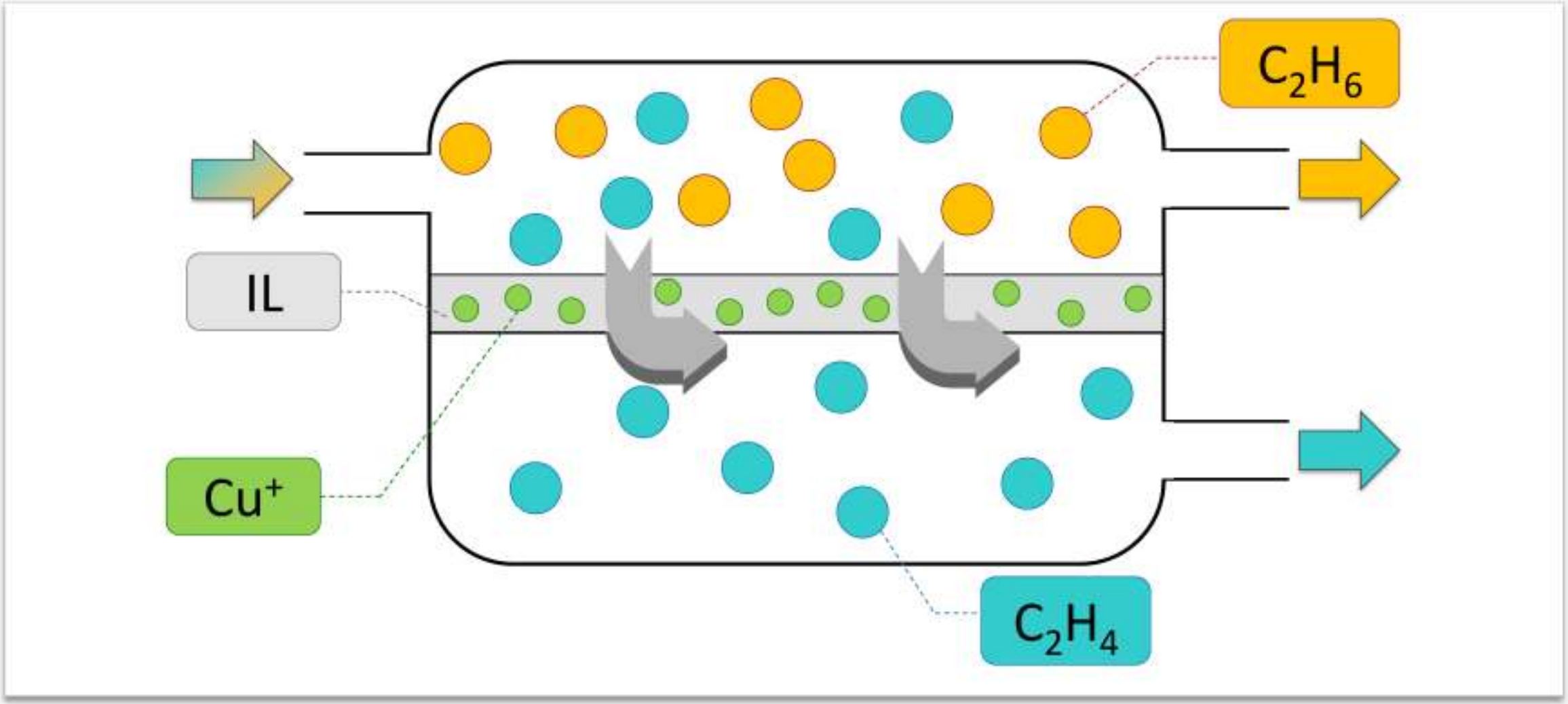


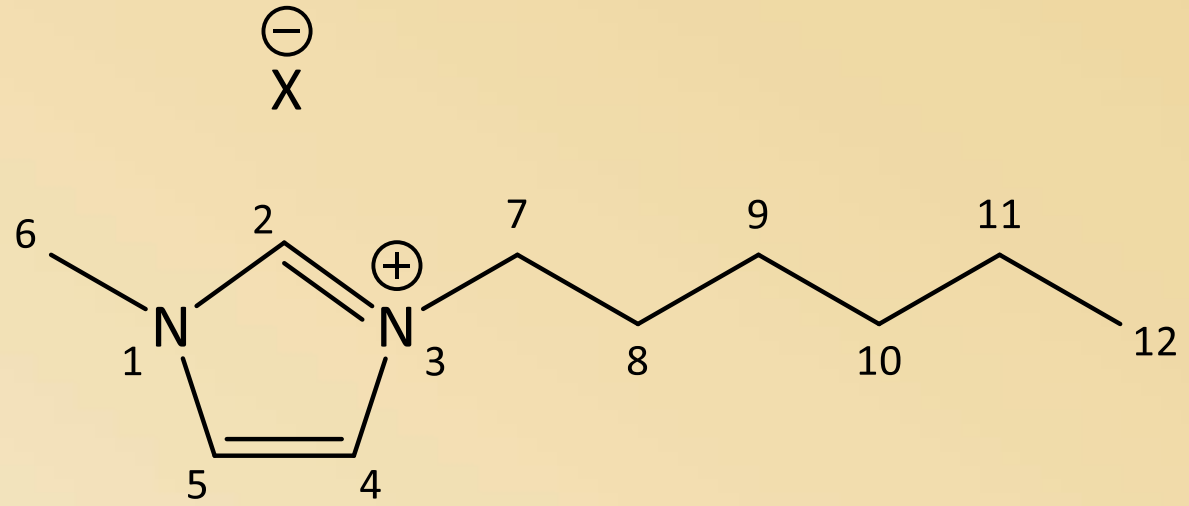
Fig. 1 - Dewar-Chatt model of π-bond complexation

Olefin/Paraffin Separation



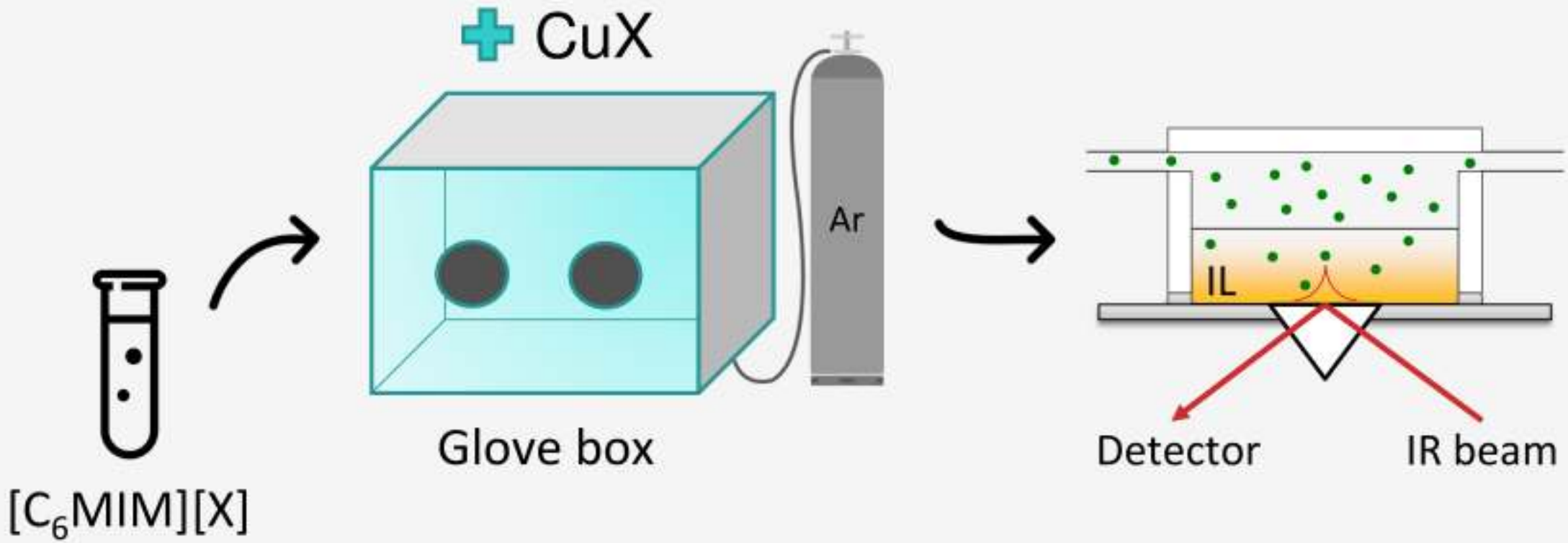
The aim of investigation

To study the effect of Cu(I) additives on the ethylene sorption capacity of $[C_6MIM][X]$ (X=Cl, Br, I) ILs by *in situ* ATR-FTIR spectroscopy.



1-hexyl-3-methyl-imidazolium halides $[C_6MIM][X]$

Experimental



Attenuated total reflection (ATR) mode

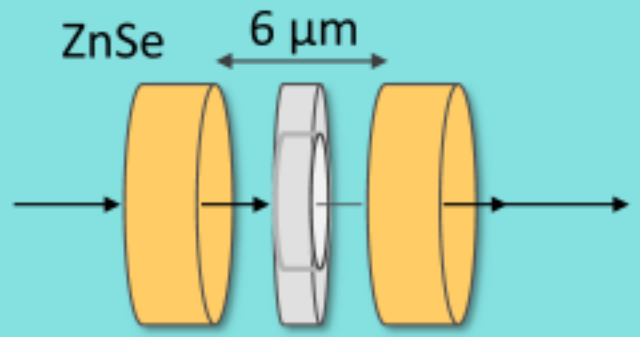


Fig. 1 - High-pressure transmission cell

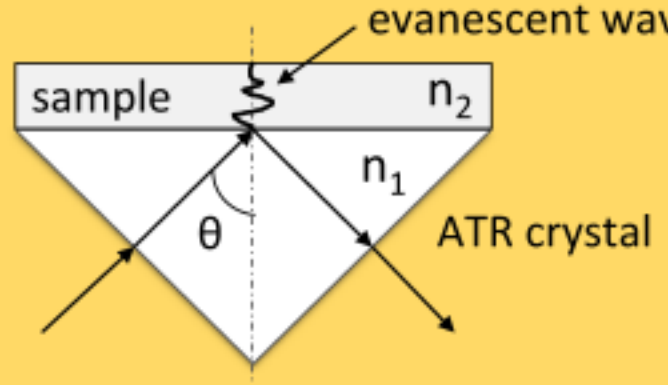
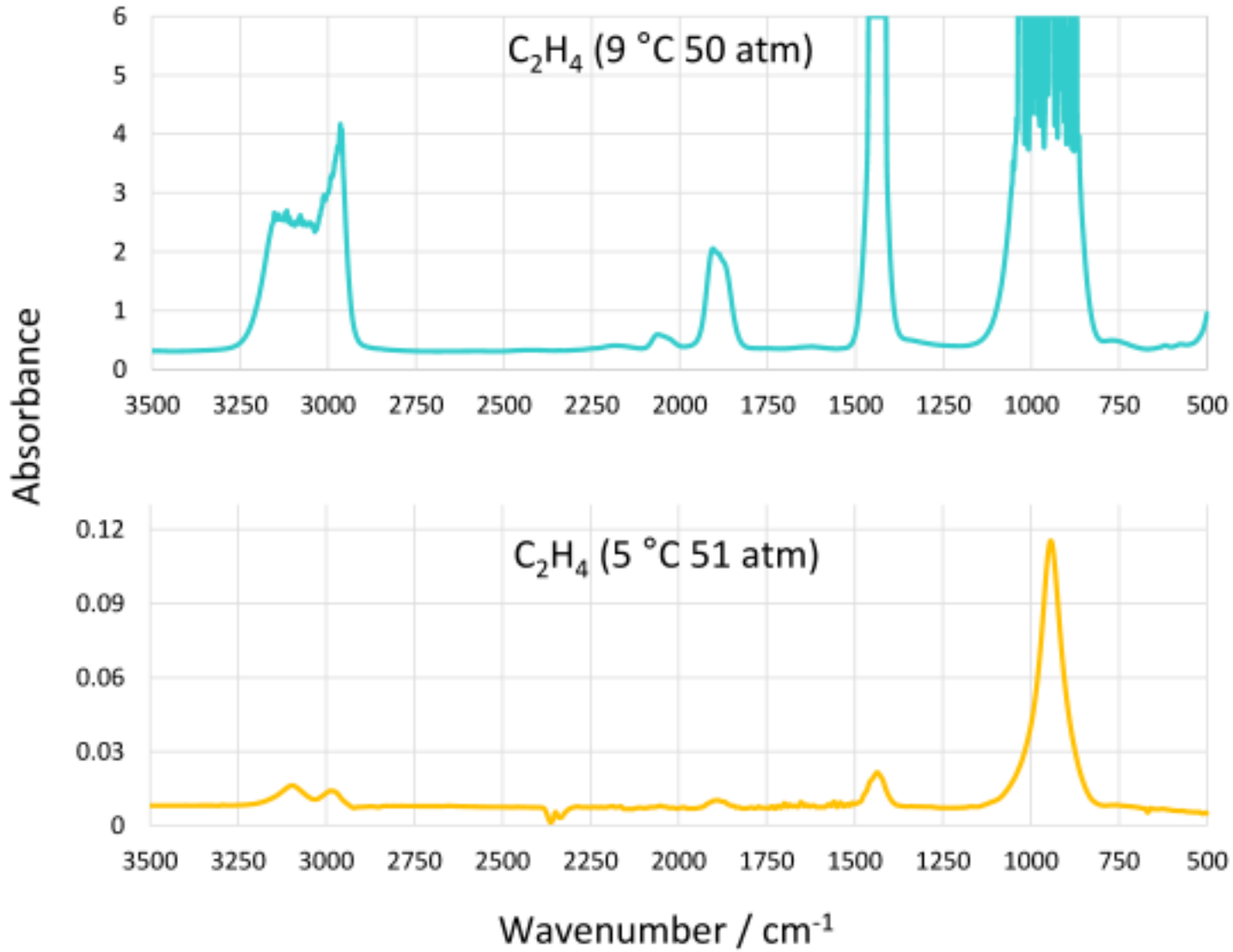
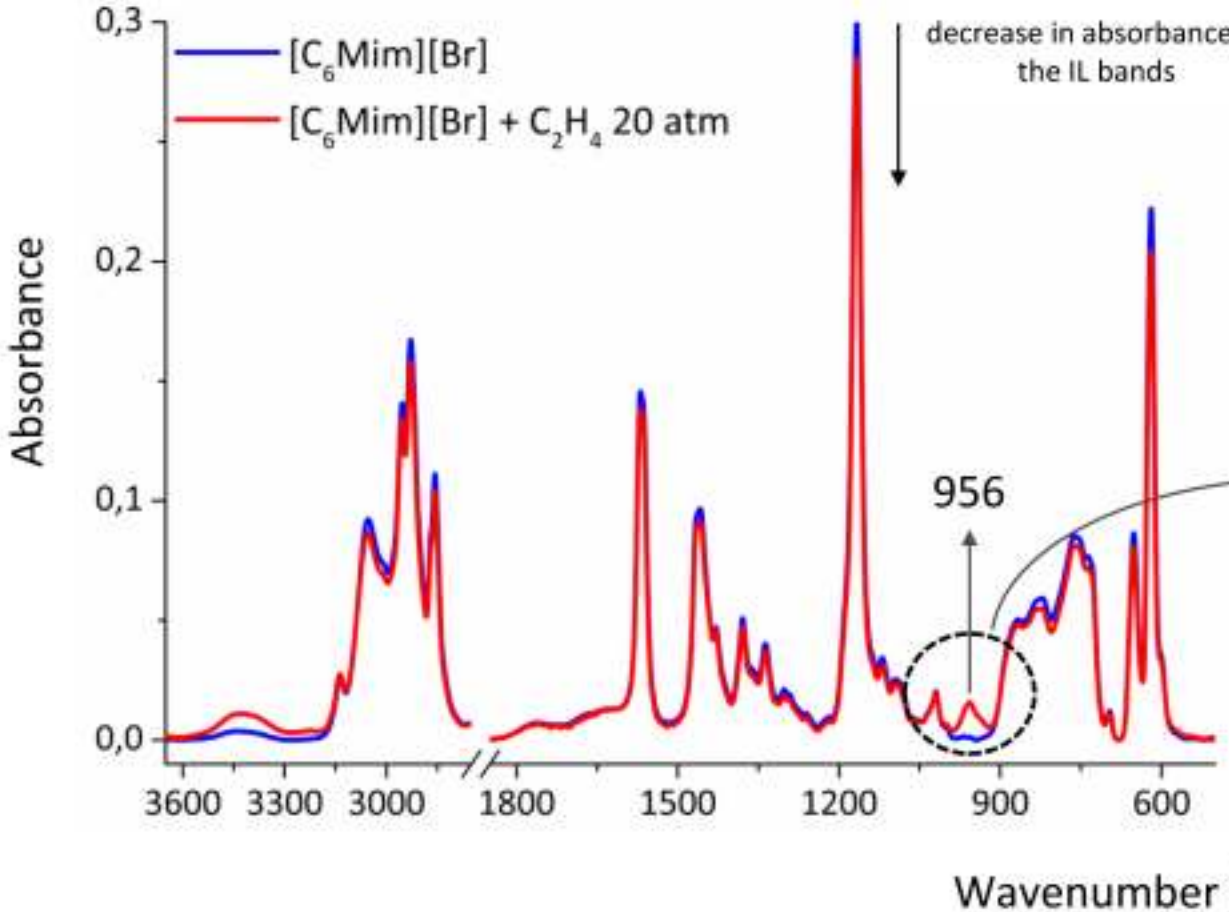
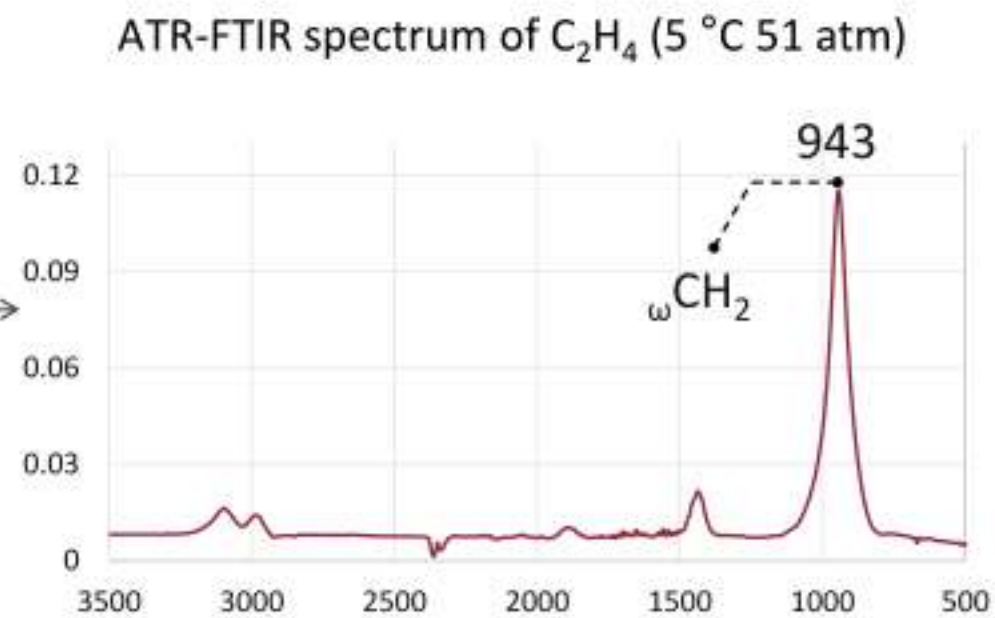


Fig. 2 - ATR accessory

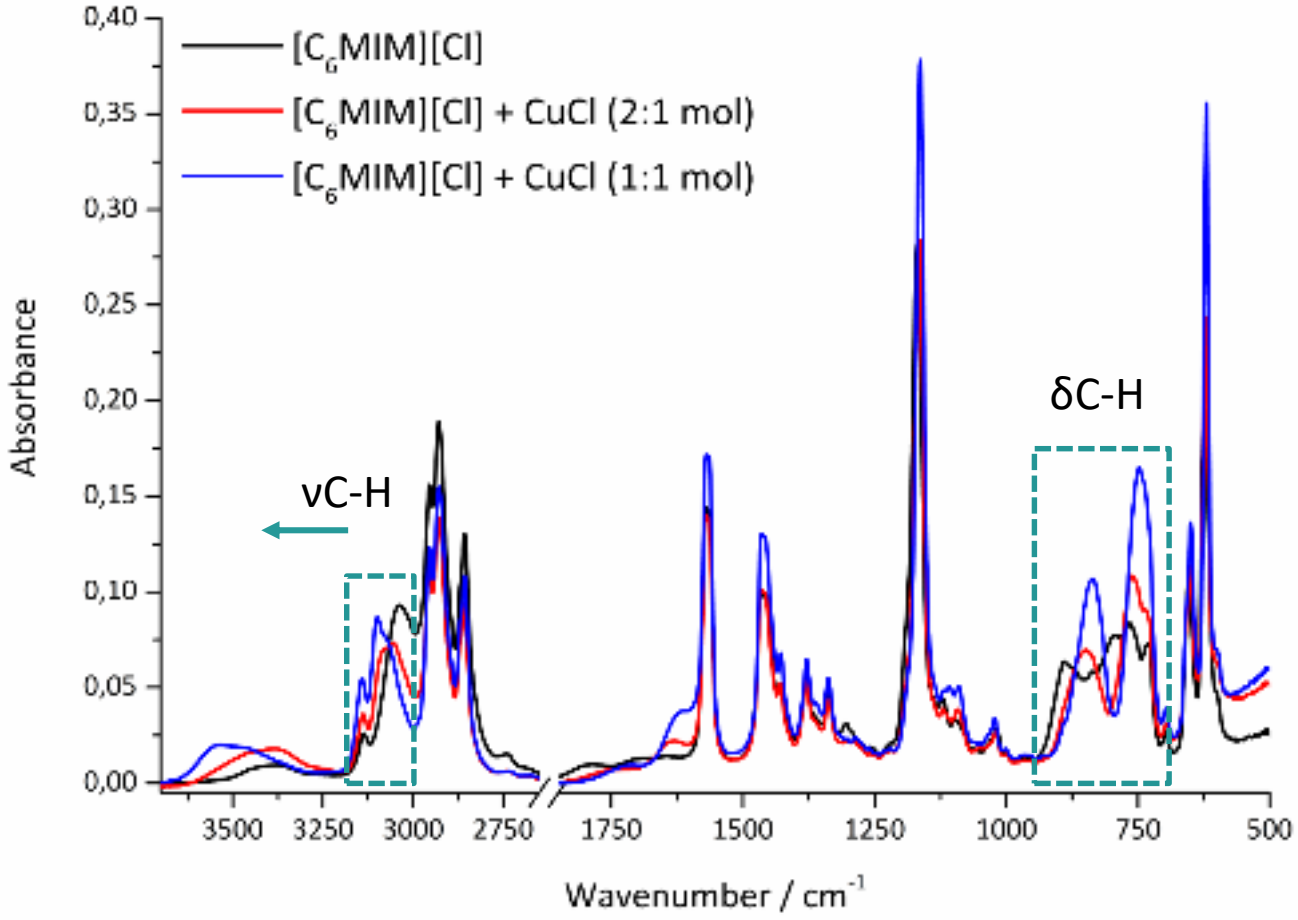


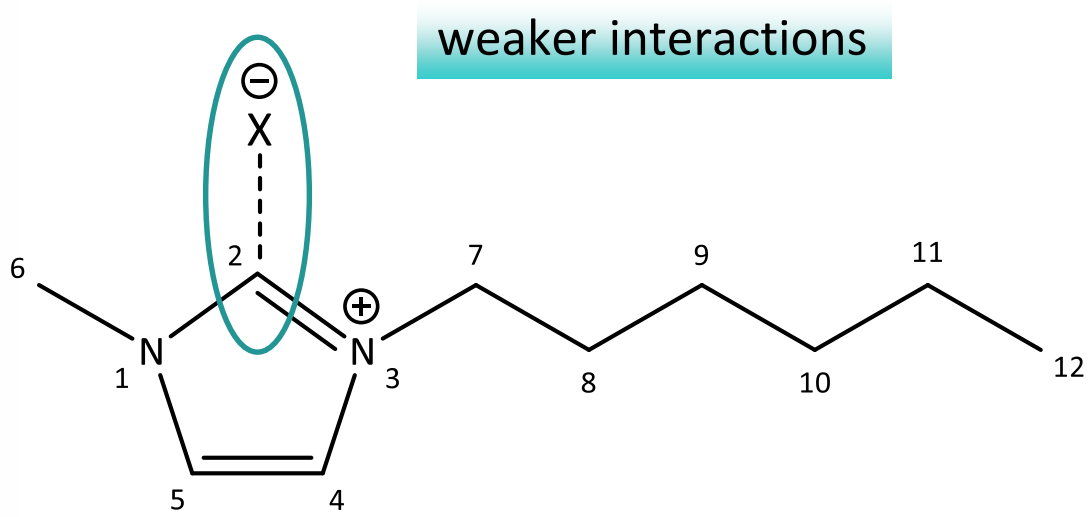
ATR-FTIR spectra of [C_6MIM][Br] IL



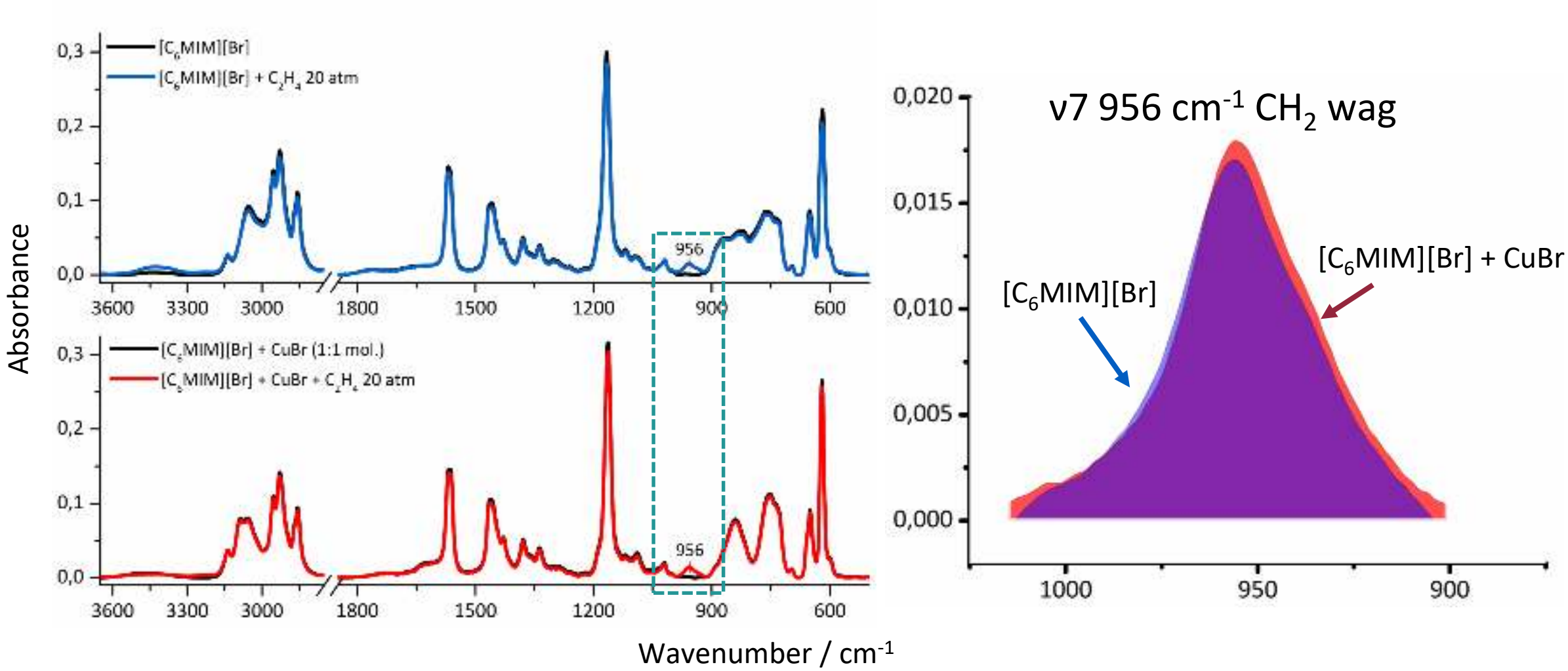


ATR-FTIR spectra of [C_6MIM][Cl] IL with CuCl

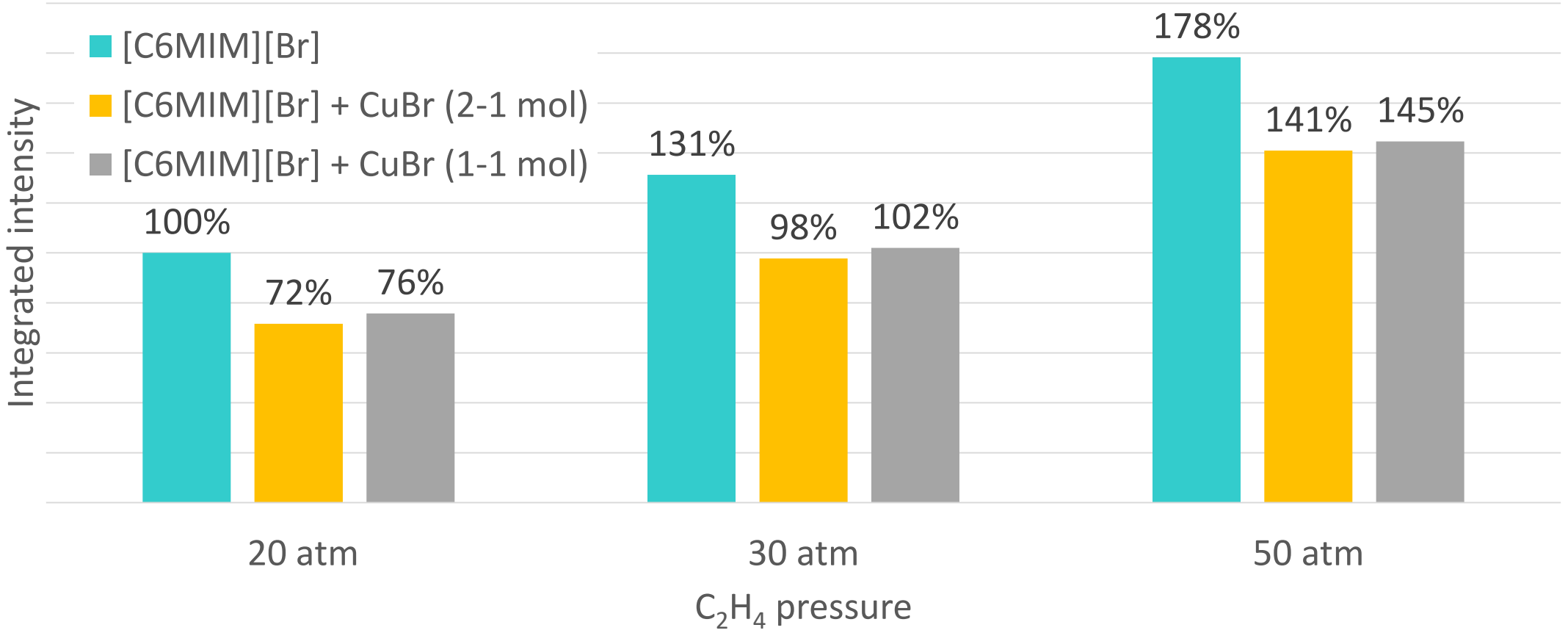




ATR-FTIR spectra of [C_6MIM][Br] IL



The comparison of IL capacity

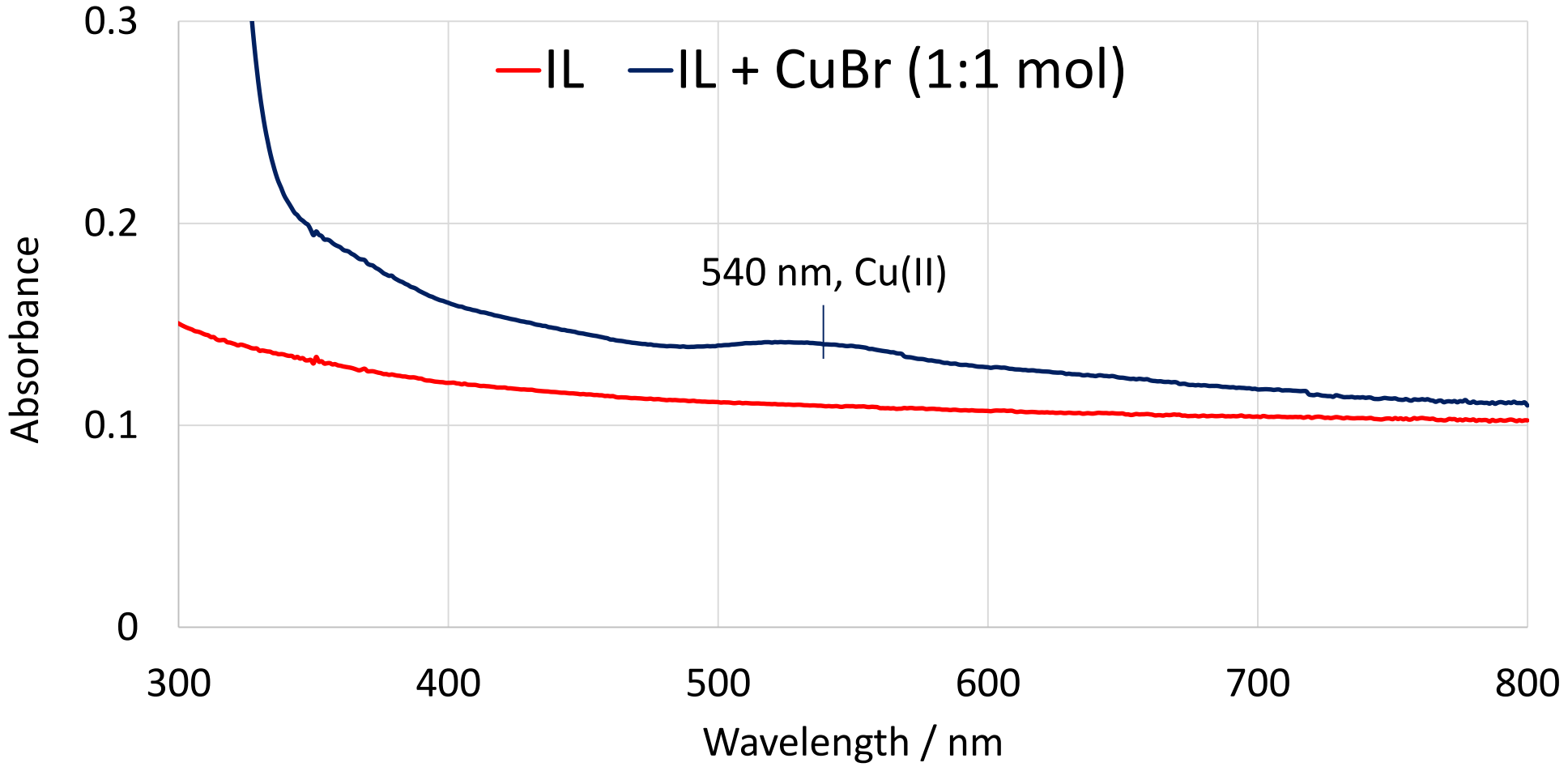


Conclusions

- Cu(I) salts do not lead to an increase in the amount of sorbed ethylene during IL sorption.
- Spectroscopically, the formation of a π-complex between absorbed ethylene and Cu (I) cannot be detected.
- For modified ILs, a decrease in the interaction between the cationic and anionic fragments is observed.

Thank you for attention!

UV-Visible Spectroscopy



$$\frac{d_{e,u}}{\lambda_1} = \frac{n_{21}cos\theta(3sin^2\theta - 2n_{21}^2 + n_{21}\,sin^2\,\theta)}{2\pi(1-n_{21}^2)[(1+n_{21}^2)\,sin^2\,\theta - n_{21}^2]\,(sin^2\theta - n_{21}^2)^{1/2}}$$

$d_{e,u}$ - effective sample depth

λ_1 - wavelength in an optically dense medium

n_{21} – n_2/n_1

n_i - refractive index