

## Smart Sensing of Alcohol Vapours with a Molybdenum Coordination Complex



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### INTRODUCTION & AIM

The selective and sensitive detection of volatile alcohol such as methanol or ethanol at ambient conditions is of great importance in environmental monitoring,<sup>1</sup> industrial process control,<sup>2</sup> and public health<sup>3</sup> due to their widespread use and potential toxicity. Transition metal coordination complexes, particularly those of molybdenum, have shown great semiconductor properties,<sup>4</sup> making them ideal candidates for molecular recognition and sensor applications. Their ability to engage in specific interactions with hydroxyl-containing analytes,<sup>5</sup> combined with tuneable electronic properties, allows for tailored sensor design with high selectivity.

In this study, we report the synthesis and characterization of a novel molybdenum coordination complex. The sensor's response to MeOH/EtOH vapours was systematically investigated by solid-state impedance spectroscopy (SS-IS) at room temperature (RT), while electrical properties were studied in wide temperature range. The complex exhibited reversible modulation of conductivity at RT, indicating efficient and selective alcohol detection.

### METHOD

The ligand was synthesized through a condensation reaction between oxalylhydrazide and 2-hydroxy-3-methoxybenzaldehyde, yielding a Schiff base. This ligand was then coordinated to  $\{\text{MoO}_2\}^{2+}$  core in MeOH under reflux conditions to form a dinuclear molybdenum(VI) complex, formulated as  $[\text{Mo}_2\text{O}_4(\text{L})(\text{MeOH})_2] \cdot 2\text{H}_2\text{O}$ . The resulting complex was isolated as an orange powder and characterized by spectroscopic methods.

To investigate its potential as a chemical sensor, particularly for alcohol vapours, the complex was exposed to MeOH and EtOH vapours, and the changes in its conductivity were monitored using SS-IS. The electrical properties of the complex were studied via SS-IS over wide range of frequencies (0.01 Hz – 1 MHz) and temperatures (40 – 200 °C).

This approach allowed for the assessment of the complex's vapour sensing capabilities, revealing characteristic response upon exposure to MeOH vapours.

### REFERENCES

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### ACKNOWLEDGEMENTS

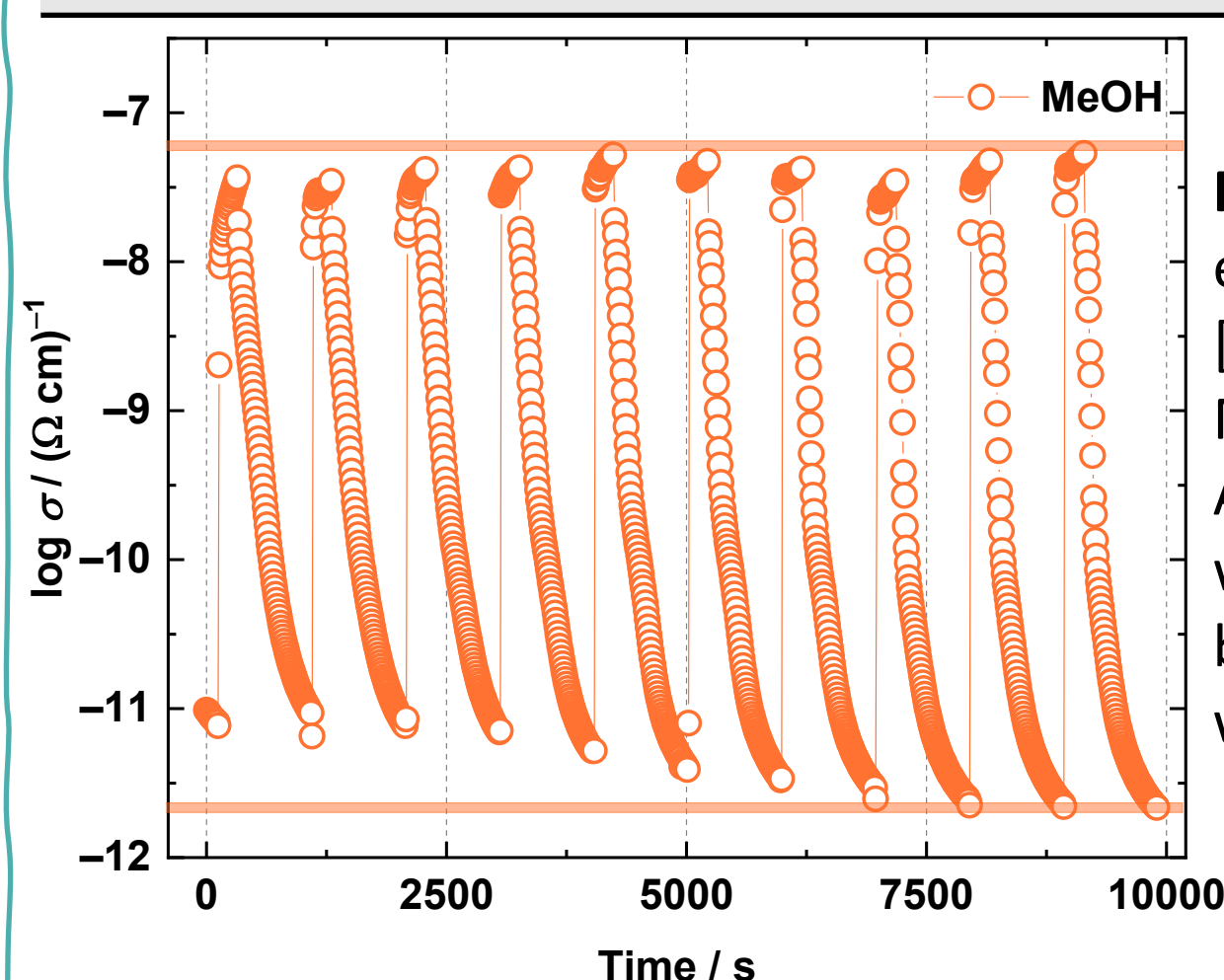
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### RESULTS & DISCUSSION

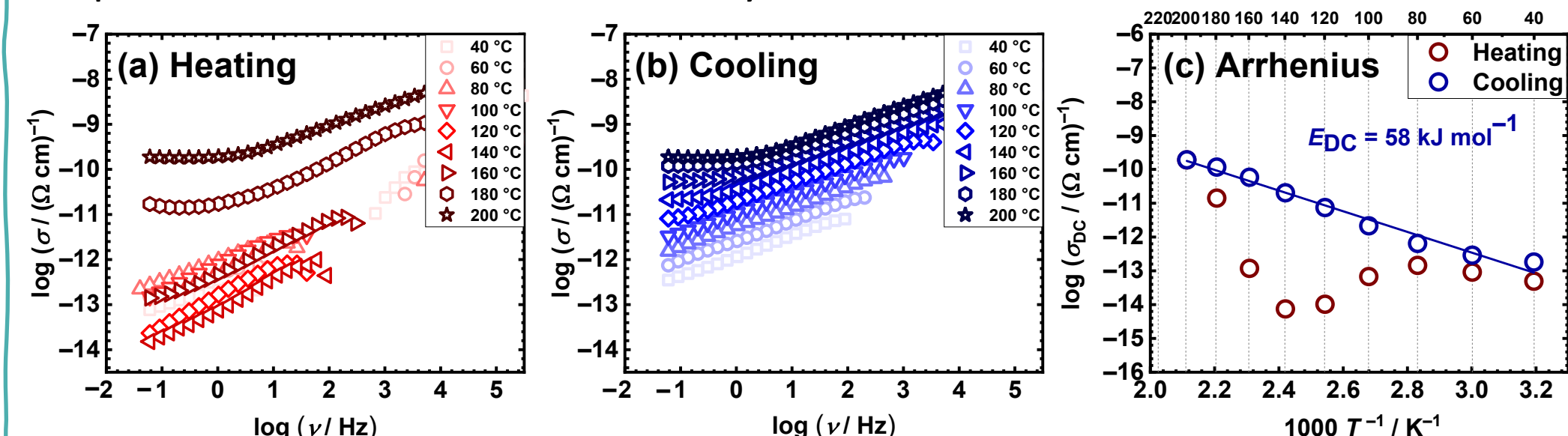
**Table 1.** Conductivity, response ( $t_{\text{res}}$ ) and recovery ( $t_{\text{rec}}$ ) time after exposure of the dinuclear complex  $[\text{Mo}_2\text{O}_4(\text{L})(\text{MeOH})_2] \cdot 2\text{H}_2\text{O}$  to methanol vapours.

| Solvent vapours | Number of cycles | Conductivity / $(\Omega \text{ cm})^{-1}$ | $t_{\text{res}} / \text{s}$ | $t_{\text{rec}} / \text{s}$ |
|-----------------|------------------|-------------------------------------------|-----------------------------|-----------------------------|
| Methanol        | 10               | $5.20 \times 10^{-8}$                     | 50                          | 540                         |



**Figure 1.** Conductivity after exposure of complex  $[\text{Mo}_2\text{O}_4(\text{L})(\text{MeOH})_2] \cdot 2\text{H}_2\text{O}$  to MeOH vapours over 10 cycles. After initial exposure, the sample was left in air to relax before being re-exposed. Measurement was carried out at 1 Hz.

Analog measurements to EtOH vapour were performed over five cycles, with a response time of 1250 s and recovery time at 1060 s.



**Figure 2.** Conductivity spectra for  $[\text{Mo}_2\text{O}_4(\text{L})(\text{MeOH})_2] \cdot 2\text{H}_2\text{O}$  in heating (a) and cooling (b) runs, and (c) temperature dependence of DC conductivity ( $\log(\sigma_{\text{DC}})$  vs.  $1000/T$ ) for both runs (red circle—heating, blue circle—cooling).

### CONCLUSION

The dinuclear molybdenum(VI) complex  $[\text{Mo}_2\text{O}_4(\text{L})(\text{MeOH})_2] \cdot 2\text{H}_2\text{O}$  was successfully synthesized and characterized.

#### Selective methanol sensing:

The complex demonstrated selective vapour sensing properties towards MeOH. Electrical conductivity increased significantly to  $5.2 \times 10^{-8} (\Omega \text{ cm})^{-1}$  upon exposure to MeOH. Response and recovery times were fast, at 50 s and 540 s, respectively, representing great performance at RT. Reproducibility tests over 10 sensing cycles confirmed the material's stability and suitability for practical sensor applications.

#### Temperature-dependent conductivity:

The complex exhibited a temperature-dependent increase in electrical conductivity, consistent with semiconducting behaviour. At 200 °C, the conductivity was measured at  $1.91 \times 10^{-10} (\Omega \text{ cm})^{-1}$ . Both the conductivity value and the activation energy of  $58 \text{ kJ mol}^{-1}$  are in close agreement with those reported for related molybdenum-based systems.<sup>4,6</sup>

#### Dual functionality:

This research highlights the dual functionality of the synthesized molybdenum complex, showing promise for both sensor and electronic applications.