

# **MOLECULAR EMITTERS AS A TUNABLE LIGHT SOURCE FOR OPTICAL MULTISENSOR SYSTEMS**

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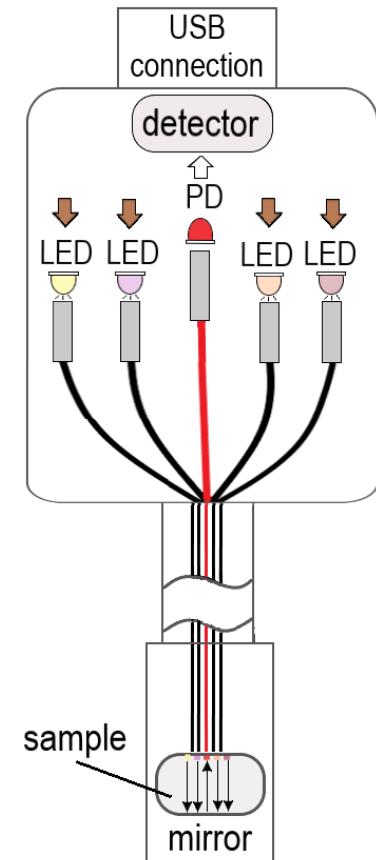
# OPTICAL MULTISENSOR SYSTEM (OMS)

- Multisensor system – an analytical device
  - composed of two or more sensors
  - optimized for a particular analytical task
  - employs chemometrics to maintain accuracy

- OMS composed of
  - light sources
  - photodetectors
  - optical fibers
  - 3D-printed parts, etc.

- Advantages
  - inexpensive
  - portable
  - on-site/on-line implementation

Example of OMS <sup>a</sup>



# PURPOSE OF THIS STUDY

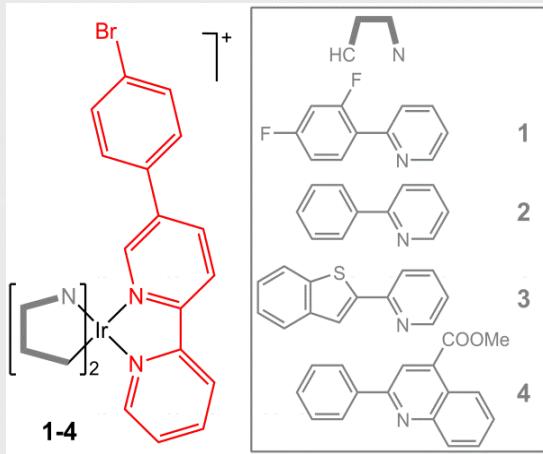
- To develop OMS prototype based on molecular emitters as a tunable light source
- To study a real-life applicability of the developed prototype

# MOLECULAR EMITTERS AS A LIGHT SOURCE

- Properties
  - laser diode excites the emission of molecular emitters
- Requirements to choose emitters
  - absorption spectrum must not overlap with emission spectrum
  - excitation radiation must fit into the absorption maximum
  - brightness (quantum yield of emission)
  - emission wavelength in solid phase
- Advantages
  - high versatility
  - short analysis time
  - adjustment of the emission wavelength for a specific application

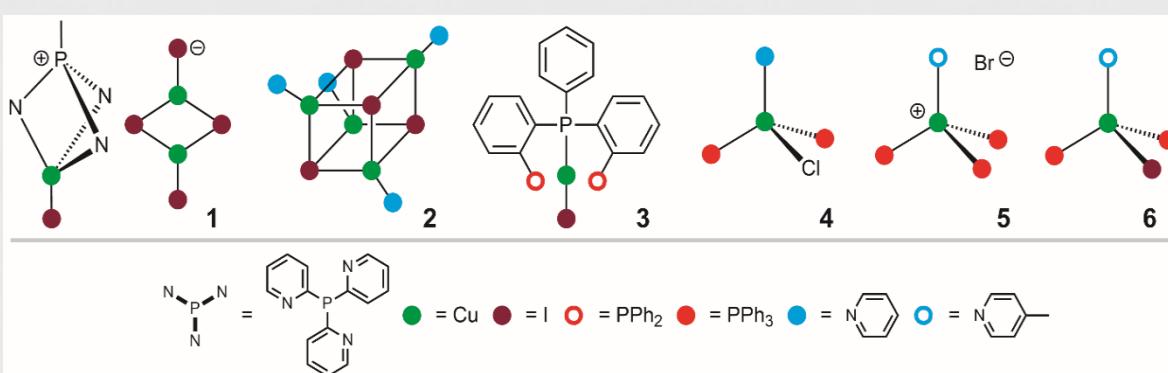
# EXAMPLES OF MOLECULAR EMITTERS

## Ir(III) complexes



- [Ir(dfppy)<sub>2</sub>(bpypy)]PF<sub>6</sub> (1)
- [Ir(ppy)<sub>2</sub>(bpypy)]PF<sub>6</sub> (2)
- [Ir(pybt)<sub>2</sub>(bpypy)]PF<sub>6</sub> (3)
- [Ir(mpqc)<sub>2</sub>(bpypy)]PF<sub>6</sub> (4)

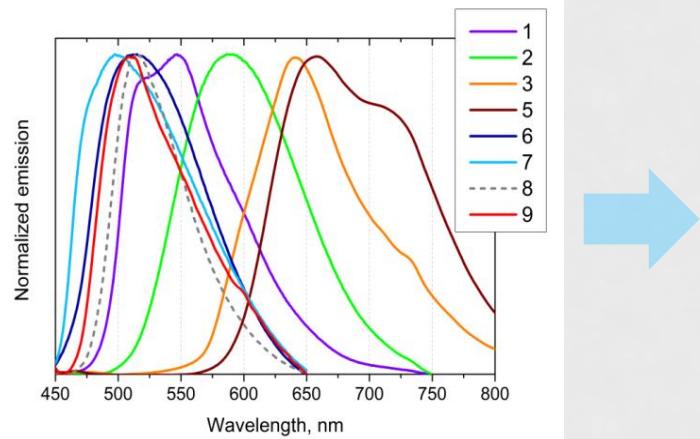
## Cu(II) complexes



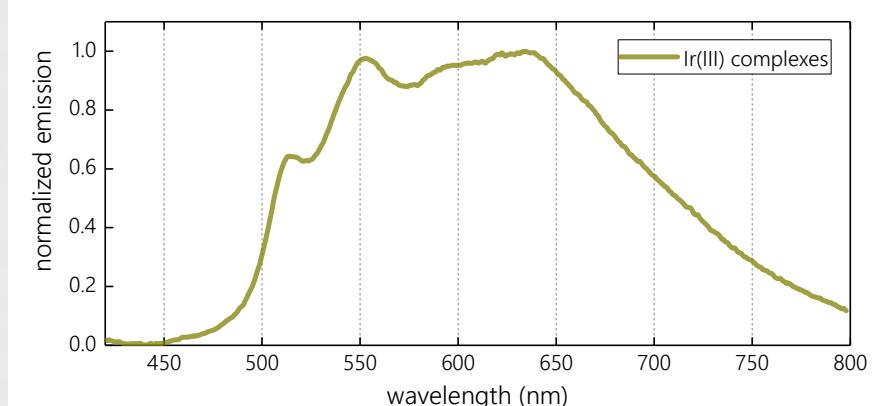
- [Cu(MePPY<sub>3</sub>)I]<sub>2</sub>[Cu<sub>2</sub>I<sub>4</sub>] (1)
- [Cu<sub>4</sub>I<sub>4</sub>(py)<sub>4</sub>] (2)
- [Cu(TpdP)<sub>2</sub>I] (3)
- [CuCl(PPh<sub>3</sub>)<sub>2</sub>(py)] (4)
- [Cu(PPh<sub>3</sub>)<sub>3</sub>(4-Mepy)]Br (5)
- [CuI(PPh<sub>3</sub>)<sub>2</sub>(4-Mepy)] (6)

# MOLECULAR EMITTERS AS A LIGHT SOURCE

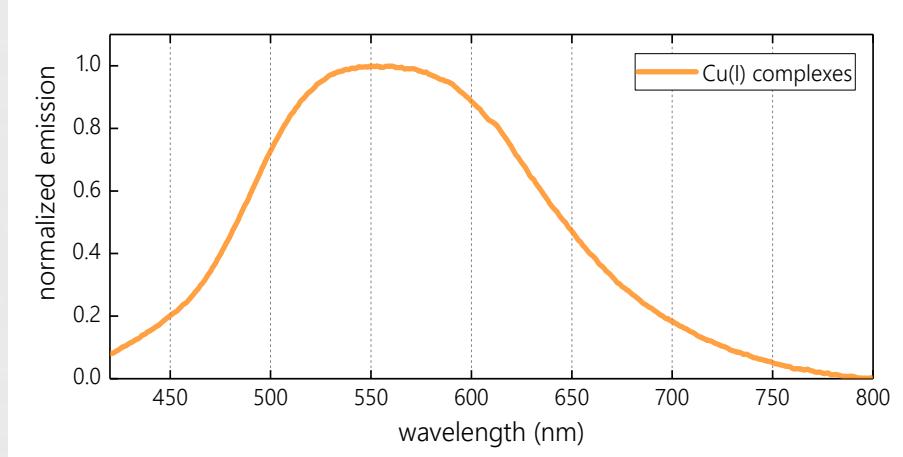
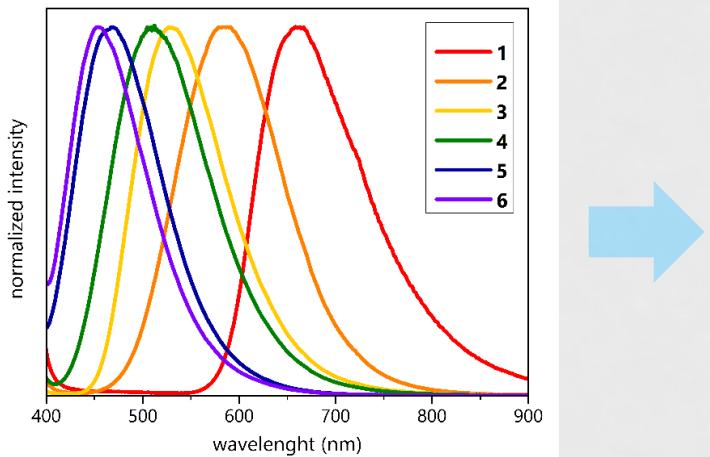
Ir(III) complexes



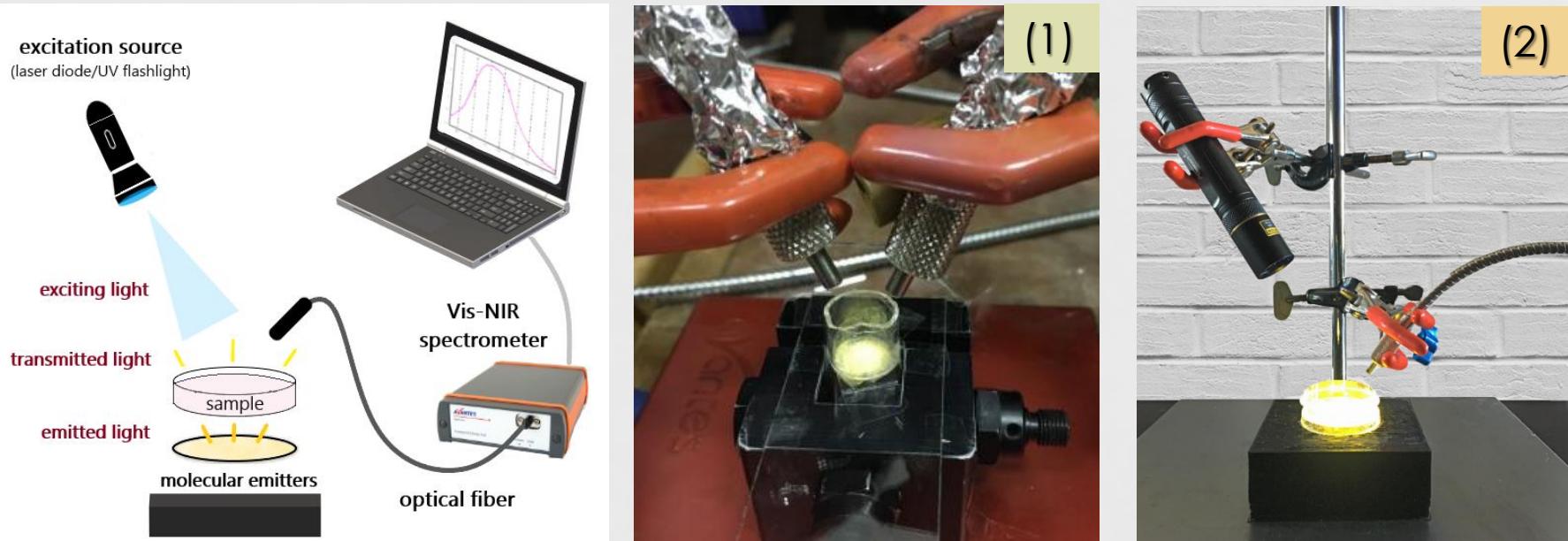
Emission spectra of the mixtures



Cu(II) complexes



# EXPERIMENTAL



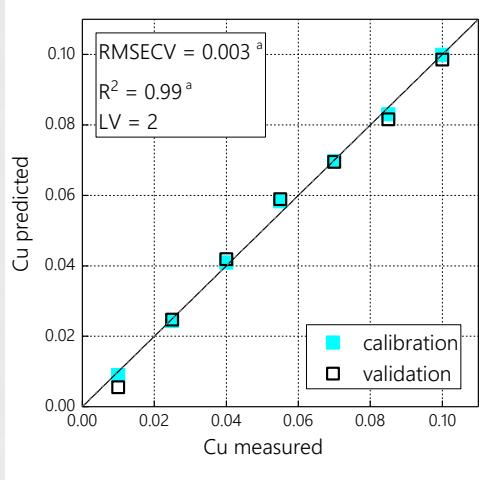
	(1) Ir(III)-based OMS <sup>a</sup>	(2) Cu(I)-based OMS
Sample volume	0.15 mL	4 mL
Sample placement	glass cup (1 cm in diameter)	polystyrene Petri dish (3.5 cm in diameter)
Excitation source	laser diode ( $\lambda_{\text{exct}} = 365 \text{ nm}$ )	laser diode ( $\lambda_{\text{exct}} = 385 \text{ nm}$ ) / UV flashlight ( $\lambda_{\text{exct}} = 365 \text{ nm}$ )
Detector	fiber-optic UV-vis spectrometer AvaSpec-ULS2048CL-EVO	

<sup>a</sup> Gitlina A.Y., Surkova A., Ivonina M.V., et al. Dyes Pigments. 2020; 180:108428. doi: 10.1016/j.dyepig.2020.108428

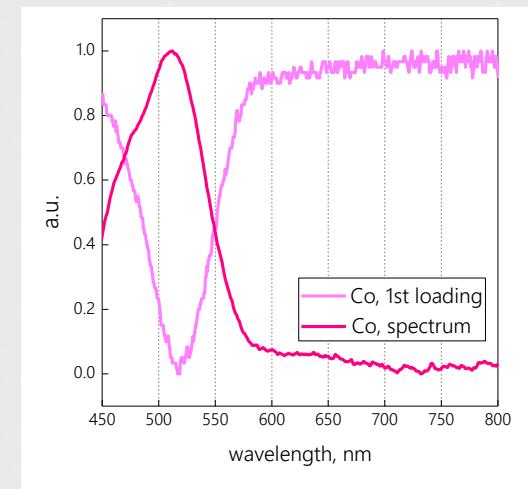
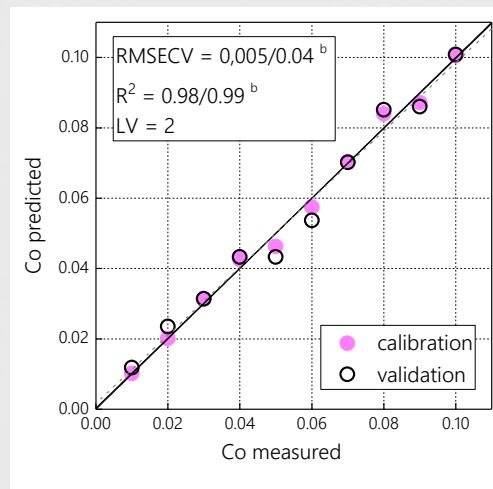
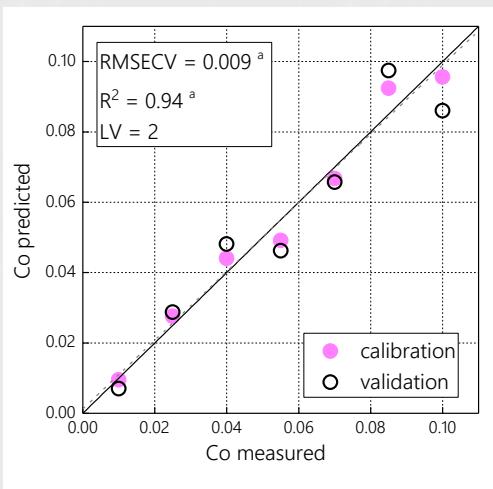
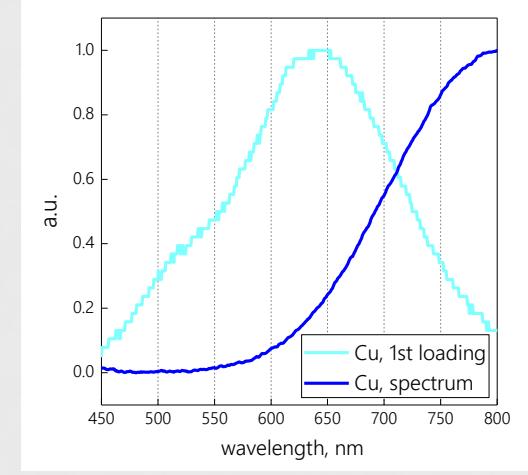
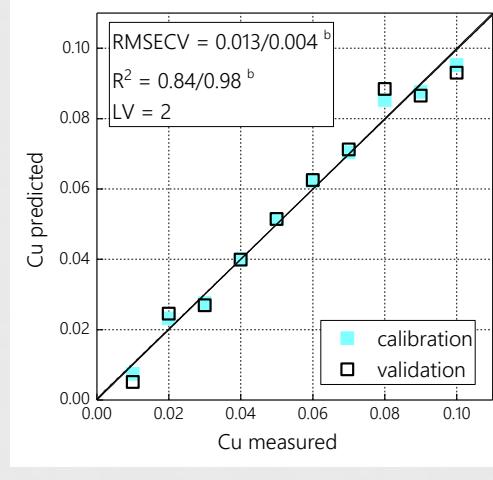
# RESULTS FOR MODEL SOLUTIONS

Individual calibration series for Co(II) and Cu(II) nitrates

Ir(III)-based OMS



Cu(II)-based OMS



excitation source: <sup>a</sup> laser diode,  $\lambda_{\text{exct}} = 365 \text{ nm}$ ; <sup>b</sup> laser diode,  $\lambda_{\text{exct}} = 385 \text{ nm}$  / UV flashlight,  $\lambda_{\text{exct}} = 365 \text{ nm}$

# PRACTICAL APPLICATION

- Calibration sample set for  $\text{PO}_4^{3-}$ 
  - 9 samples
  - 0–0.96 mg/L with 0.12 mg/L step



- Calibration sample set for  $\text{F}^-$ 
  - 11 samples
  - 0–0.4 mg/L with 0.04 mg/L step

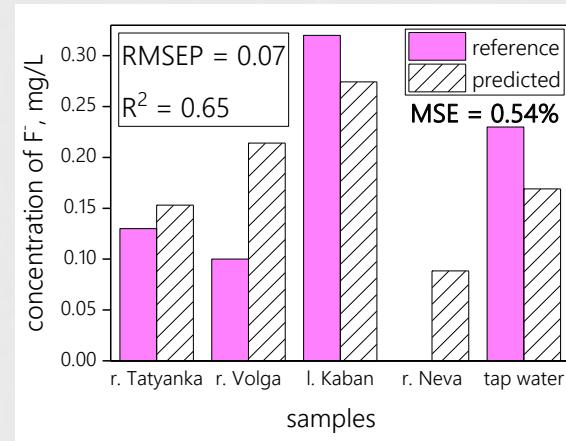
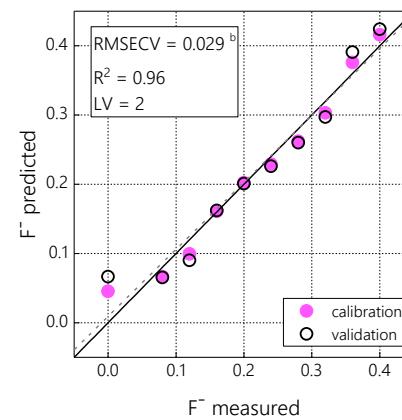
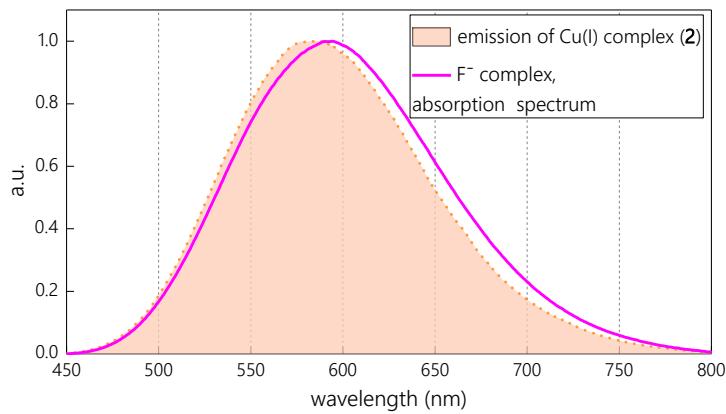
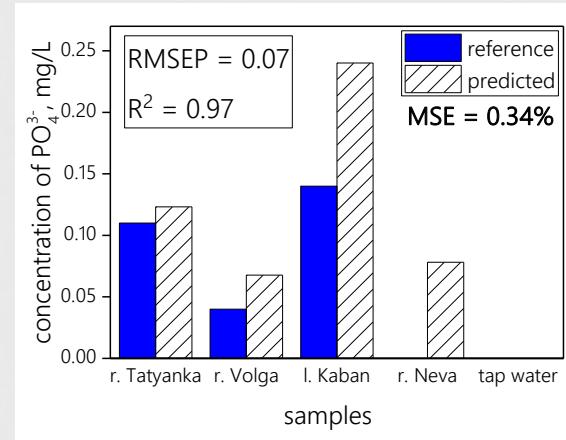
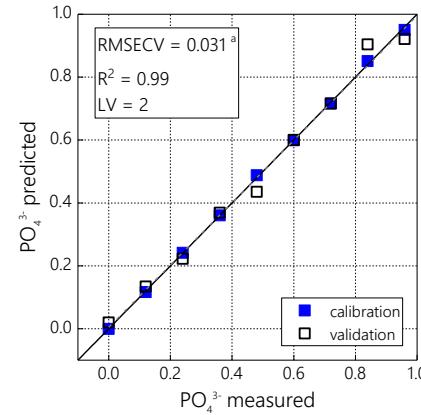
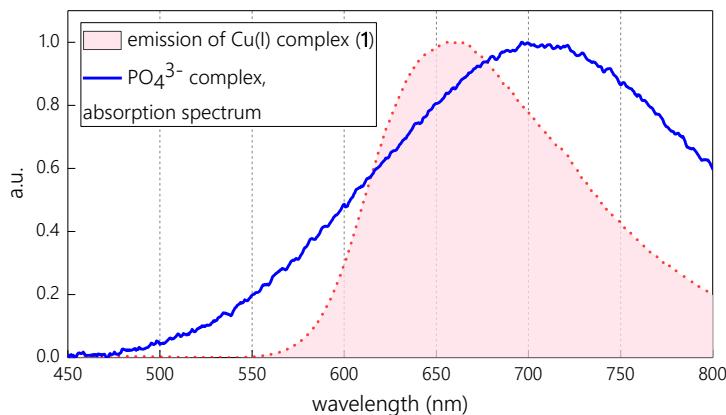


- Test set: 5 samples from tap, rivers (Neva, Volga, Tatyanka) and lake Kaban

Samples were colored in accordance with the procedures described in GOST 18309-2014 and GOST 4386-89.

# PRACTICAL APPLICATION

## Determination of fluoride and phosphate in surface water



excitation source: UV flashlight ( $\lambda_{\text{exct}} = 365 \text{ nm}$ ); interval: <sup>a</sup> 600–750 nm; <sup>b</sup> 450–800 nm

# CONCLUSIONS

- Ir(III) and Cu(I)-based complexes are suitable light sources for OMS
- Ir(III) luminescent complexes have bright controlled emission
- Cu(I) complexes are easier to produce, cheaper, and environmentally friendly
- Using UV flashlight instead of laser diode as excitation source is more convenient
- Developed OMS allows determination of fluoride and phosphate in surface waters with high accuracy

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