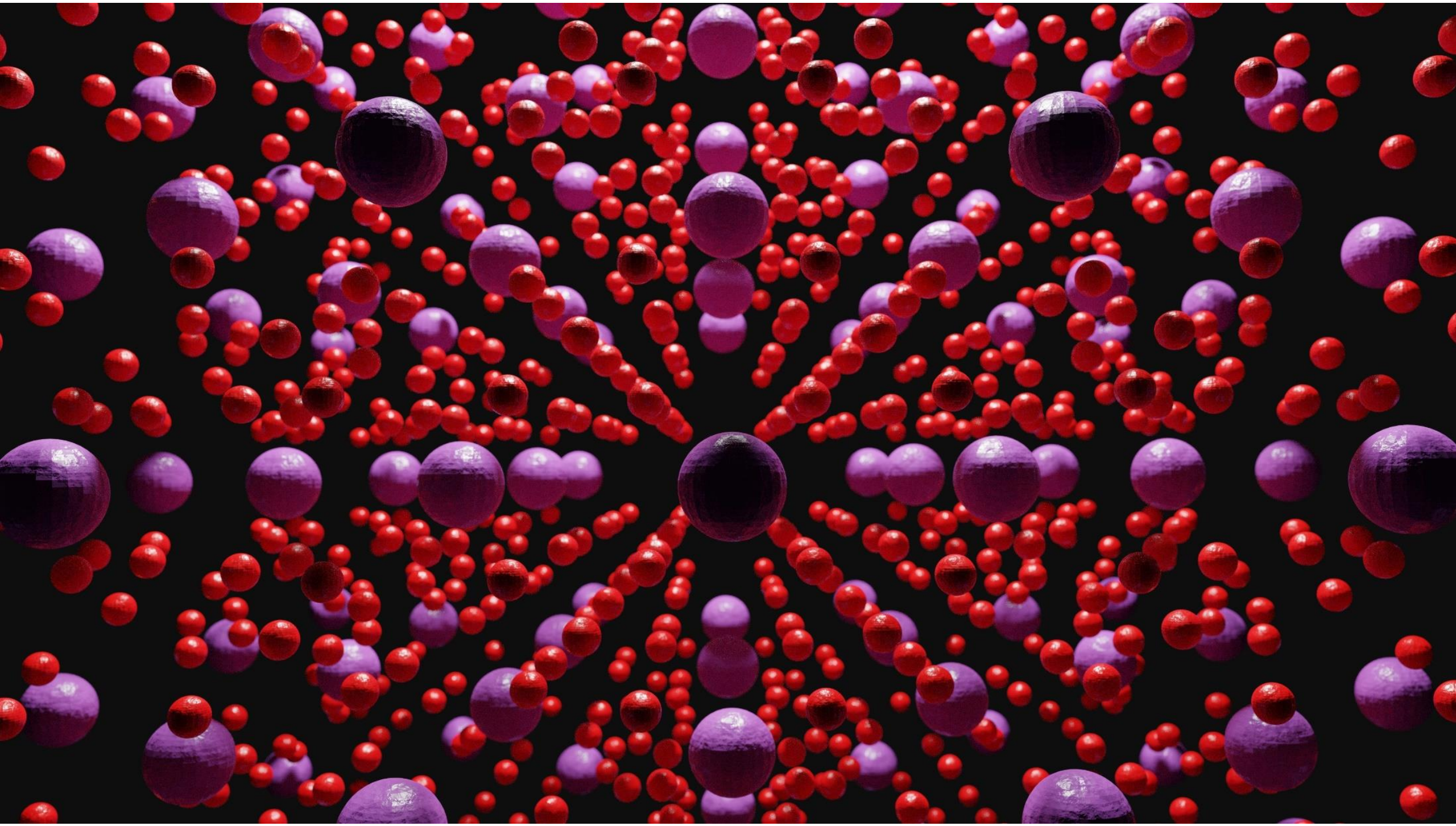
Anomalous lattice expansion of Y^{3+} and Sc^{3+} co-doped δ-Bi_2O_3 solid electrolytes for solid oxide fuel cells

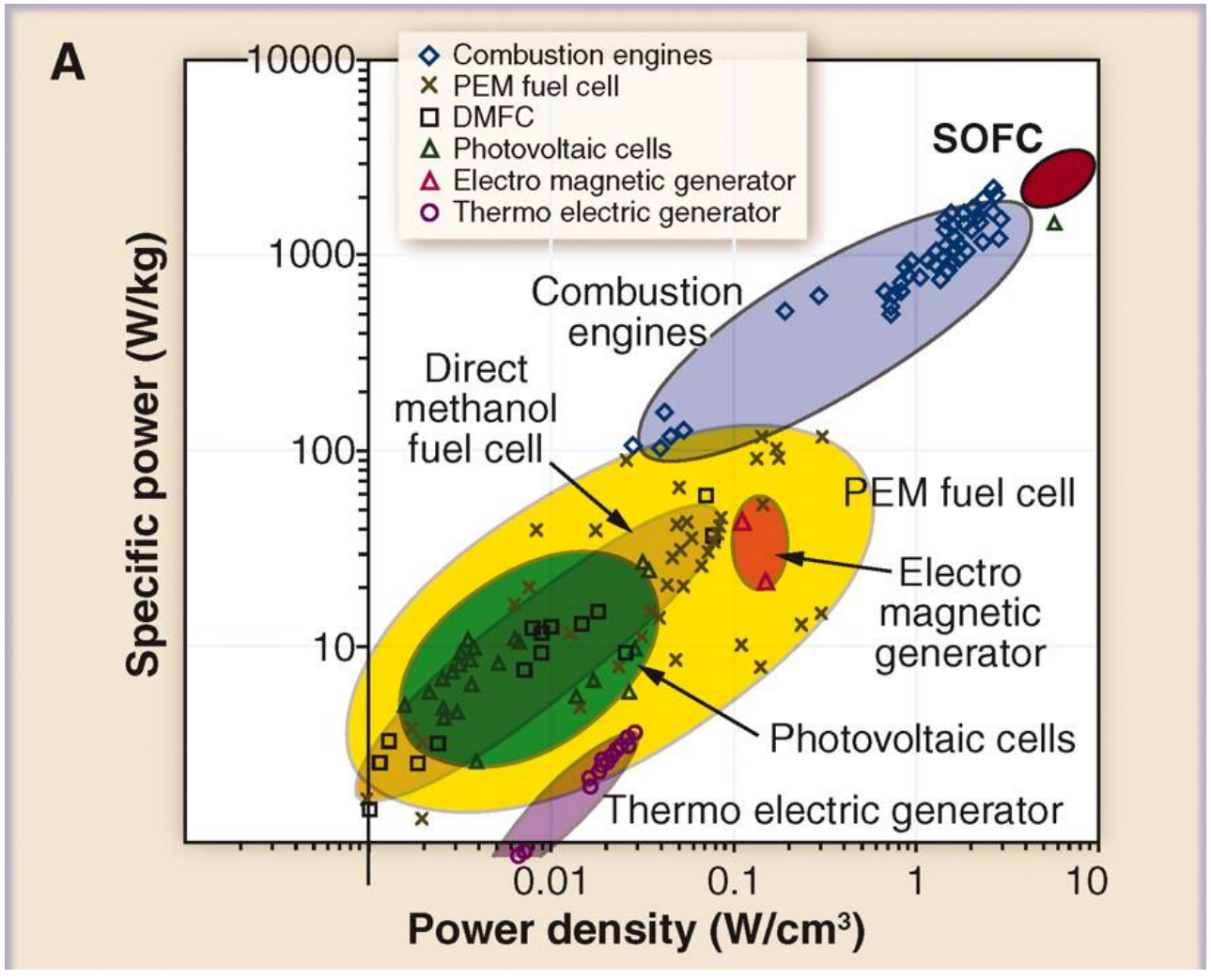


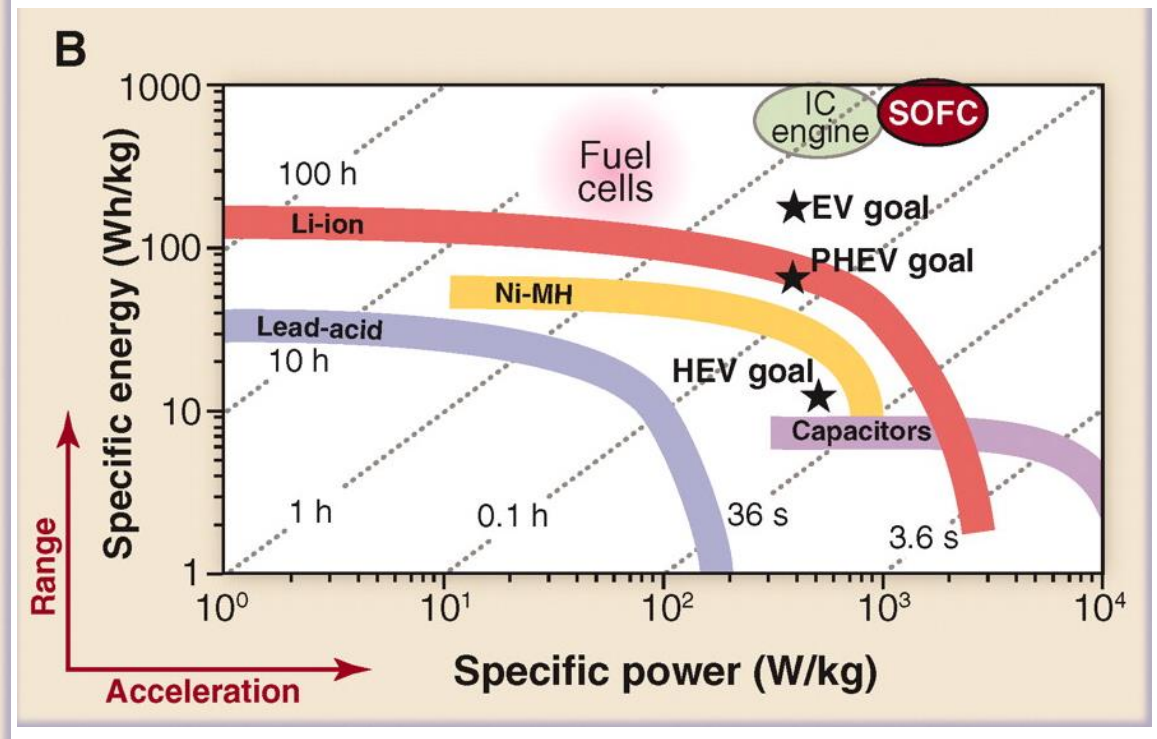
Darren Fynn[1,2], **Caren Billing**[1], **David Billing**[1,2]

[1] *Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Private Bag X3, Johannesburg, 2050, South Africa*
[2]*DSI-NRF Centre of Excellence in Strong Materials, University of the Witwatersrand, Private Bag X3, Johannesburg, 2050, South Africa*

Why solid oxide fuel cells (SOFCs)?

The search for cleaner energy





Science. **2011**, *334* (6058), 935–939.

High specific energy, specific power and power density → outperforms any other system currently available

What are SOFCs?

- Electrochemical energy conversion devices
- **Converts chemical energy from a fuel** (e.g. hydrogen, biomass, methane and other hydrocarbons, natural gas and coal) **directly into electrical energy** (*NO combustion*)

Do not require combustion as an intermediate step → higher fuel conversion efficiencies compared to combustion-based processes → can produce a given amount of energy using less fuel ∴ have lower CO_2 emissions and is more environmentally friendly

Nissan e-Bio Fuel Cell:
< 5 L/100 km
(bioethanol)

Nissan NV200 Combi:
9.8 L/100km
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https://global.nissannews.com/en/releases/nissan-unveils-worlds-first-solid-oxide-fuel-cell-vehicle?source=nng&lang=en-US

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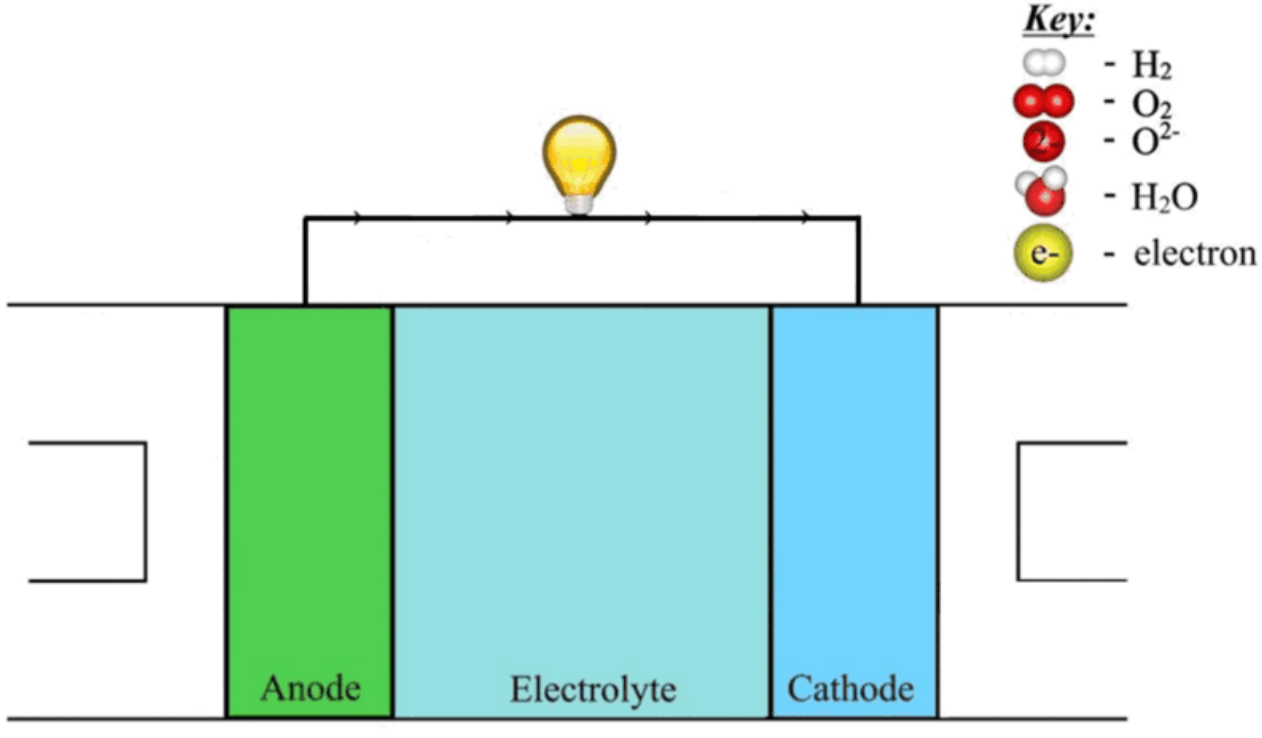
How do SOFCs work?



Energy Environ. Sci. **2016**, *9*, 1602.
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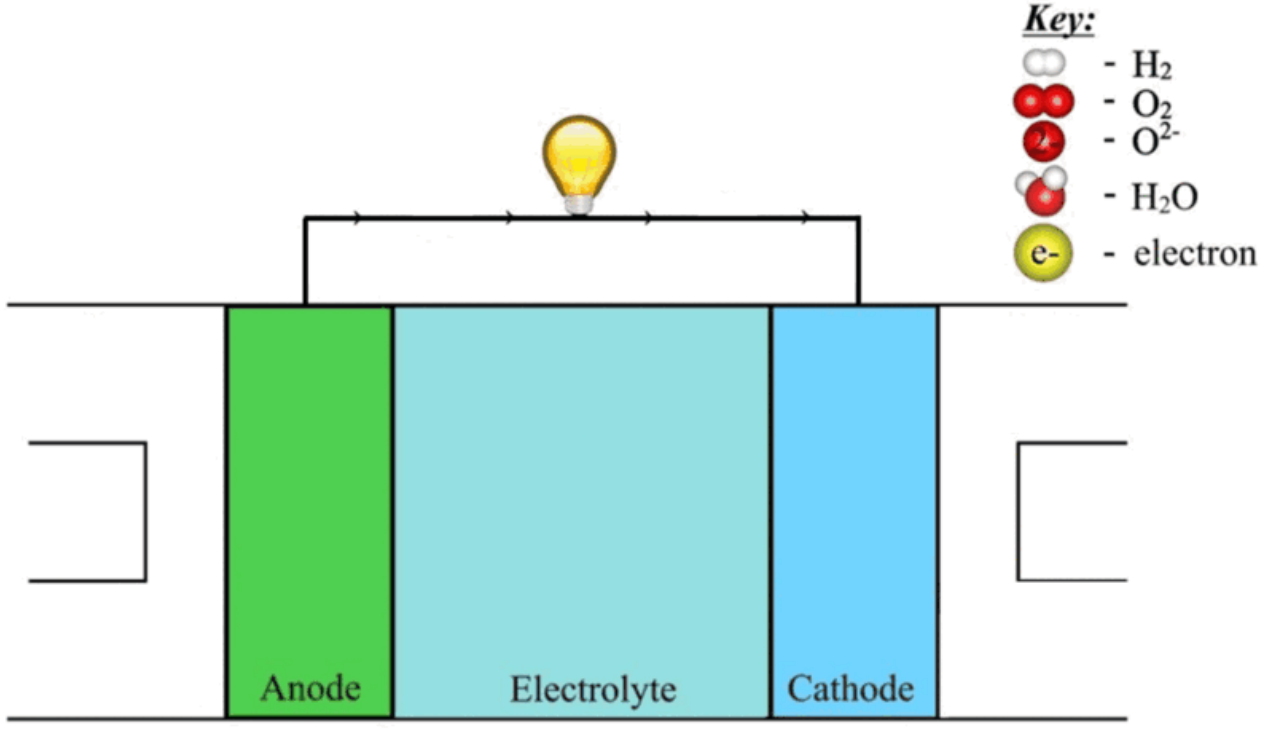

Most individual cells are small so SOFCs are usually arranged in series in a fuel cell stack in order to produce larger quantities of power

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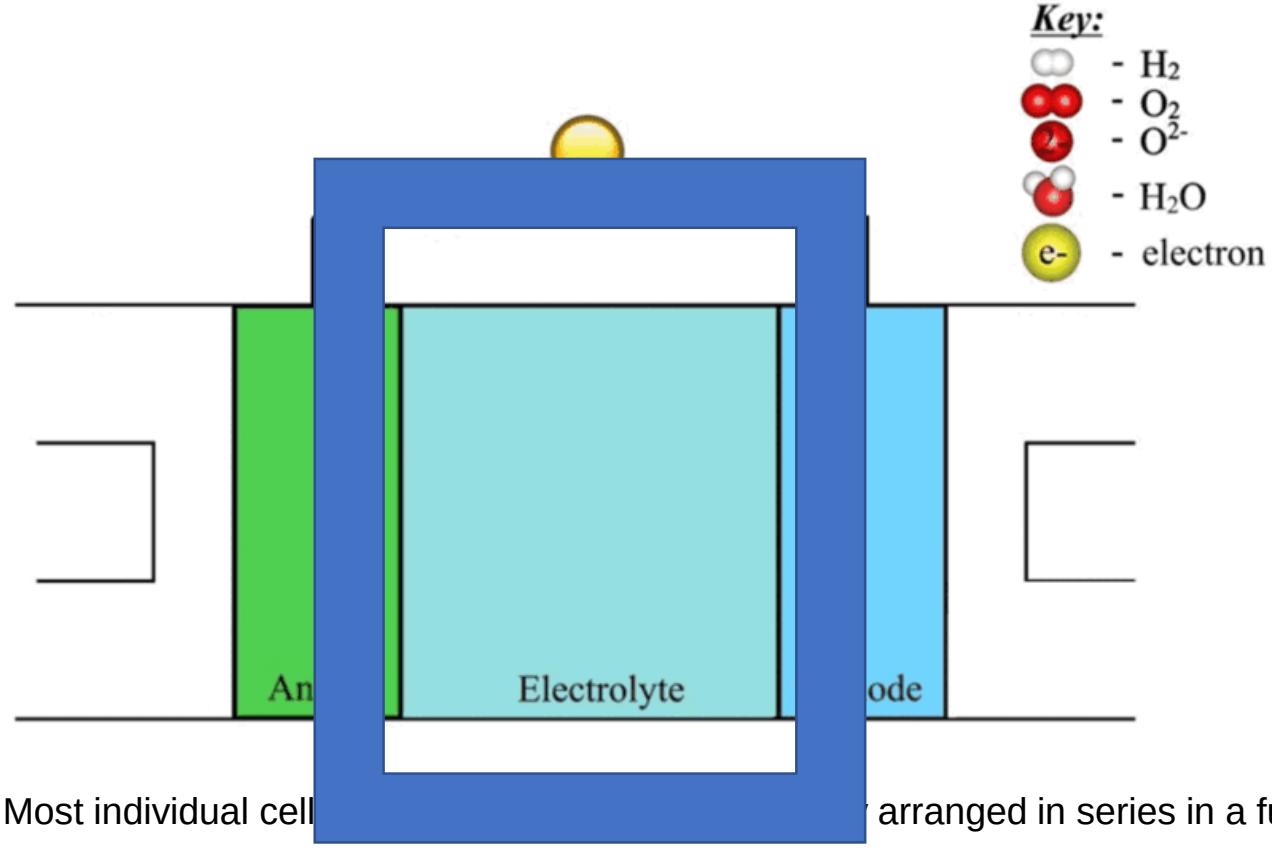

Most individual cell arranged in series in a fuel cell stack in order to produce larger quantities of power

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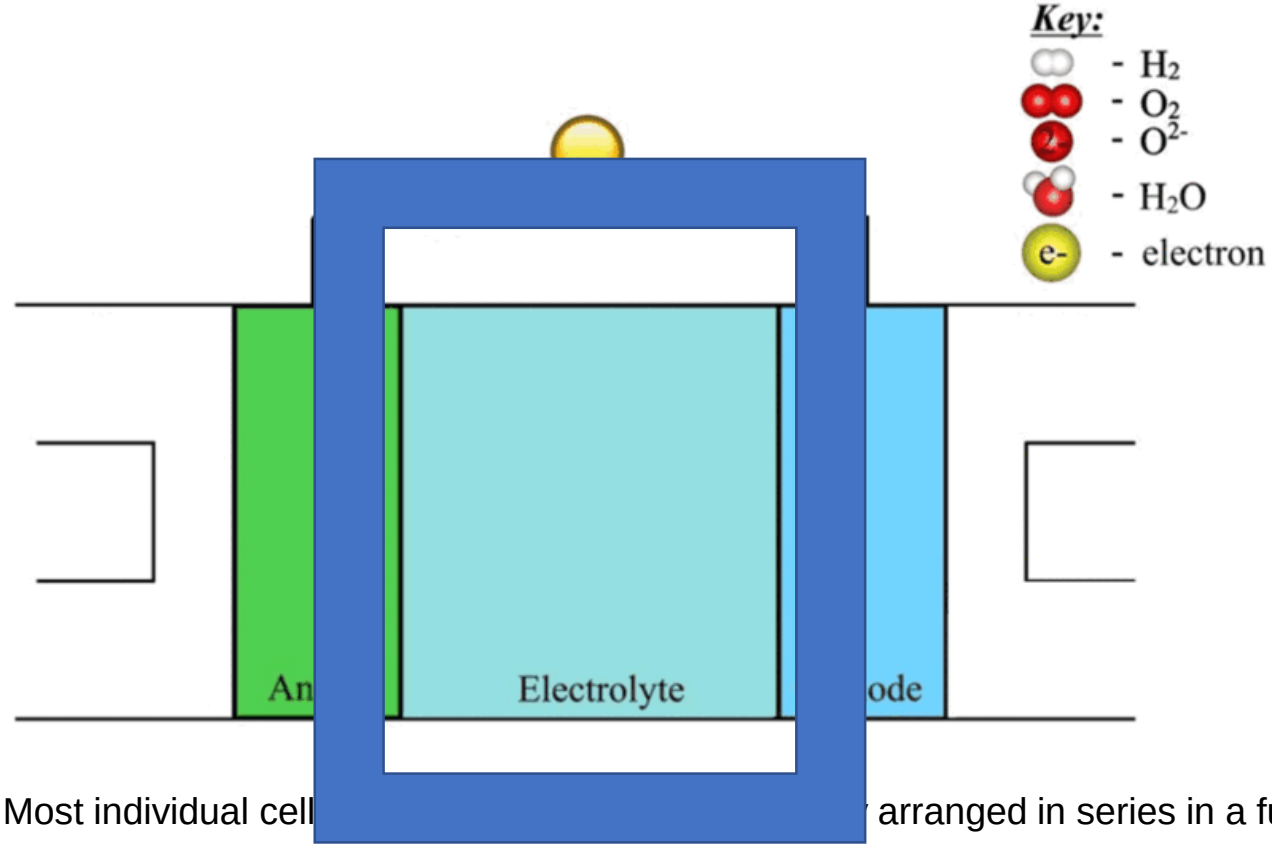

Most common electrolyte in SOFCs is yttria stabilised zirconia (**YSZ**) but requires high operating temperature (~ 1000 °C)

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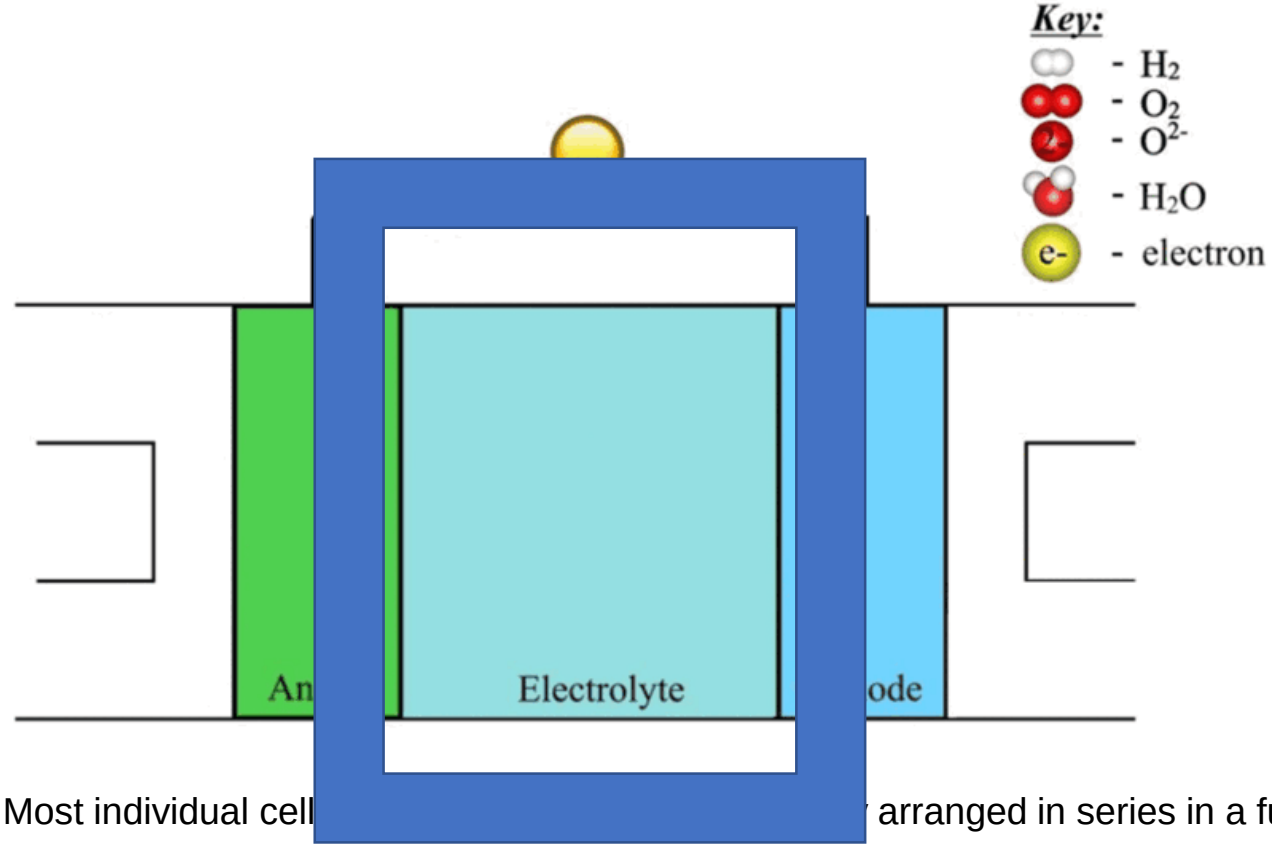

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Significant research to find electrolytes that can work at lower temperatures

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δ-Bi_2O_3

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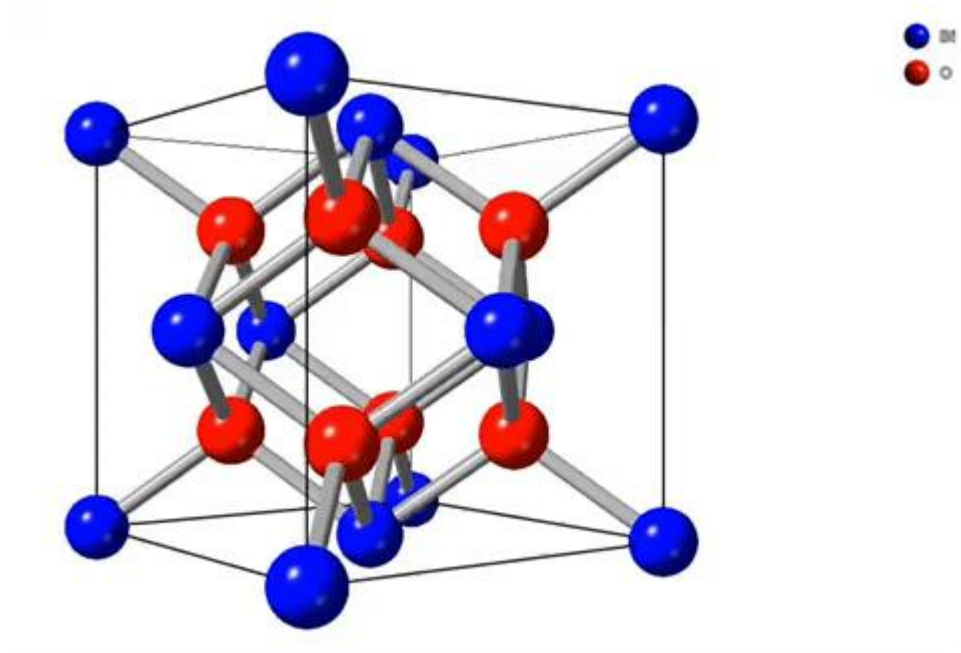
- CCP array of Bi^{3+} cations (**blue**) with oxide ions (**red**) in tetrahedral holes (25% of normal anion sites are vacant ***without any doping***)



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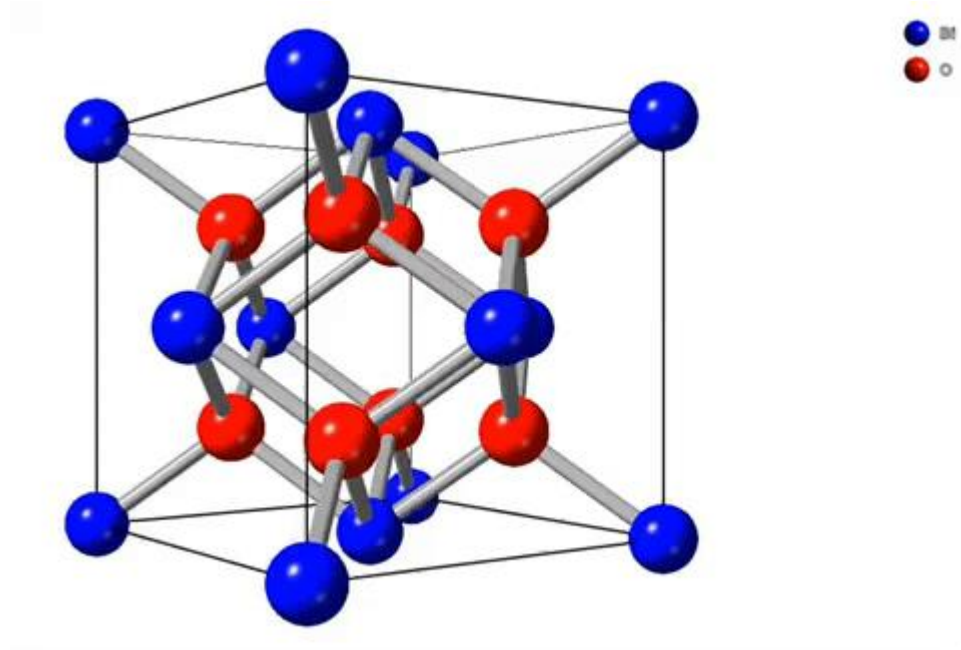

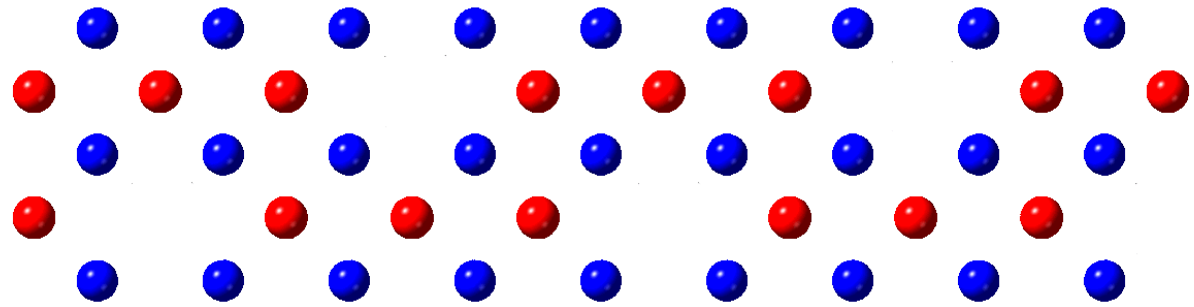

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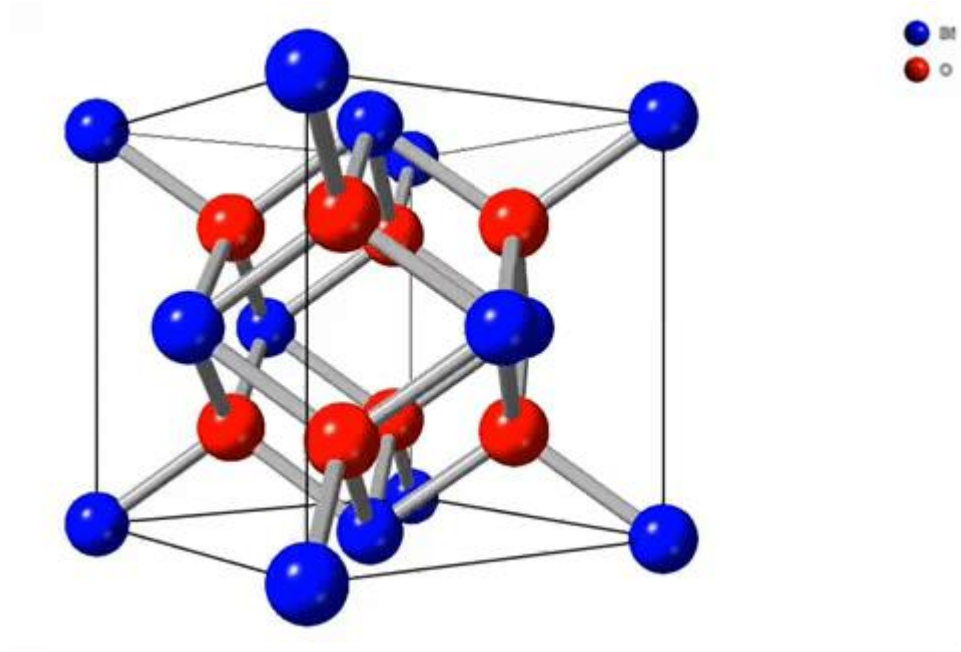
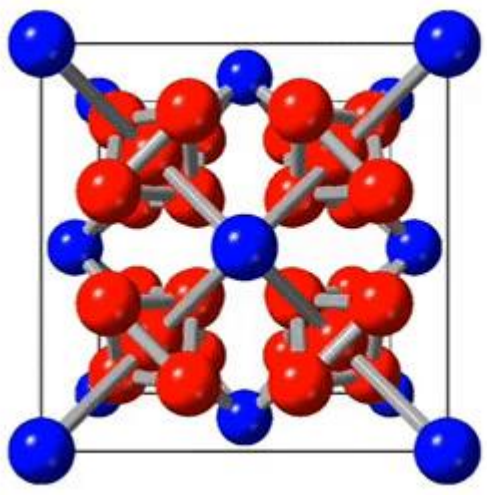
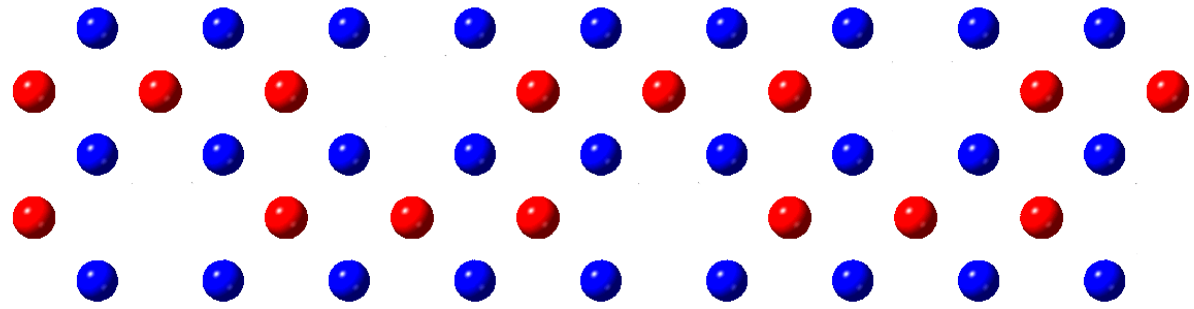
- neutron diffraction reveals an even more complicated disorder of the oxide ion sub-lattice with oxide ions occupying interstitial sites







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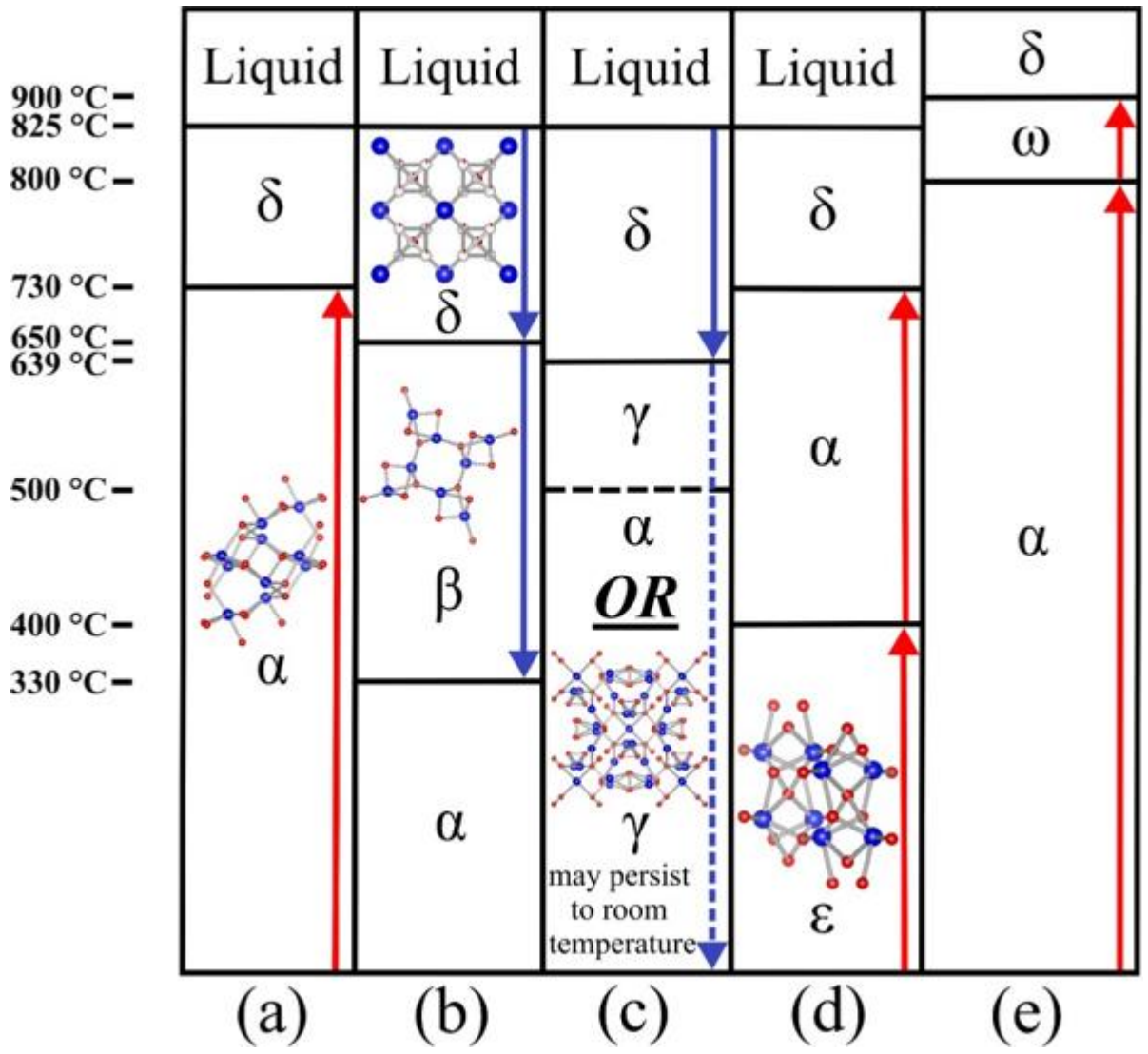
Problem with δ-Bi_2O_3



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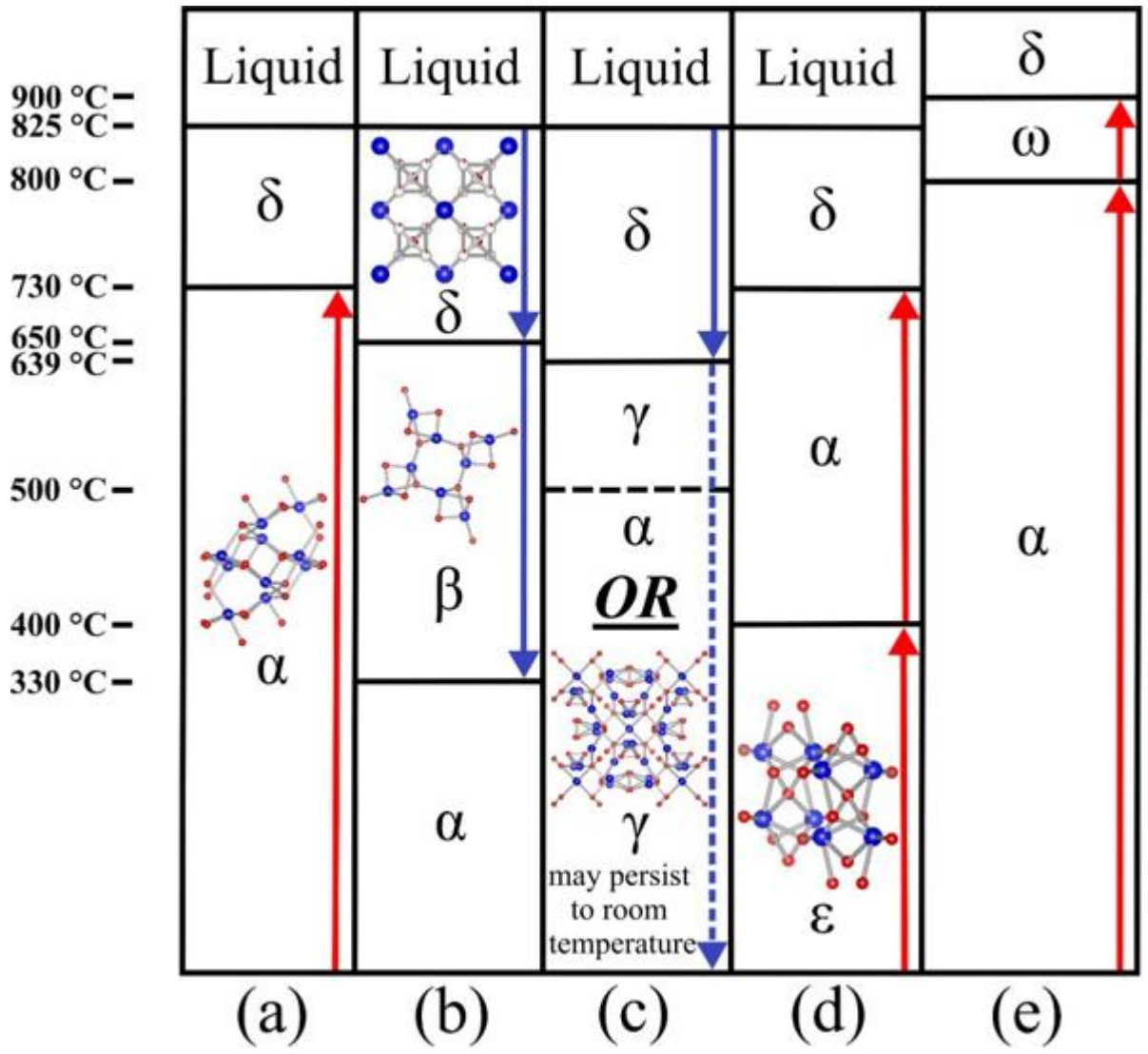

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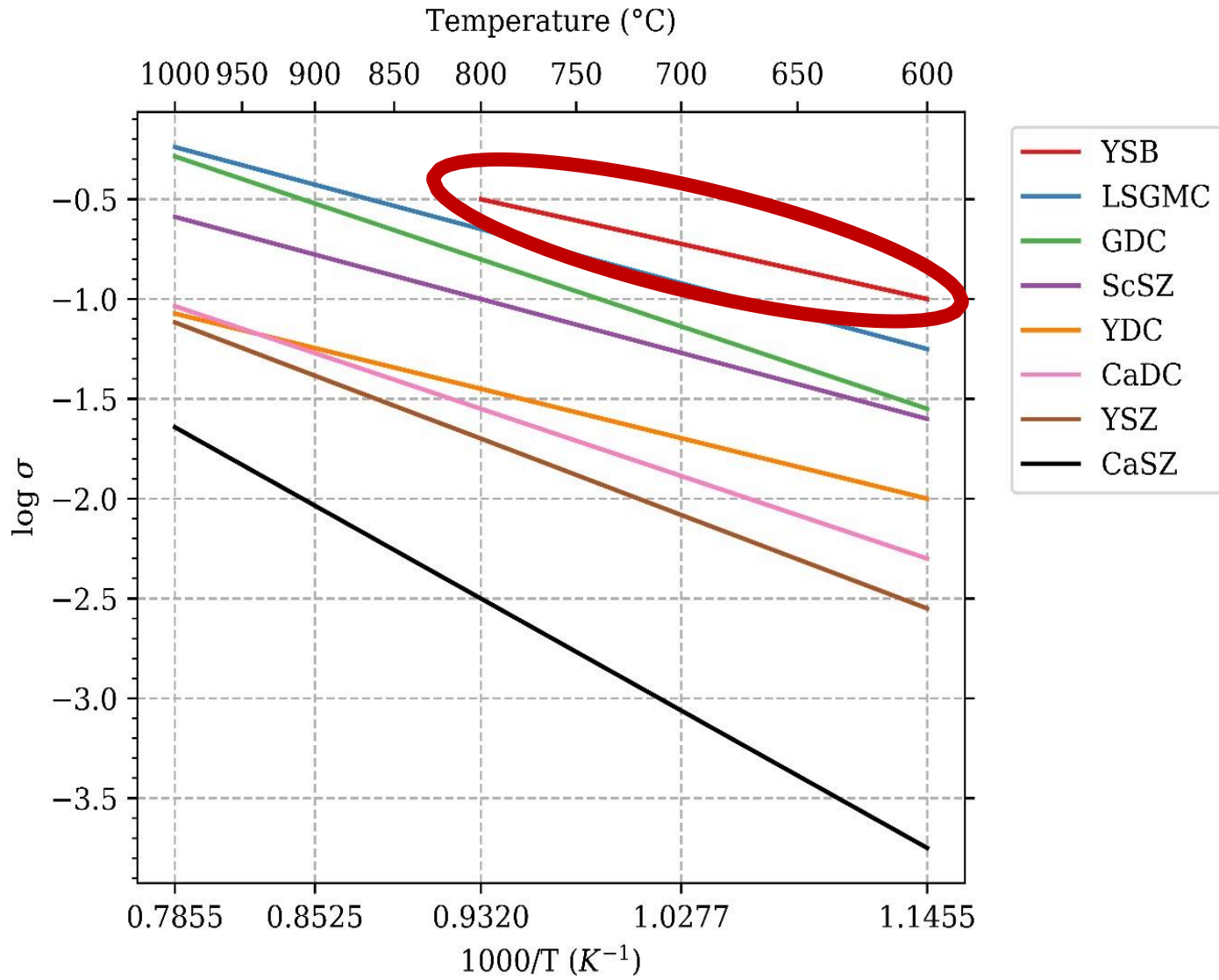

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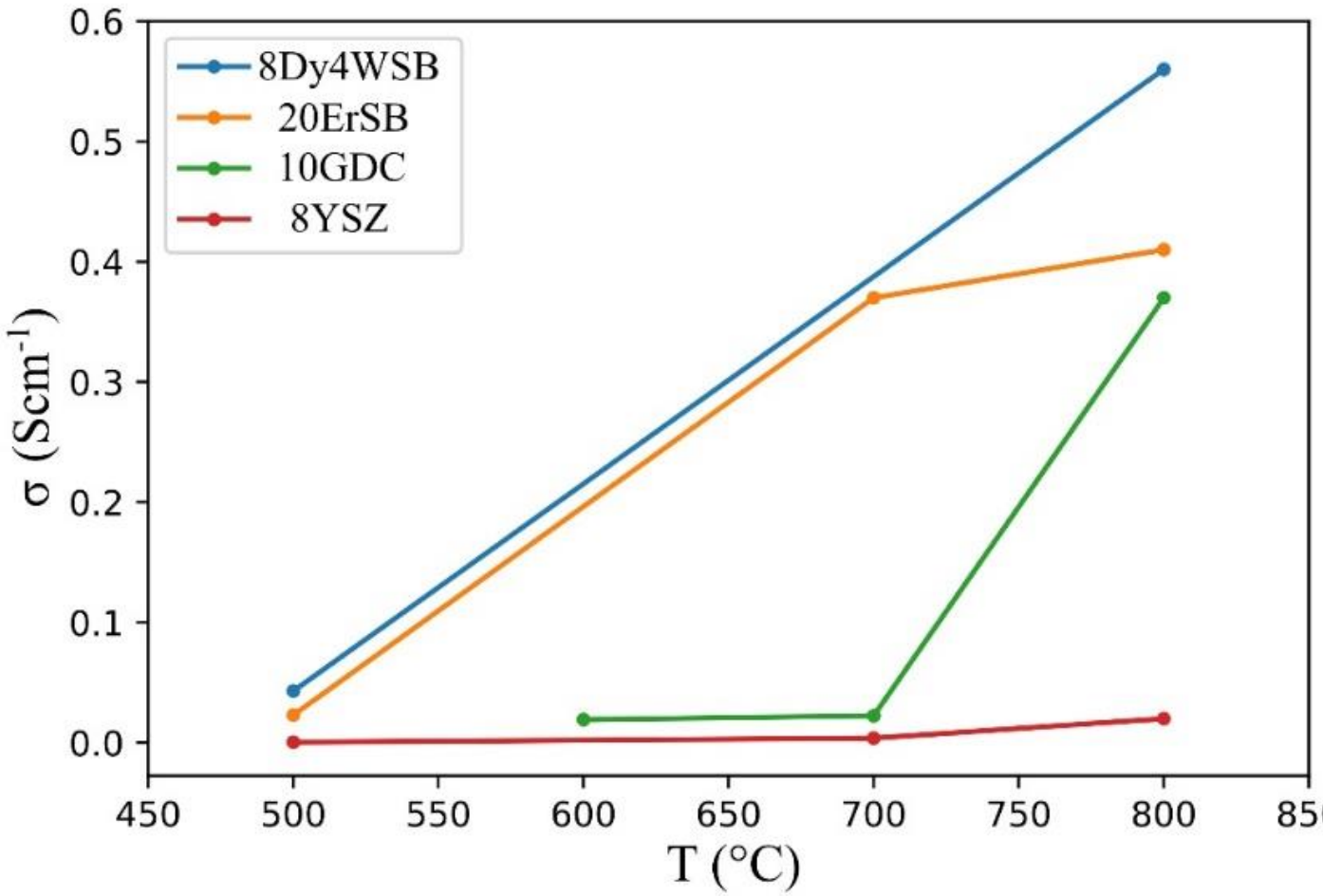

Generally results in more stable materials and requires lower total dopant concentrations than singly-doped systems, therefore have higher ionic conductivities

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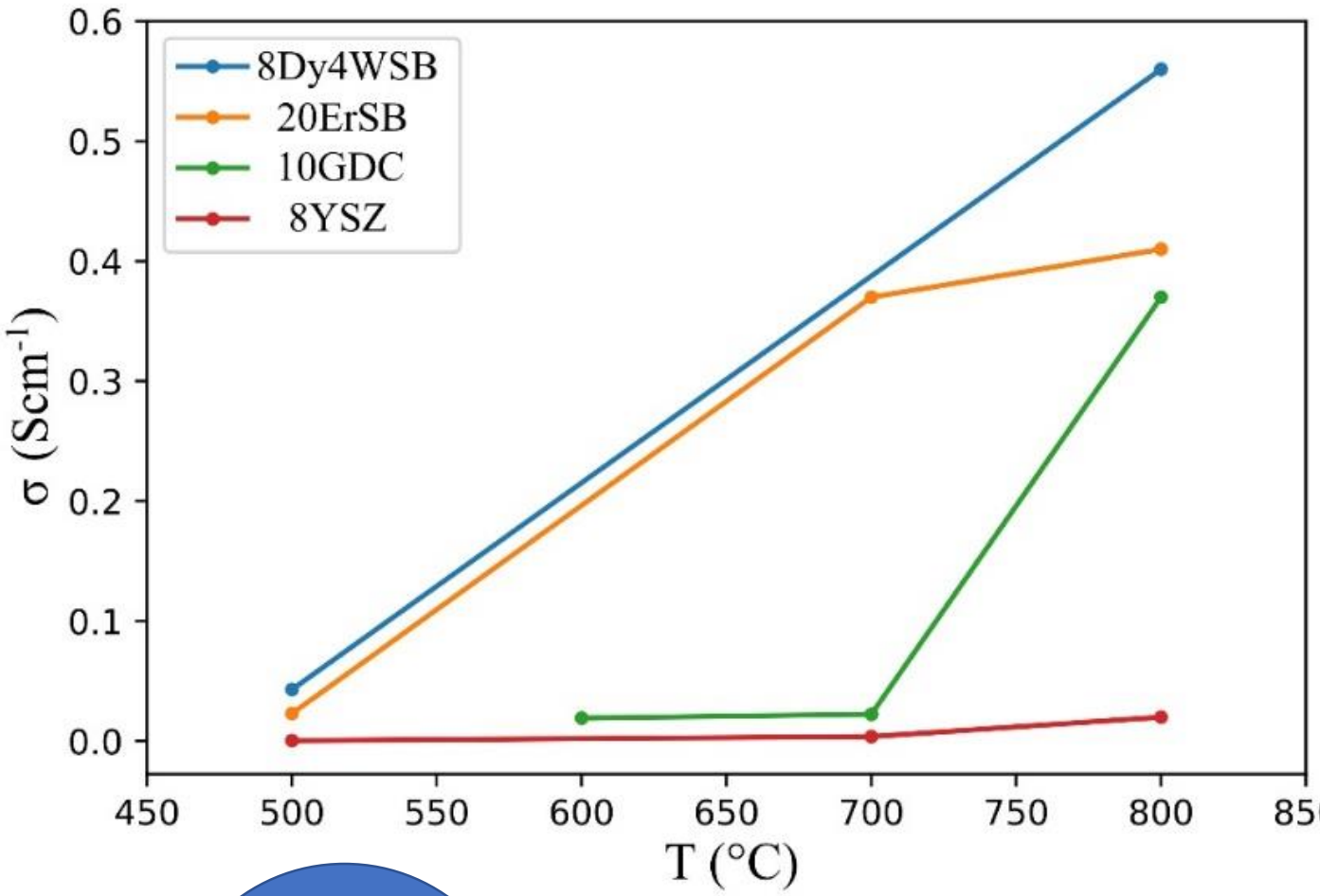

A

B

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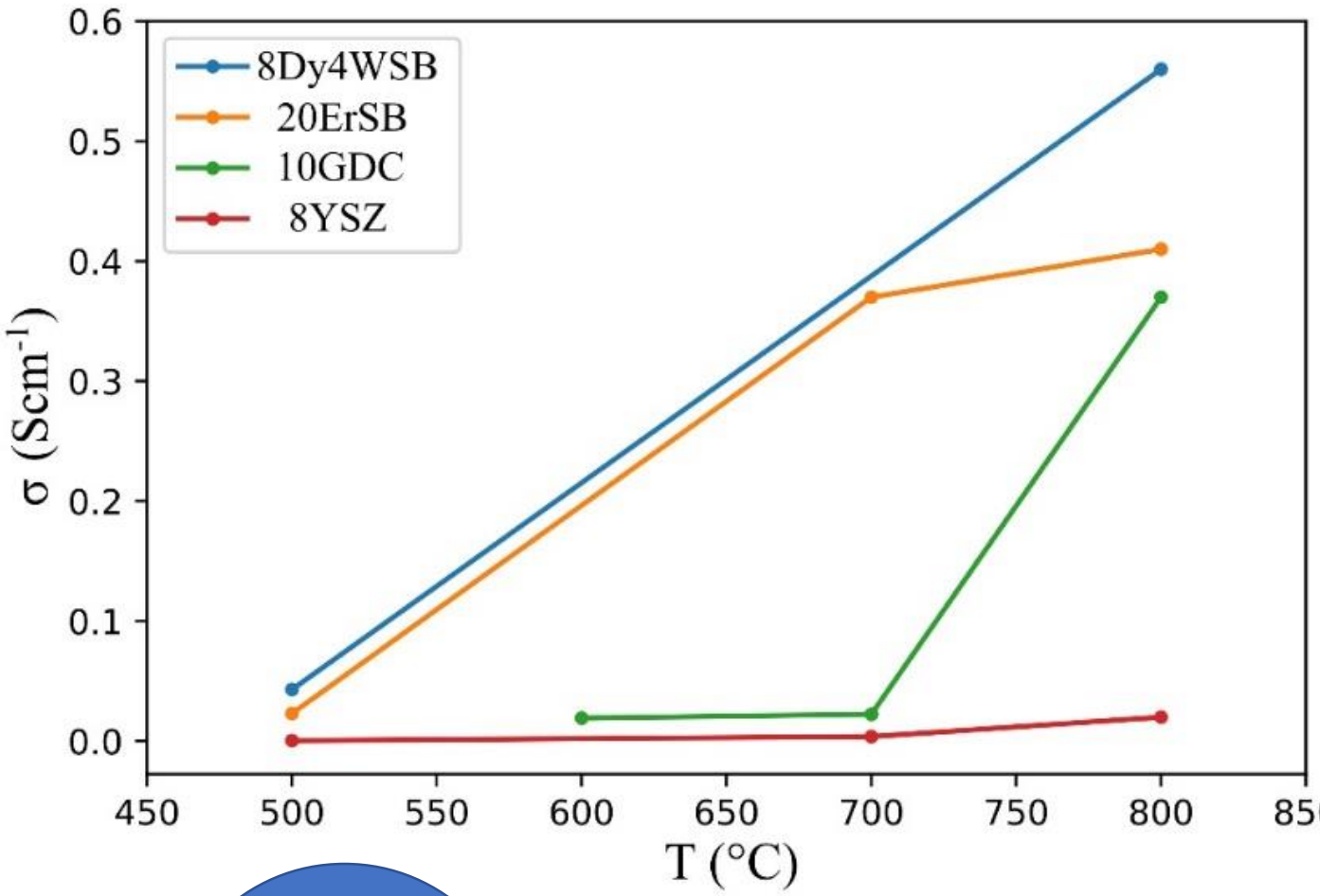

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(↑[A] ↓[B]) Lattice parameter and ionic conductivity **INCREASES**

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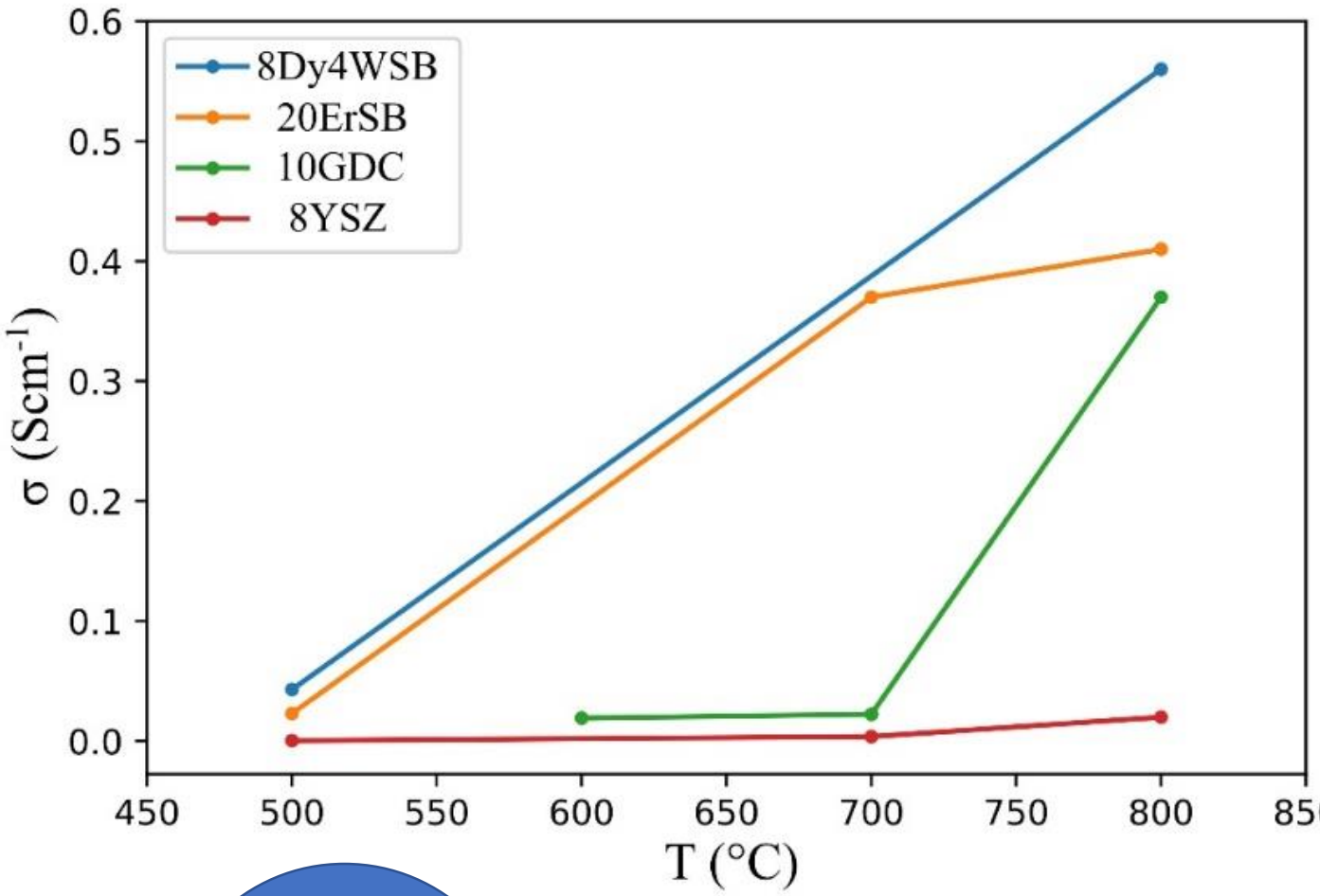

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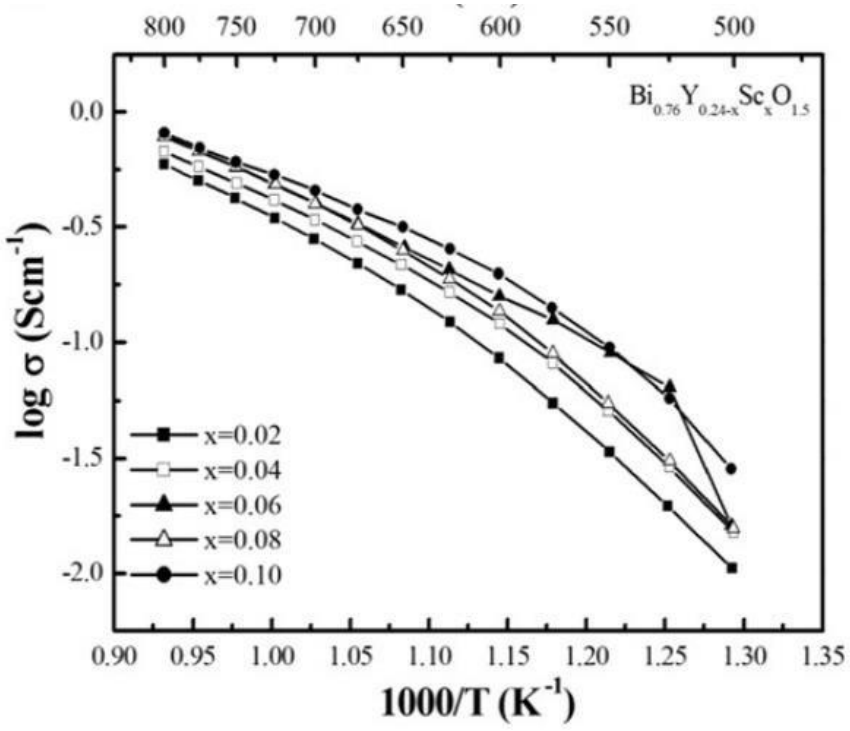
The Y^{3+} and Sc^{3+} co-doped system



J. Power Sources **2012**, *218*, 106

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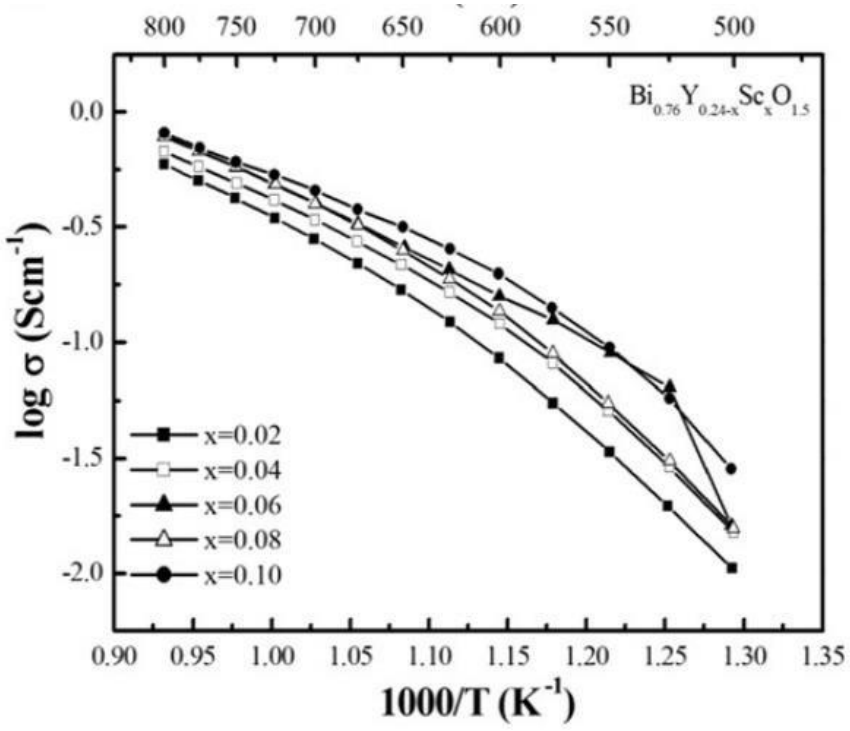

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We don't know!
Insufficient structural investigation to determine a mechanism for lattice expansion

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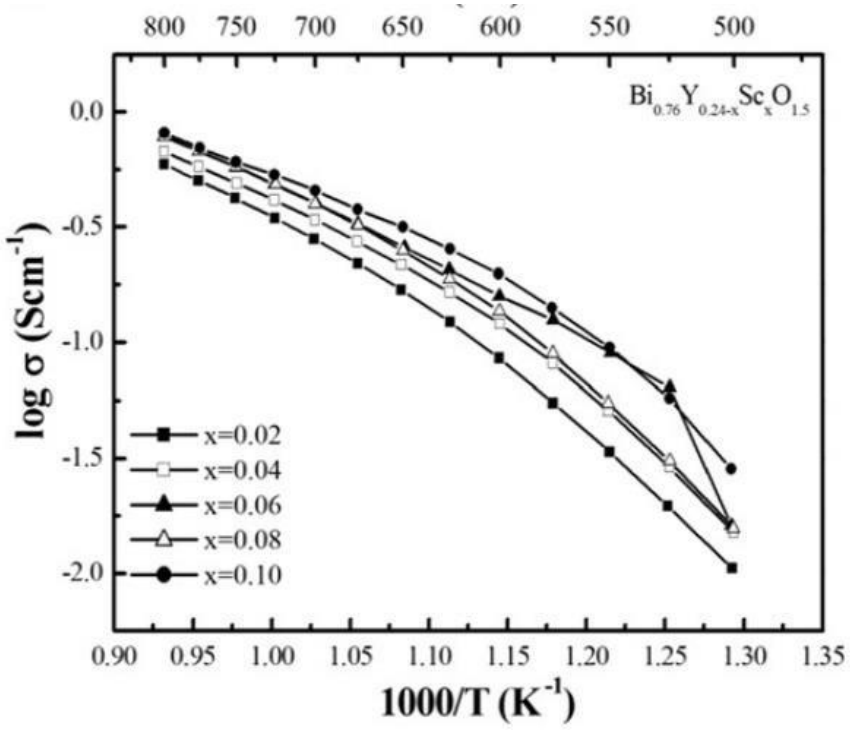

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Sc^{2+} DOES NOT EXIST

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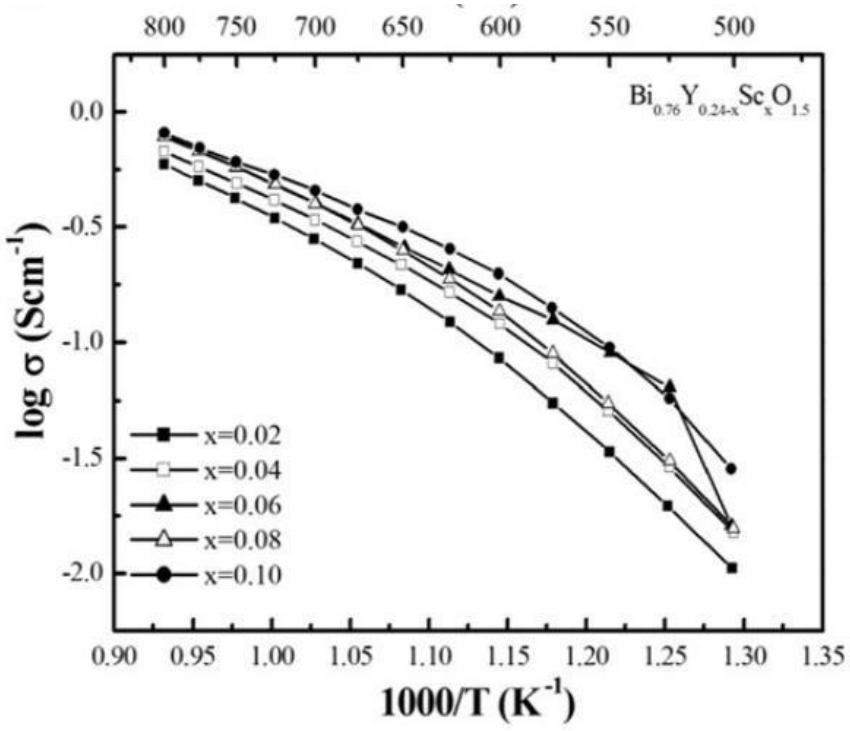

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Used a high total dopant concentration (24 mol%)

Aims and objectives

Co-dope Bi_2O_3 with Y^{3+} and Sc^{3+} at a lower total dopant concentration (20 mol%)

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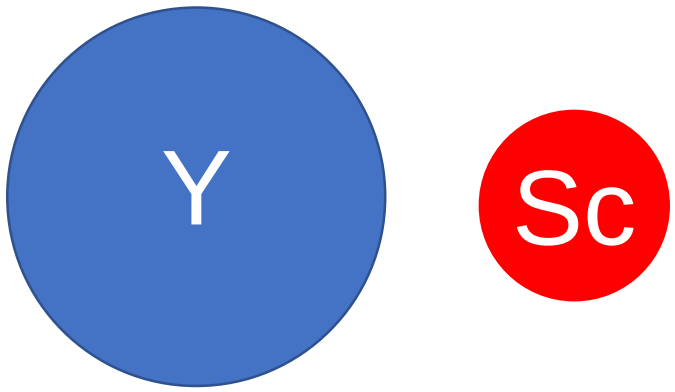
Co-dope Bi_2O_3 with Y^{3+} and Sc^{3+} at a lower total dopant concentration (20 mol%)

Provide more in-depth structural characterisation to determine the mechanism of lattice expansion

Experimental



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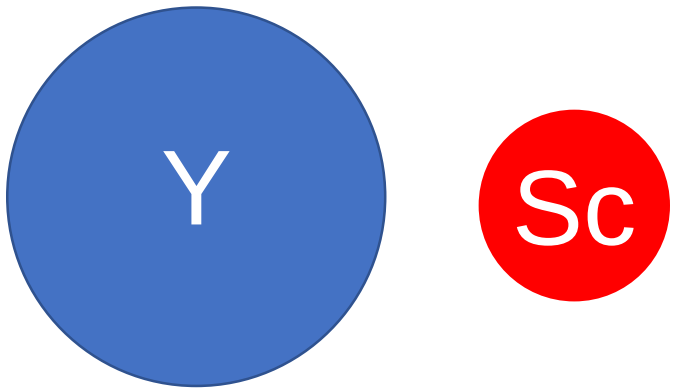

20 mol% total dopant concentration

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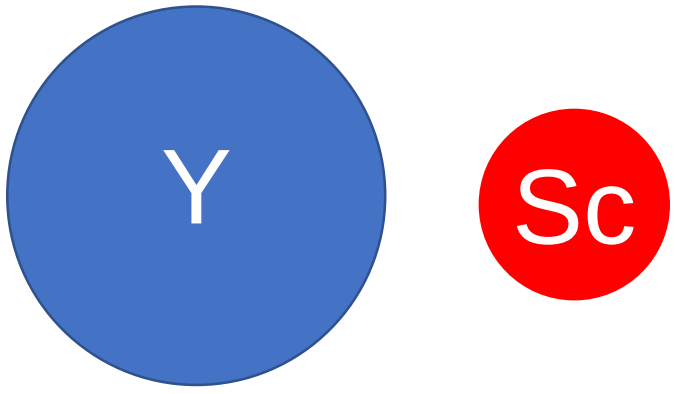

20 mol% total dopant concentration

2.5 mol% Sc(III)
5 mol% Sc(III)
7.5 mol% Sc(III)
10 mol% Sc(III)

Experimental

Y

Sc

20 mol% total dopant concentration

2.5 mol% Sc(III)
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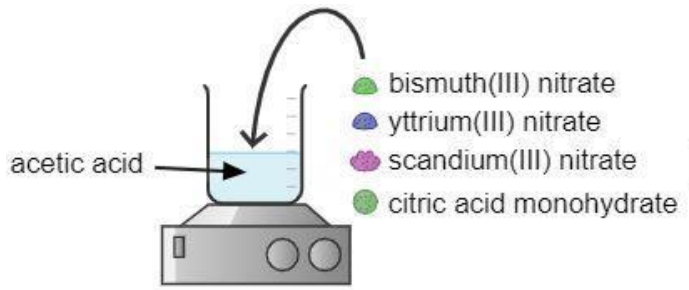

Experimental

Y

Sc

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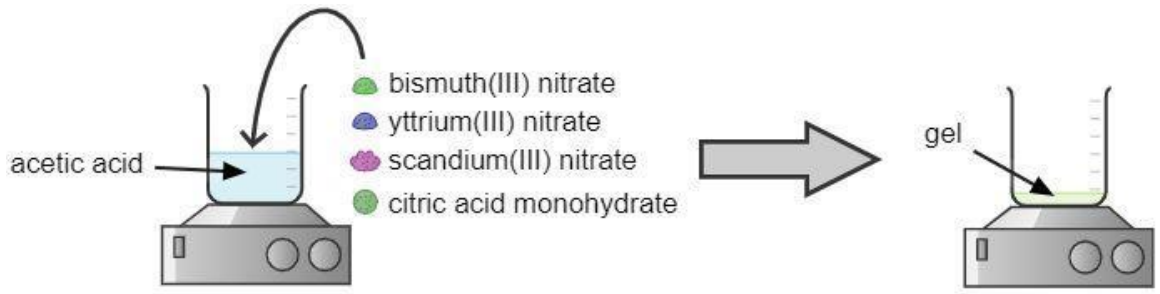

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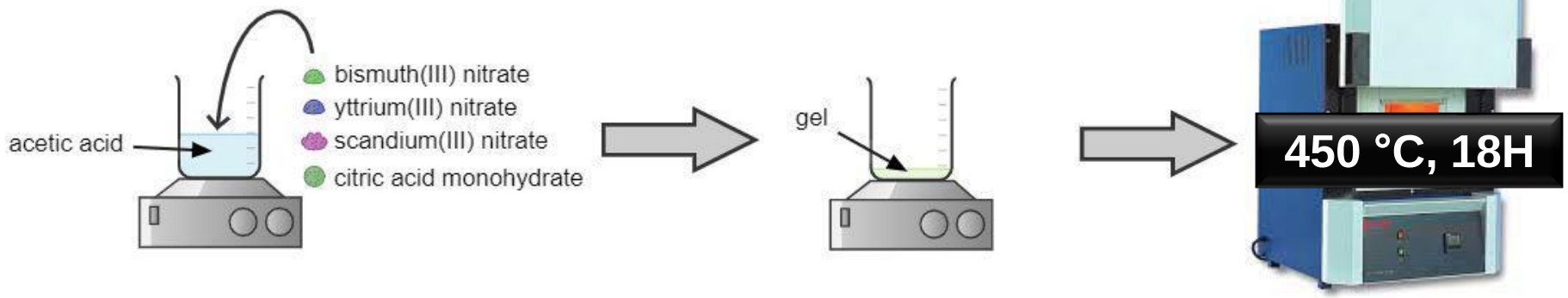

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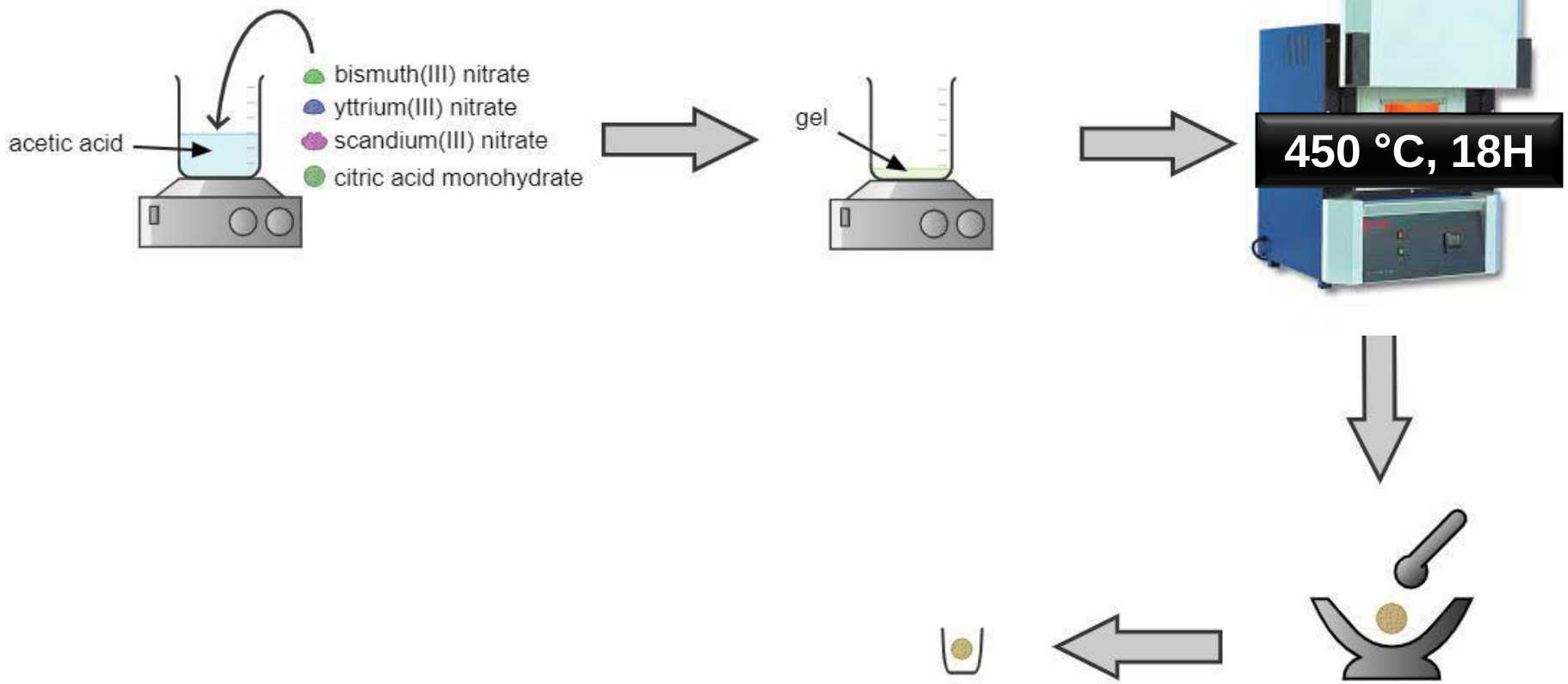

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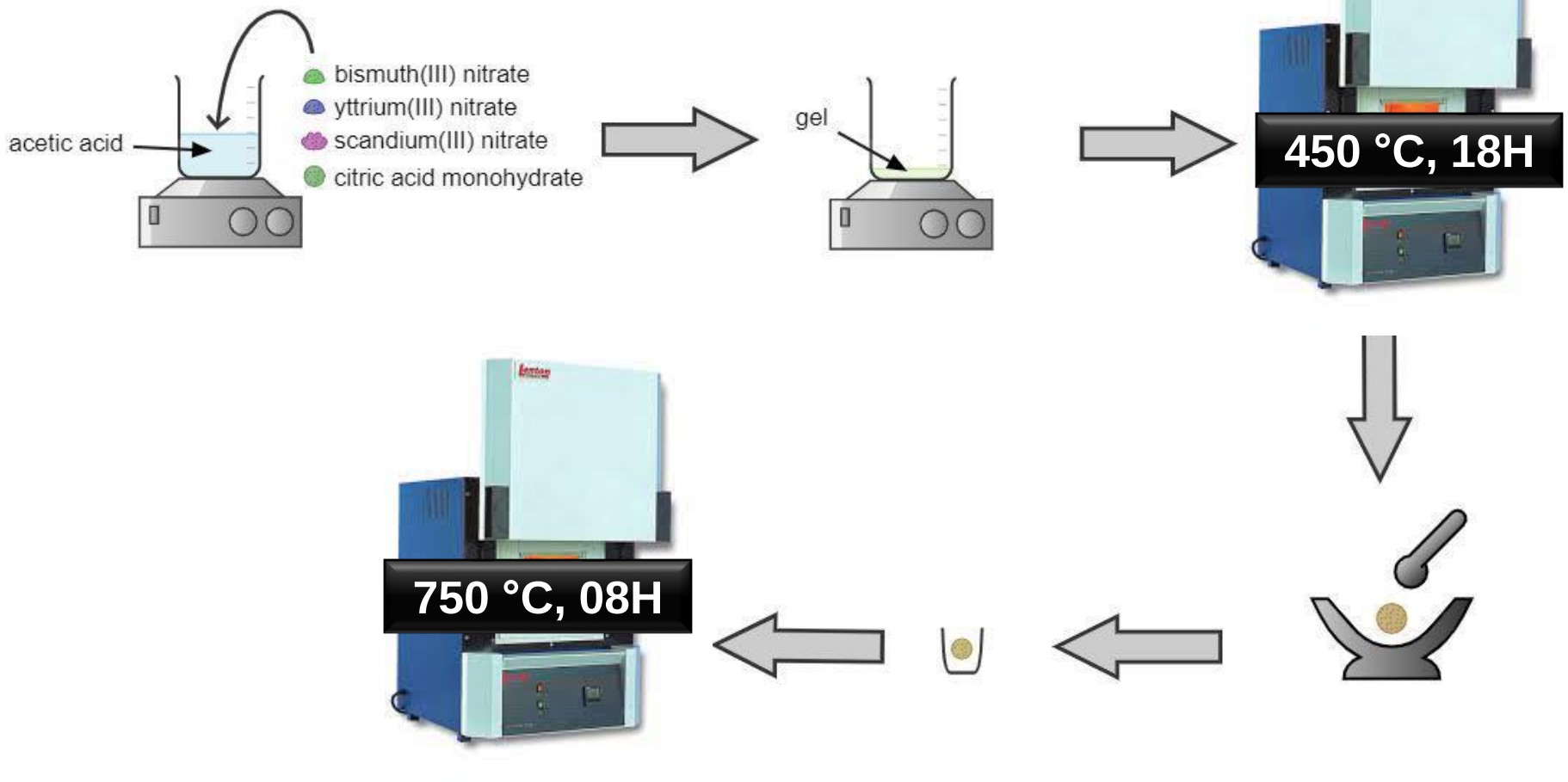
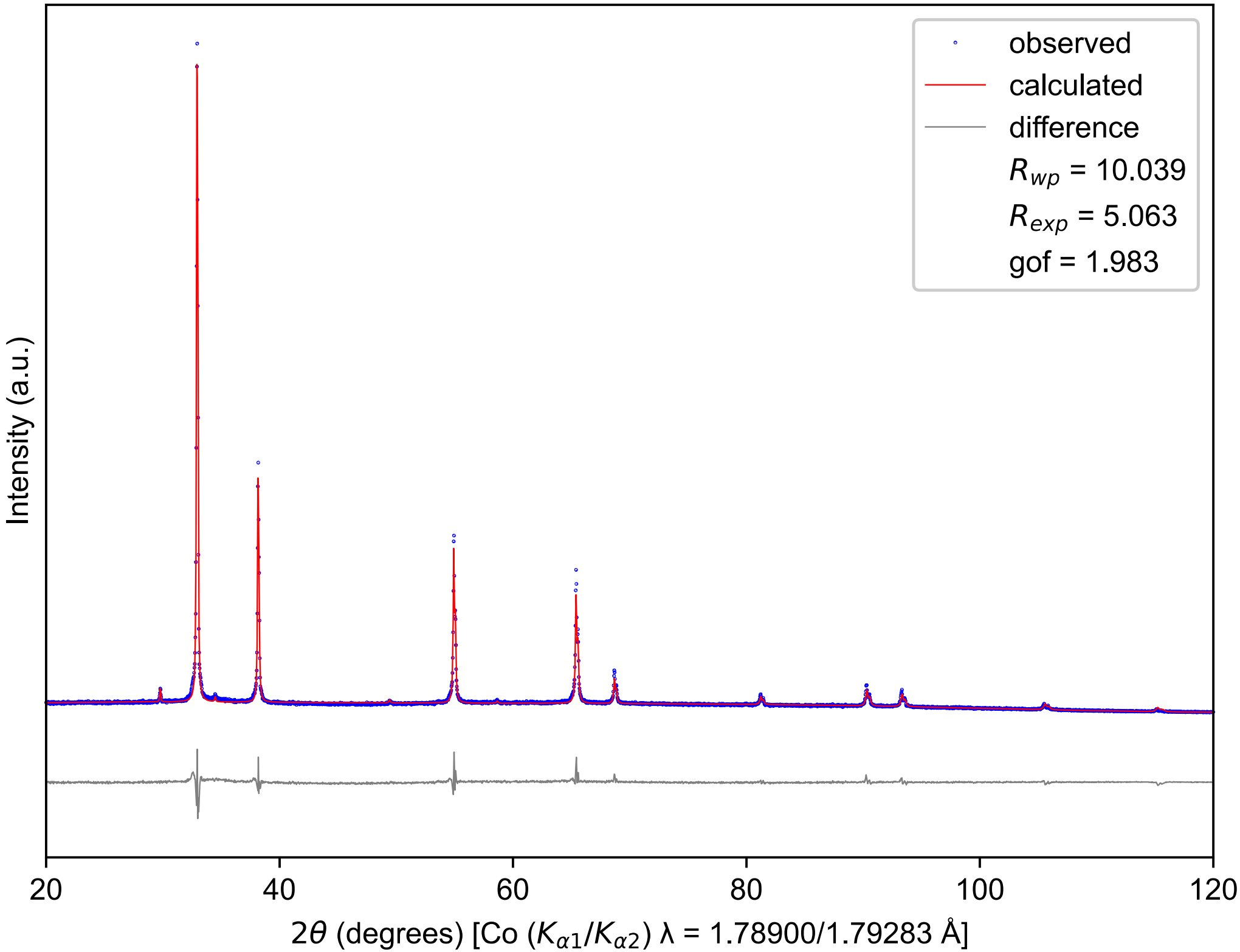


Rietveld refinements of laboratory powder X-ray diffraction data



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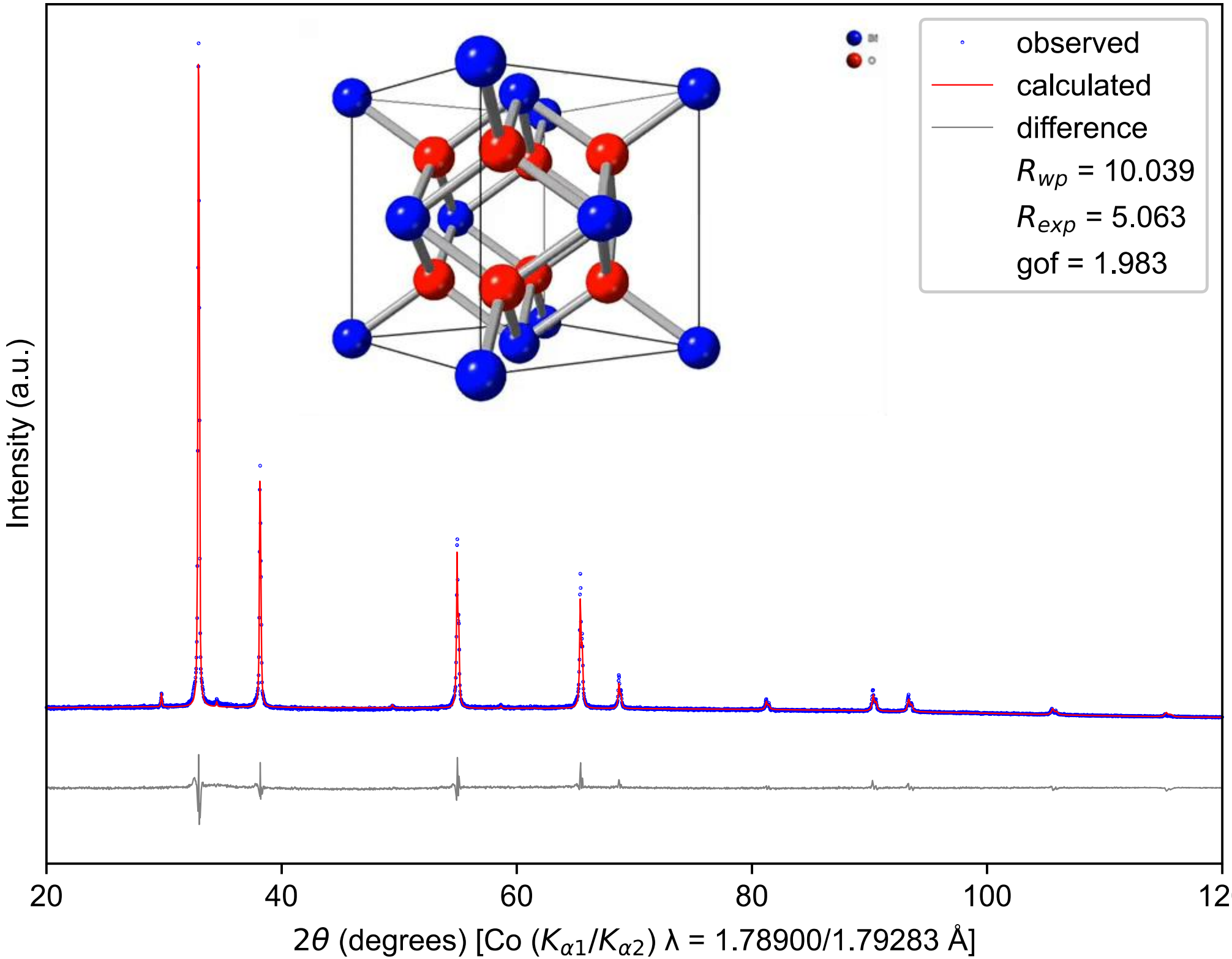

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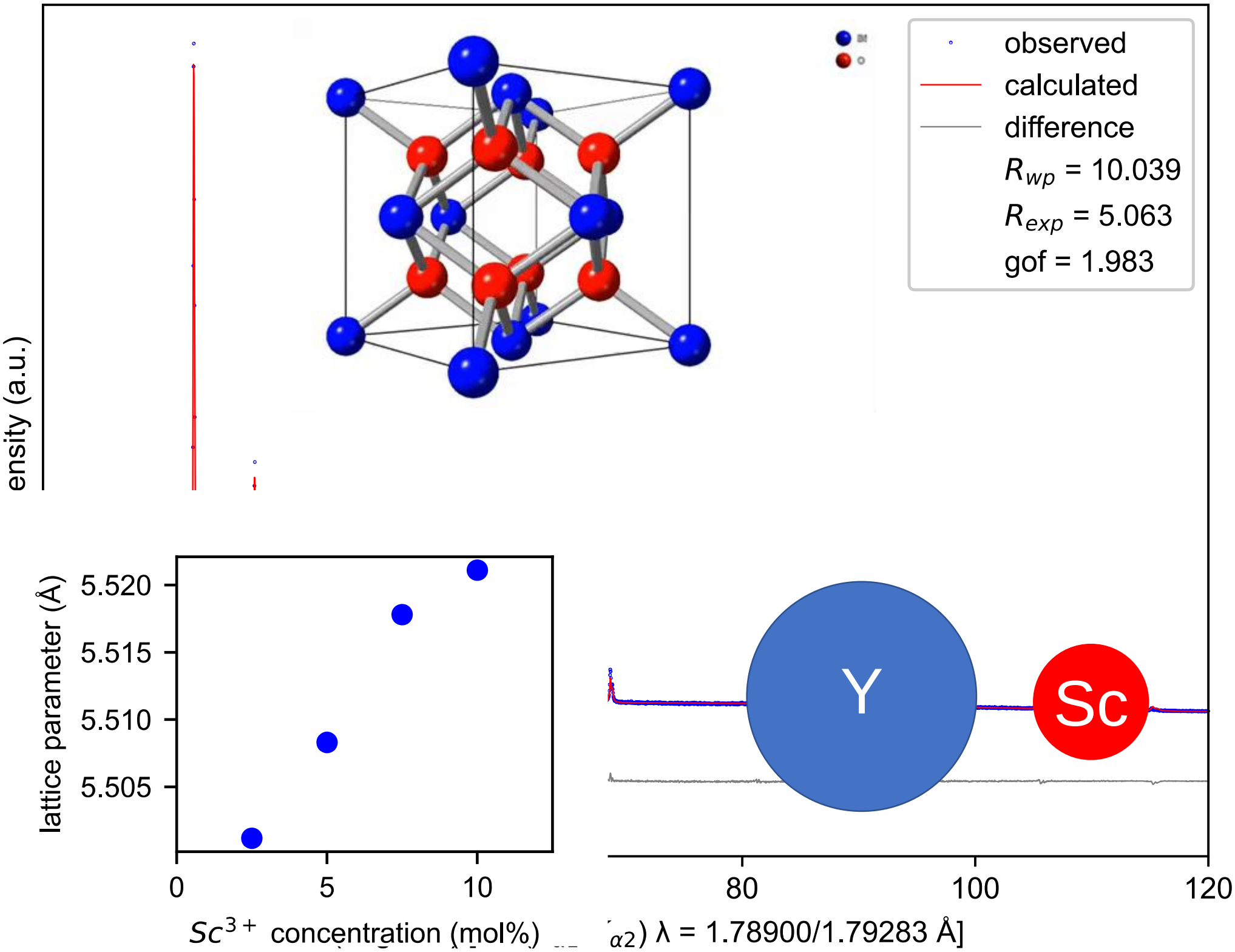

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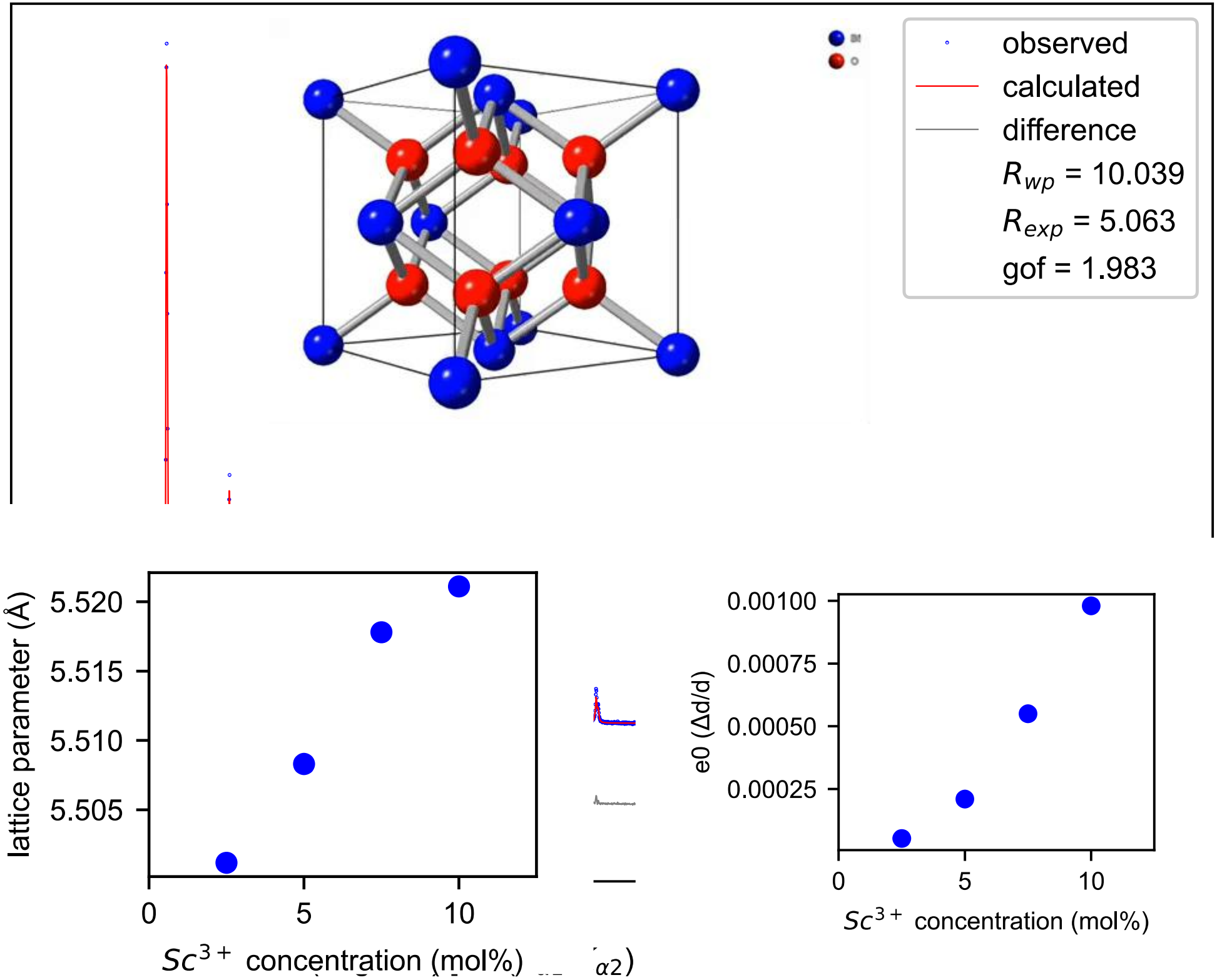
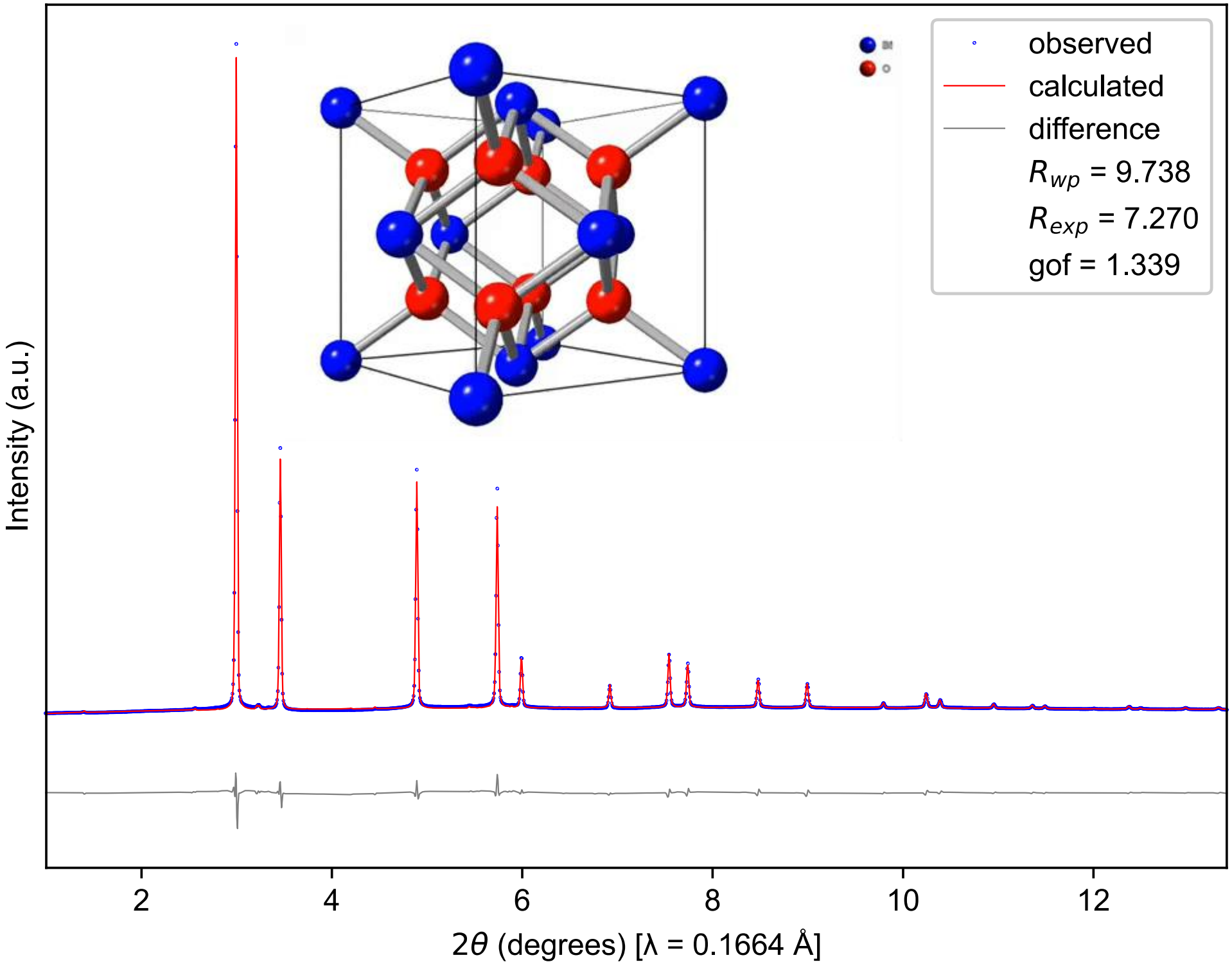


Synchrotron powder X-ray diffraction

Brookhaven National Laboratory

Beamline 28-ID-1

Synchrotron powder X-ray diffraction



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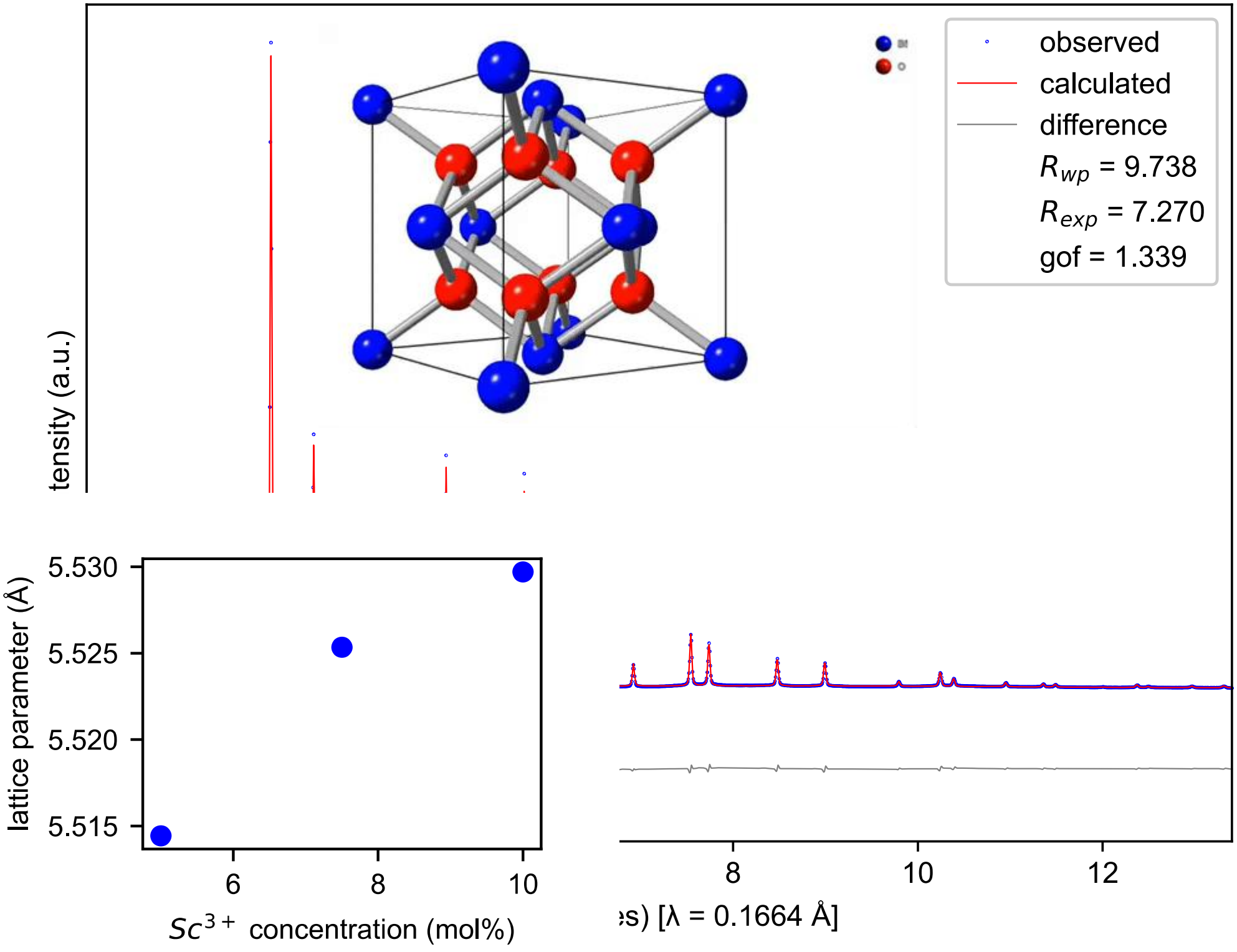

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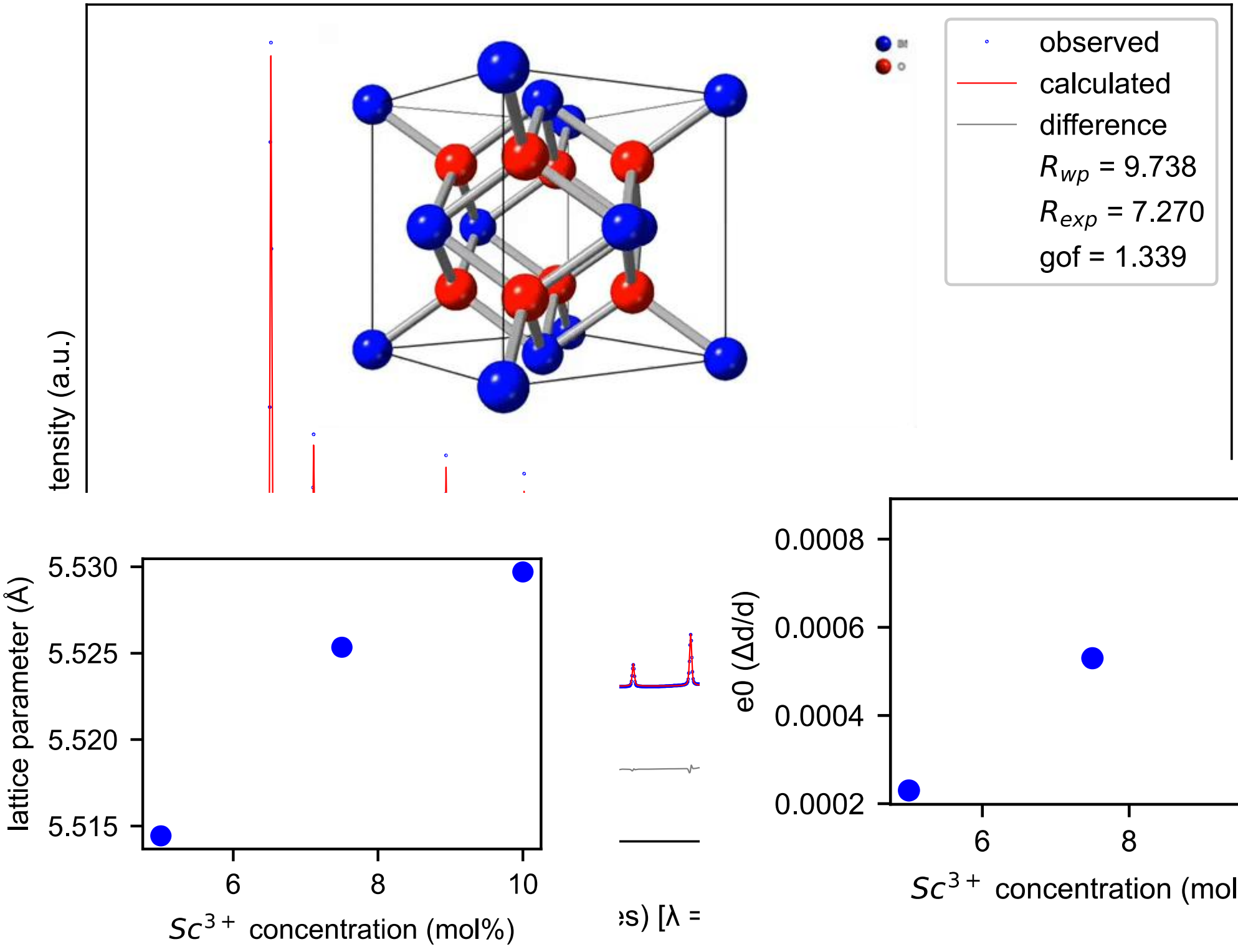

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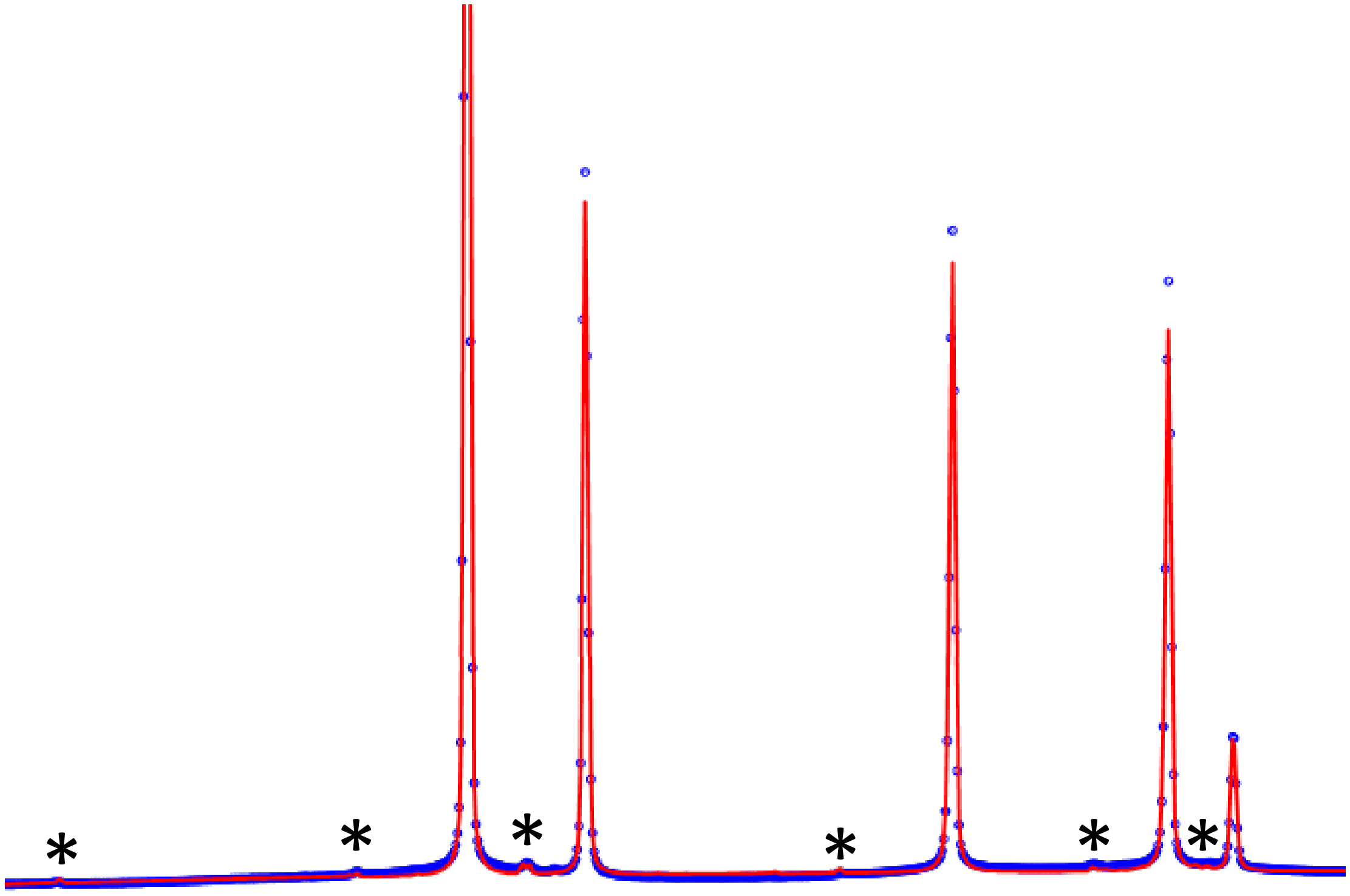

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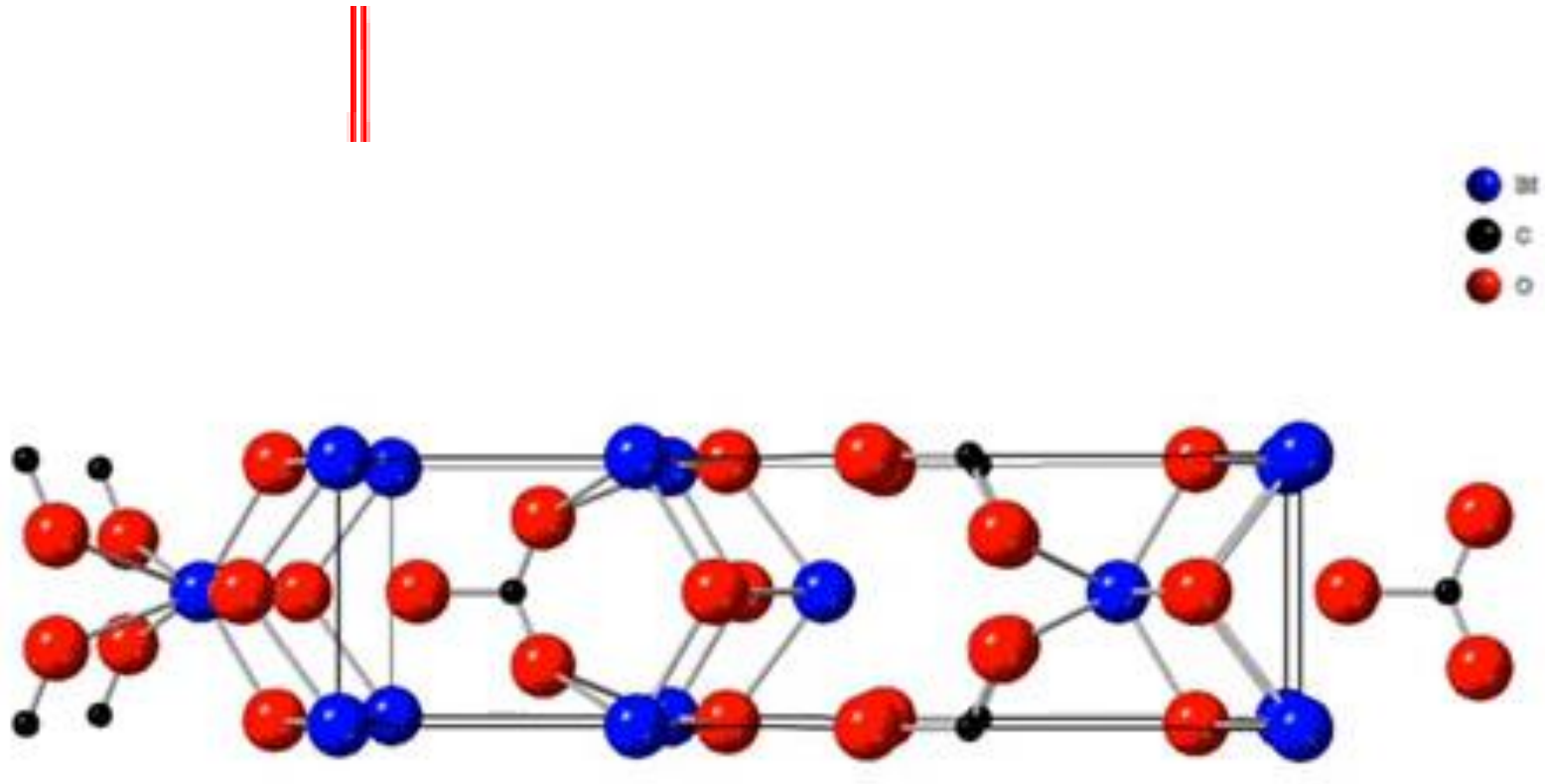
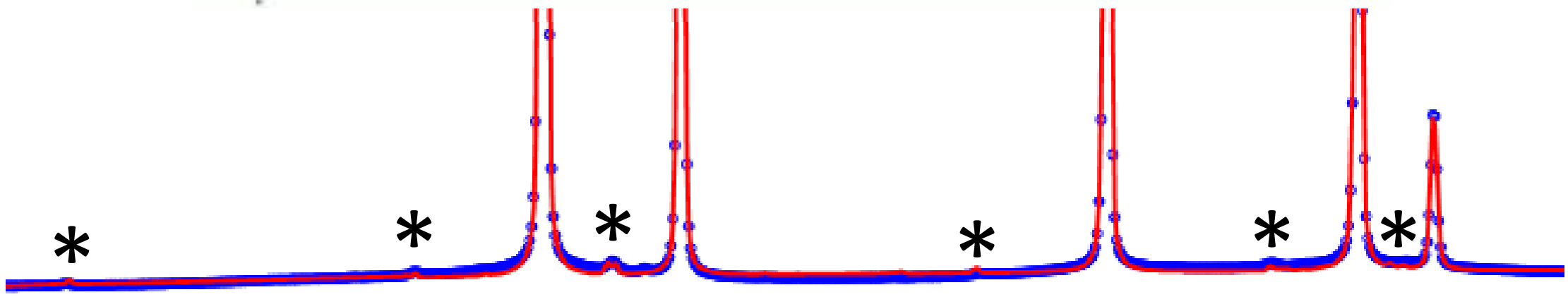


~1 wt%



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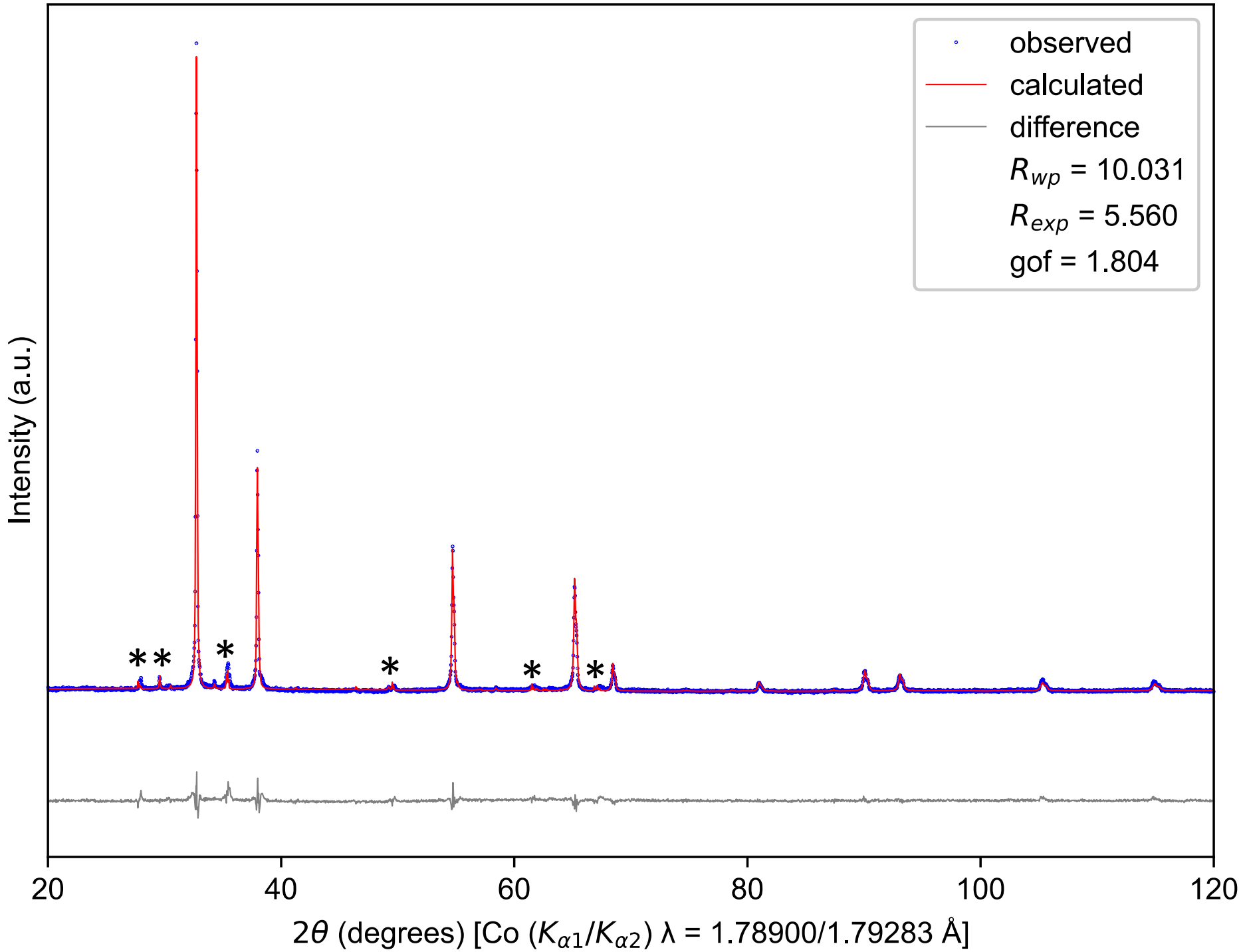

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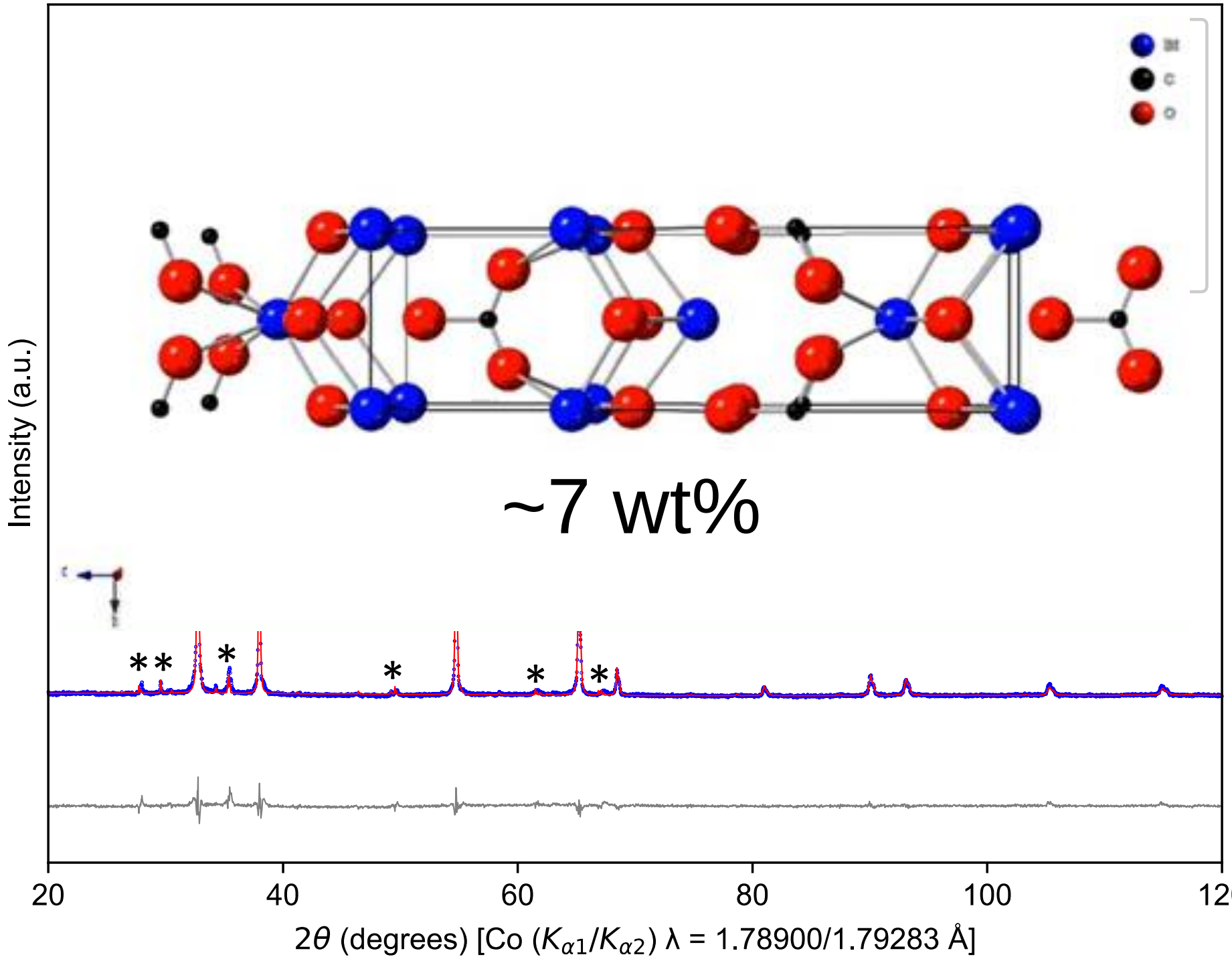

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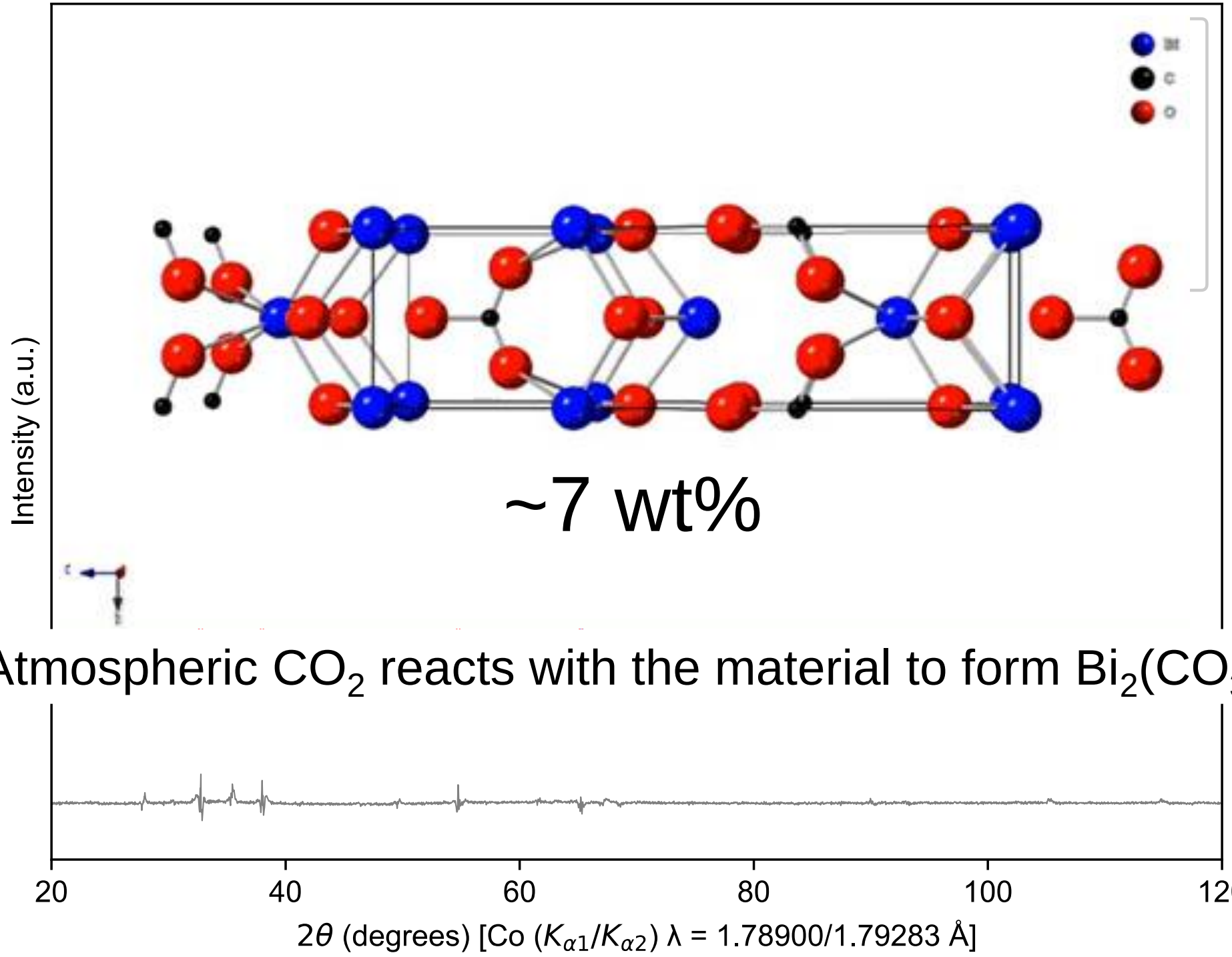

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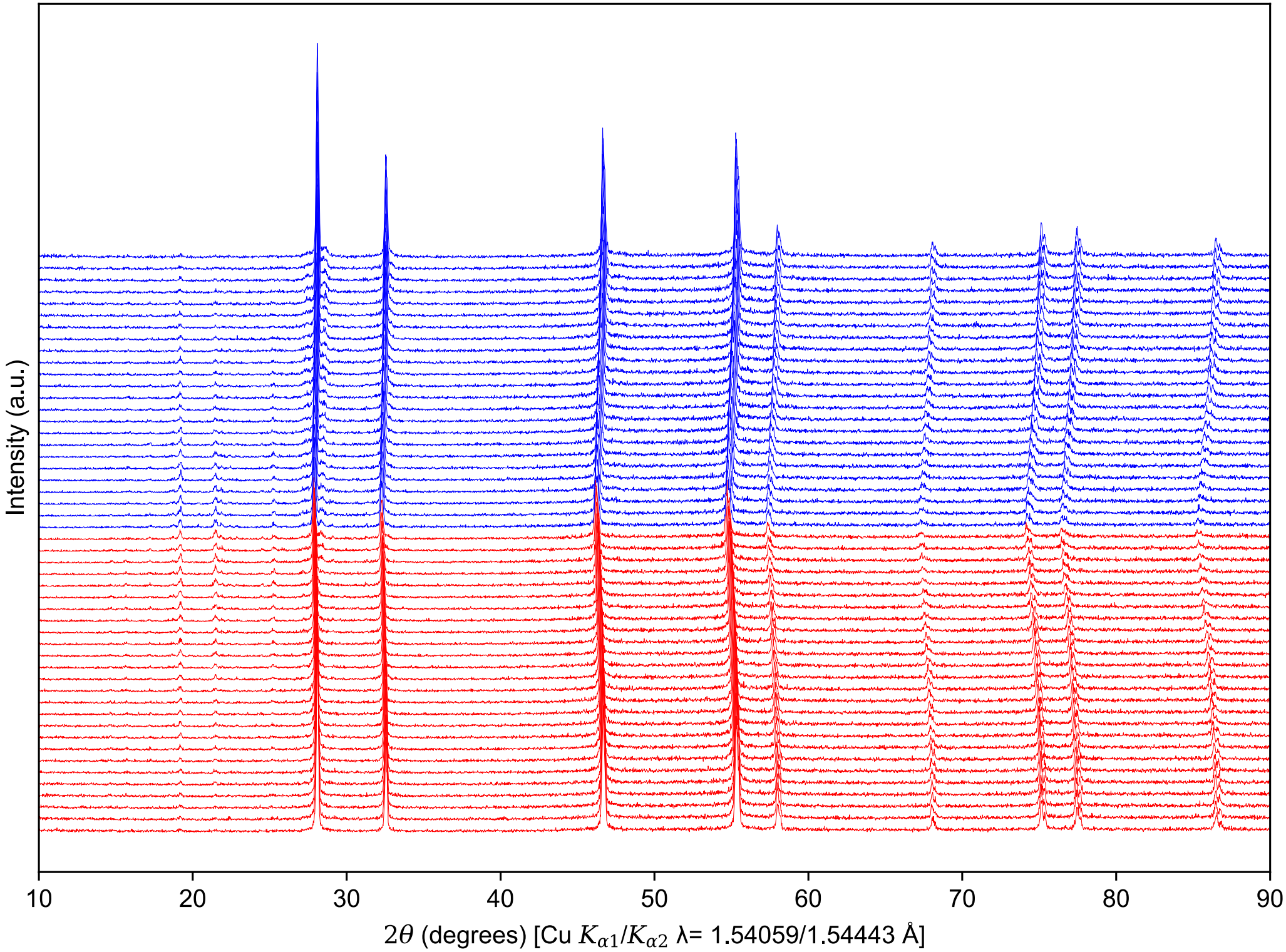

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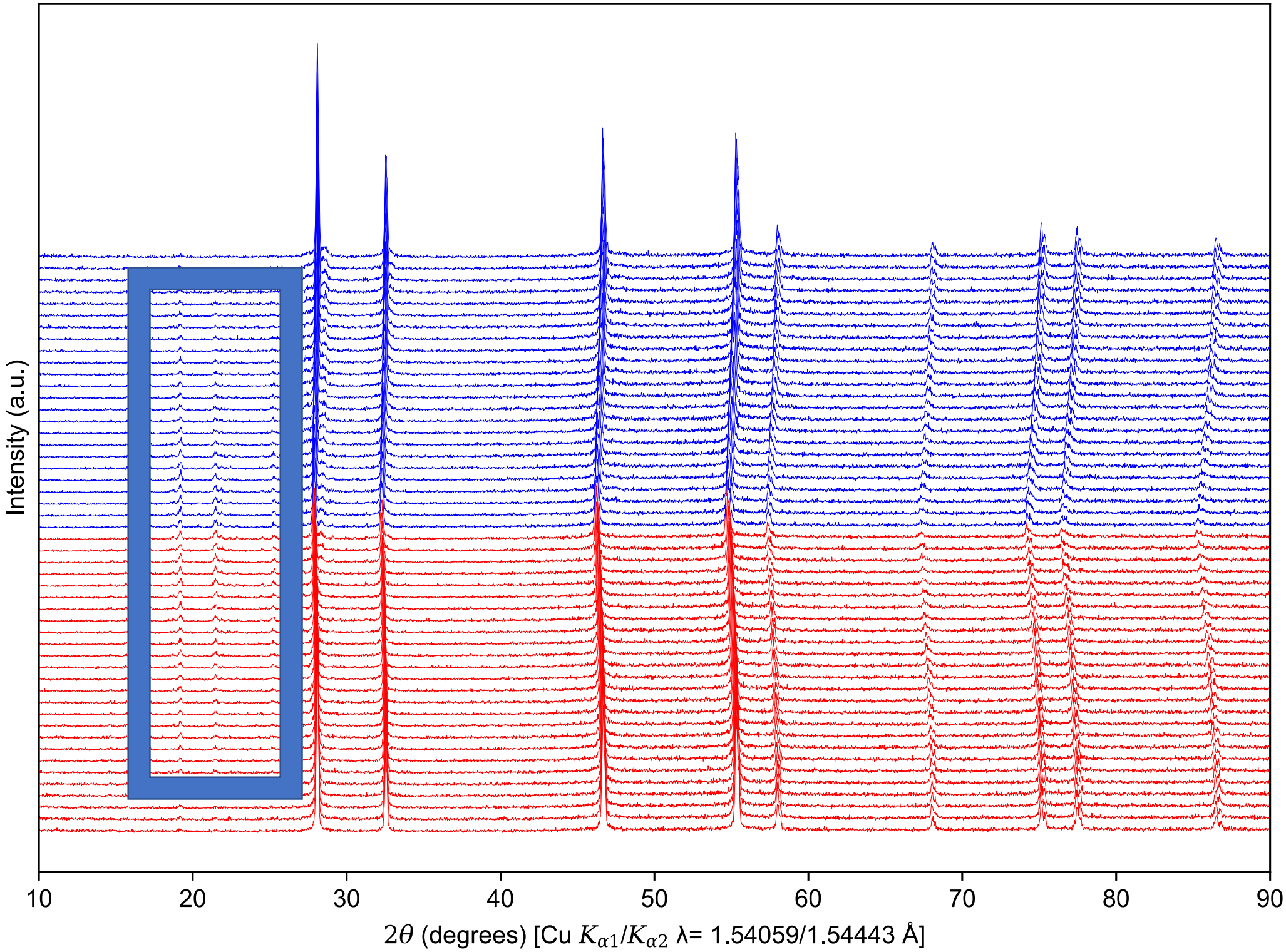

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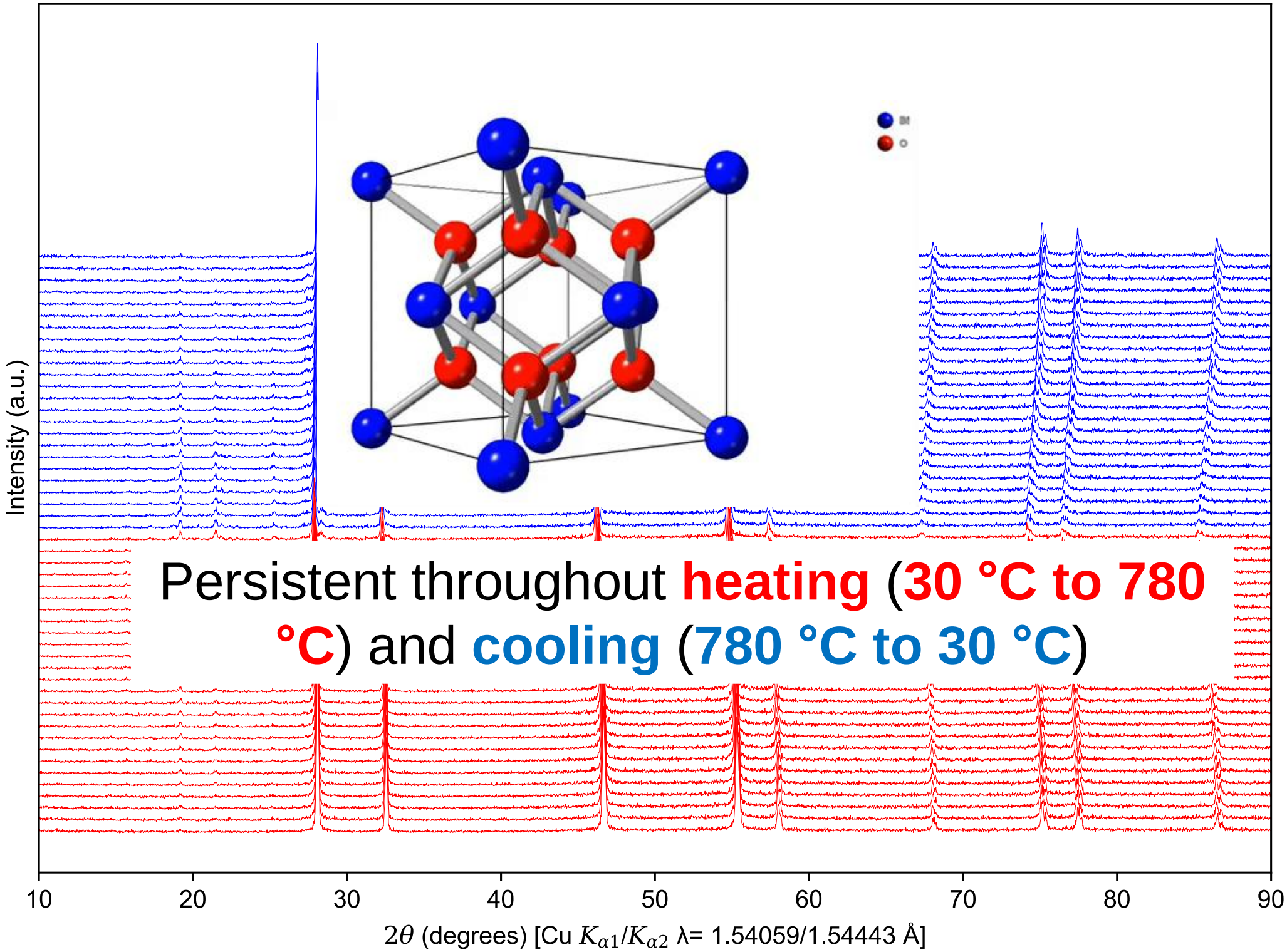
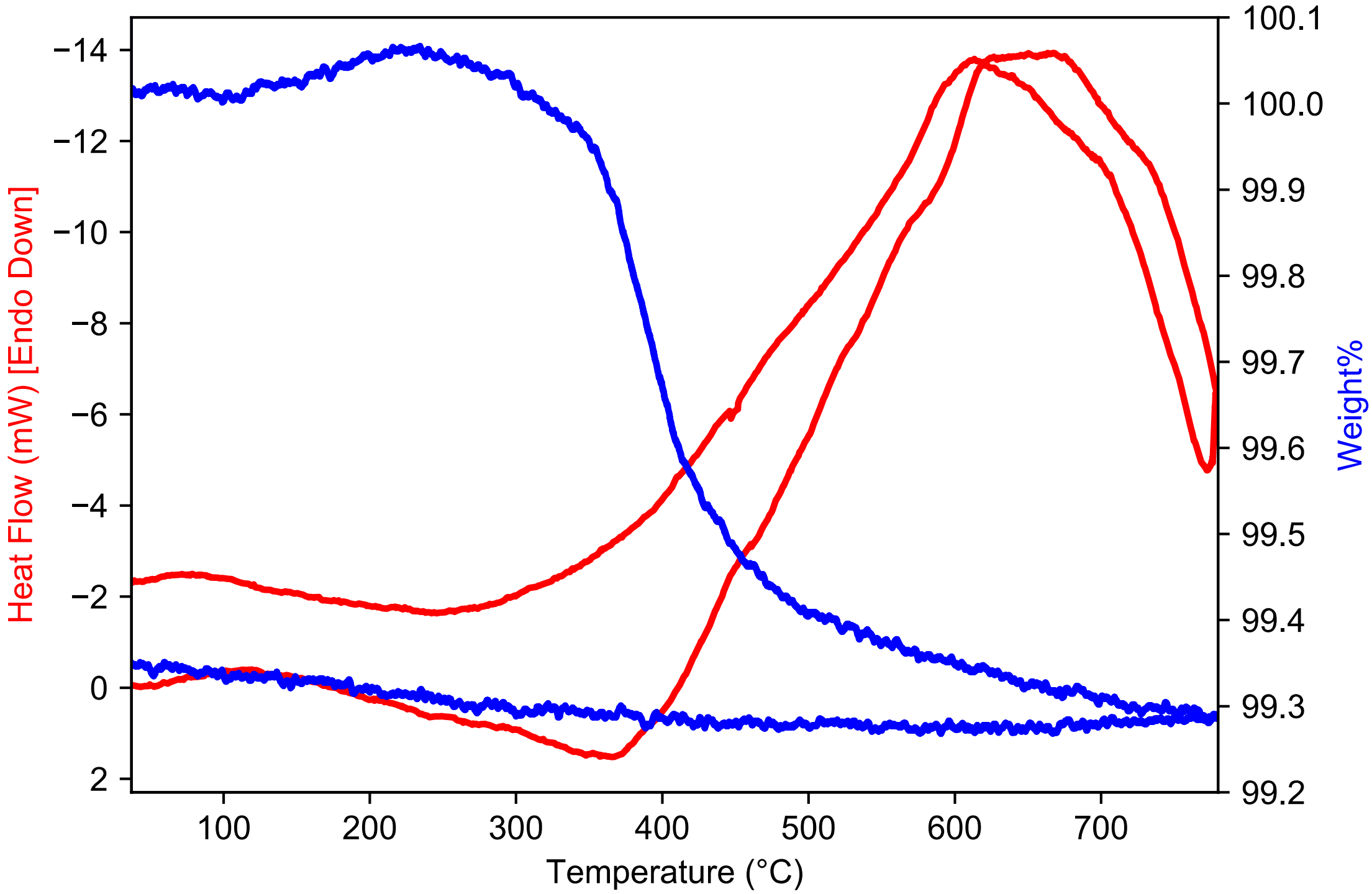


Simultaneous Thermal Analysis (STA) [DTA+TGA] of 7 months aged materials



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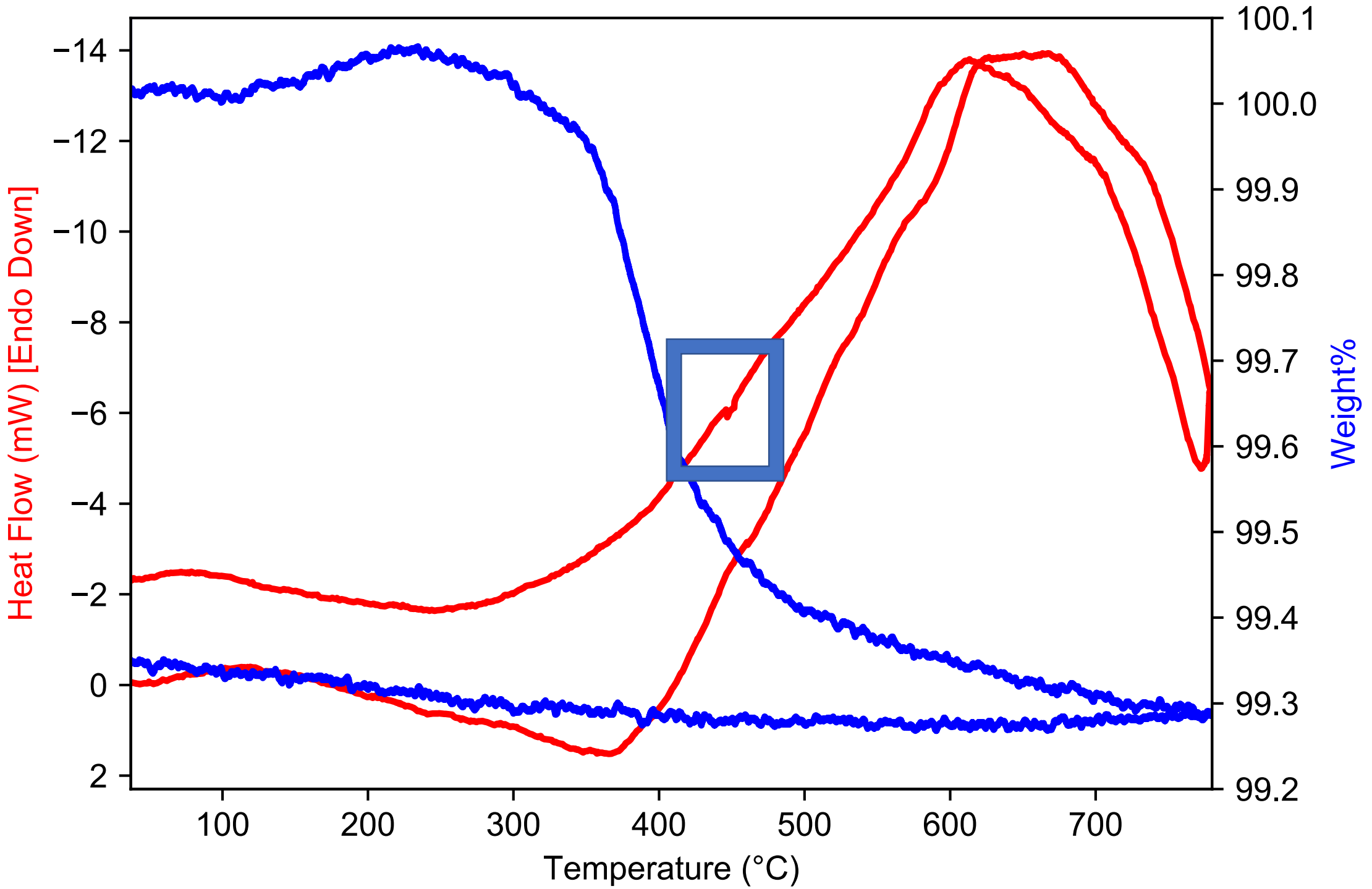

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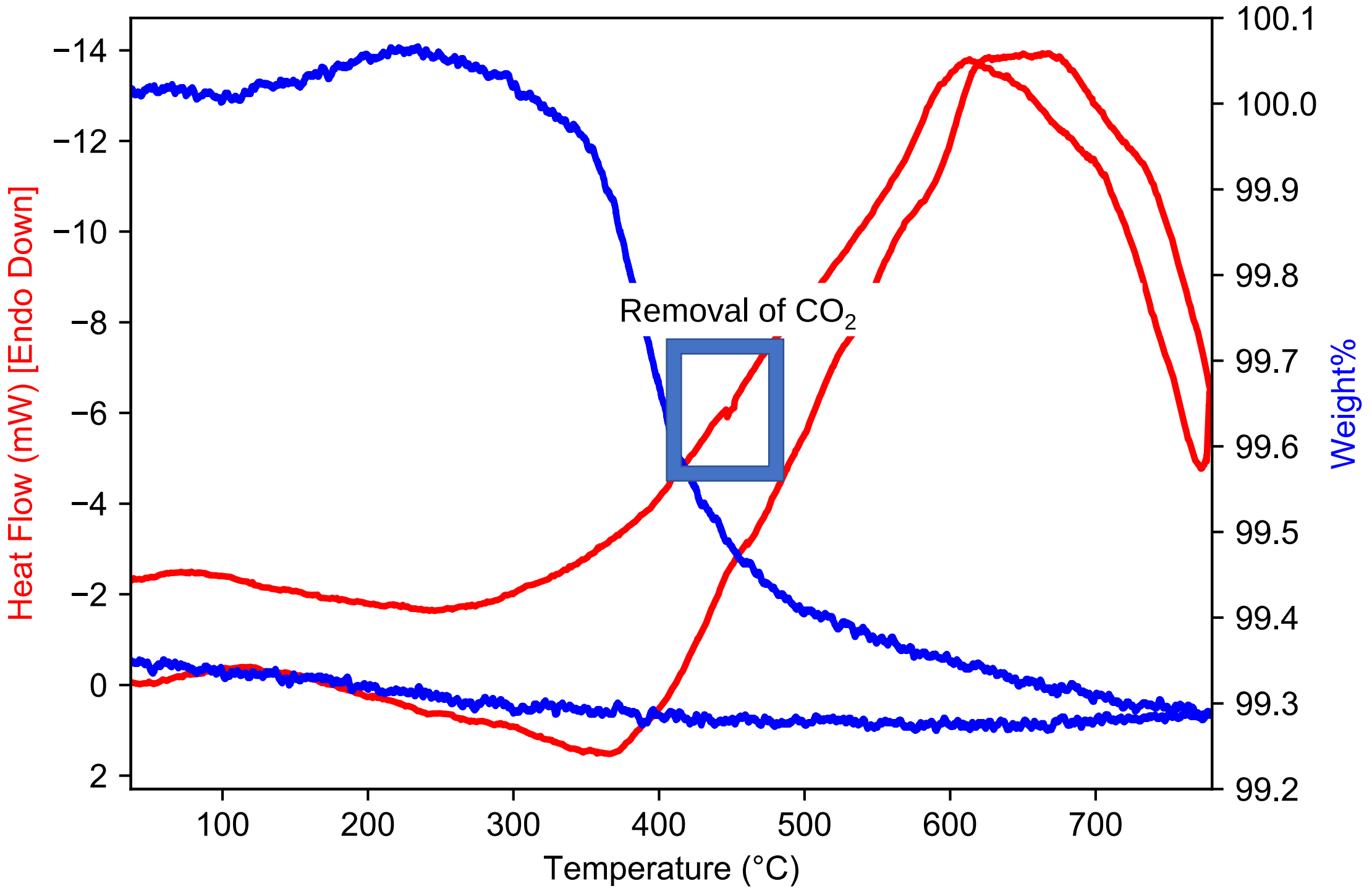

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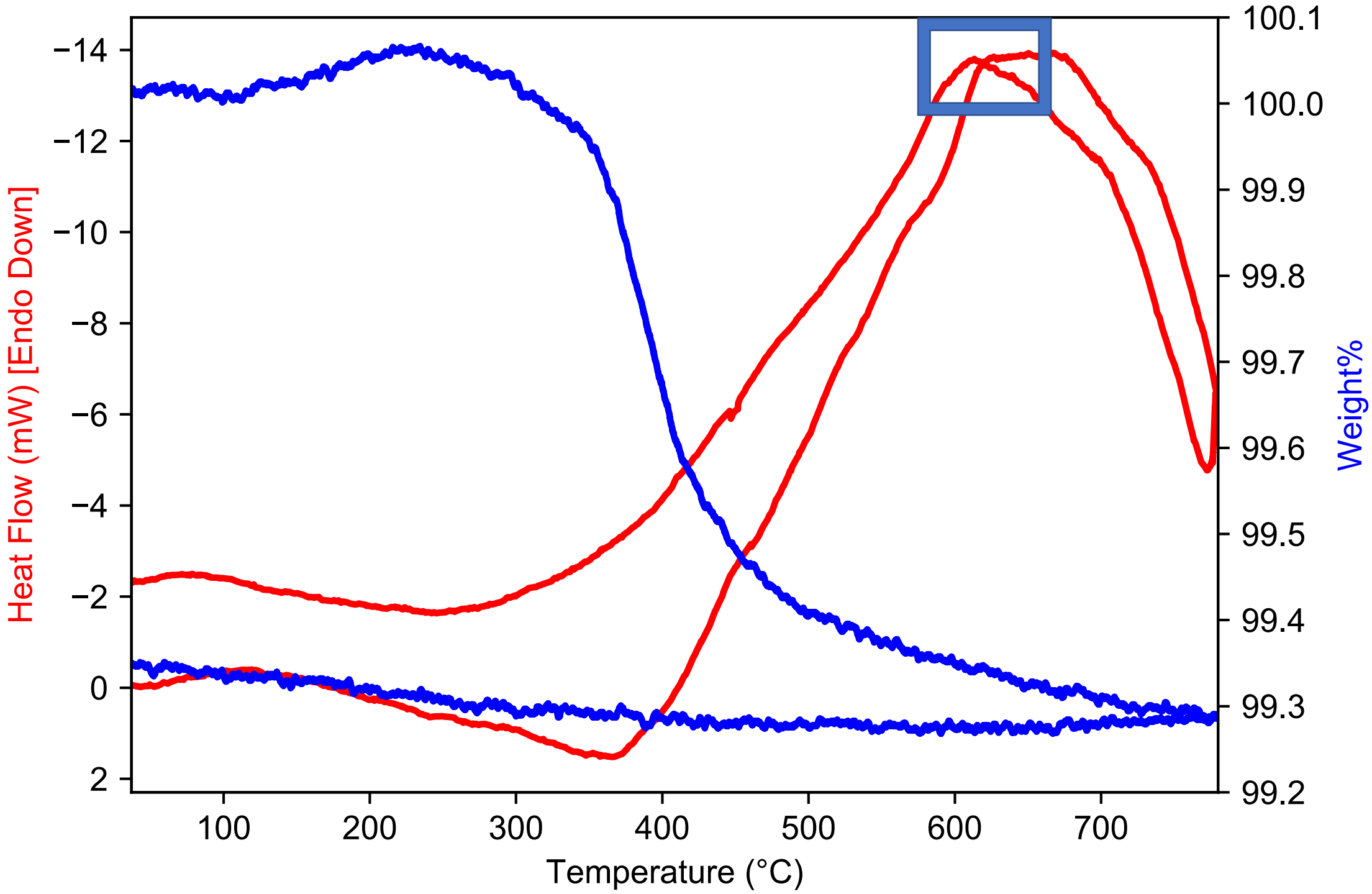

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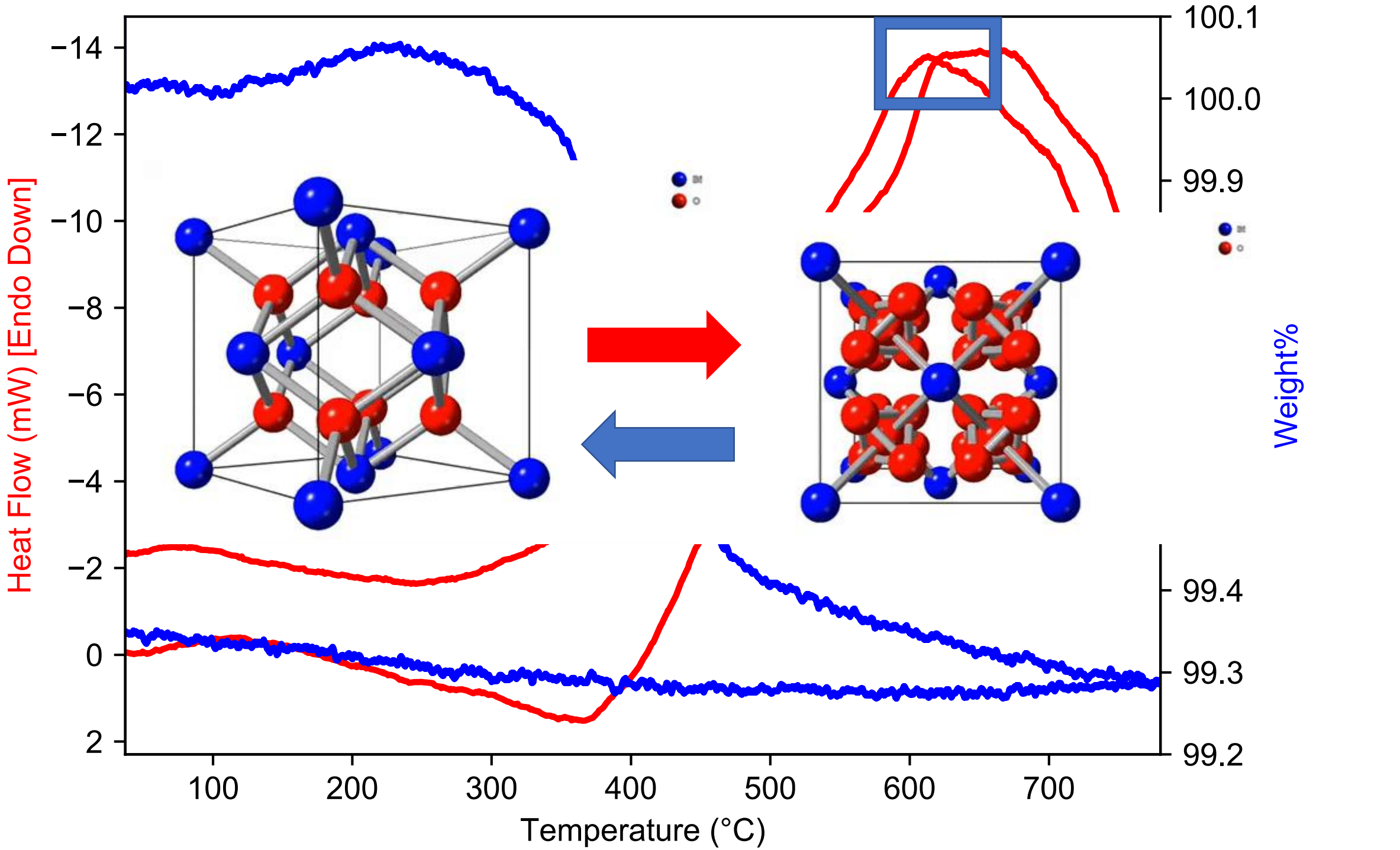

Solid State Ionics **1996**, *89*, 179.

Conclusions

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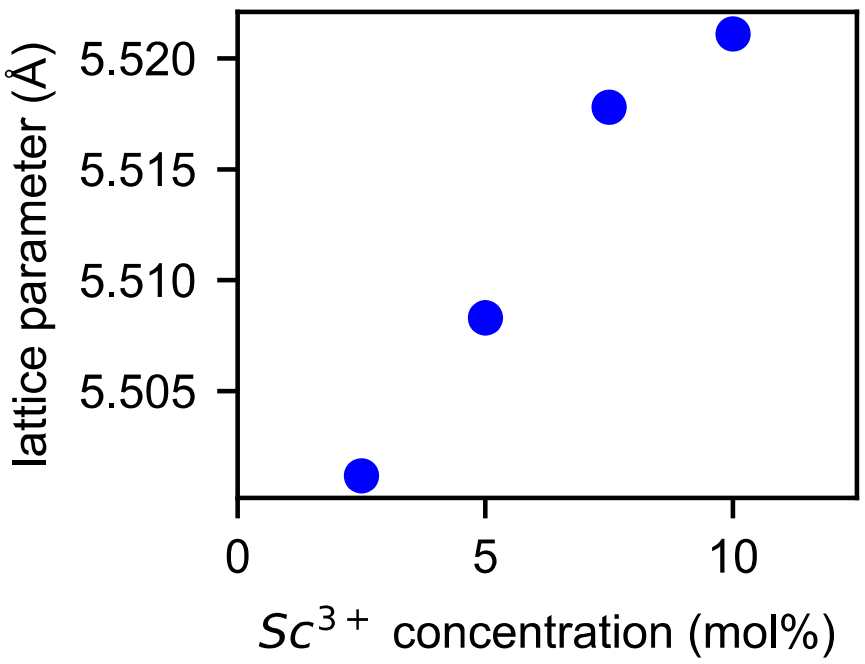

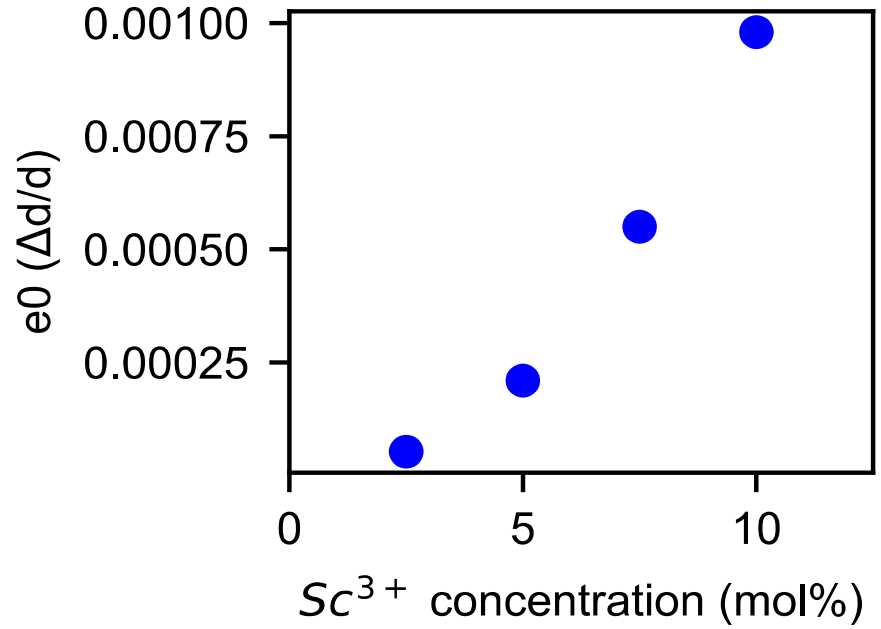

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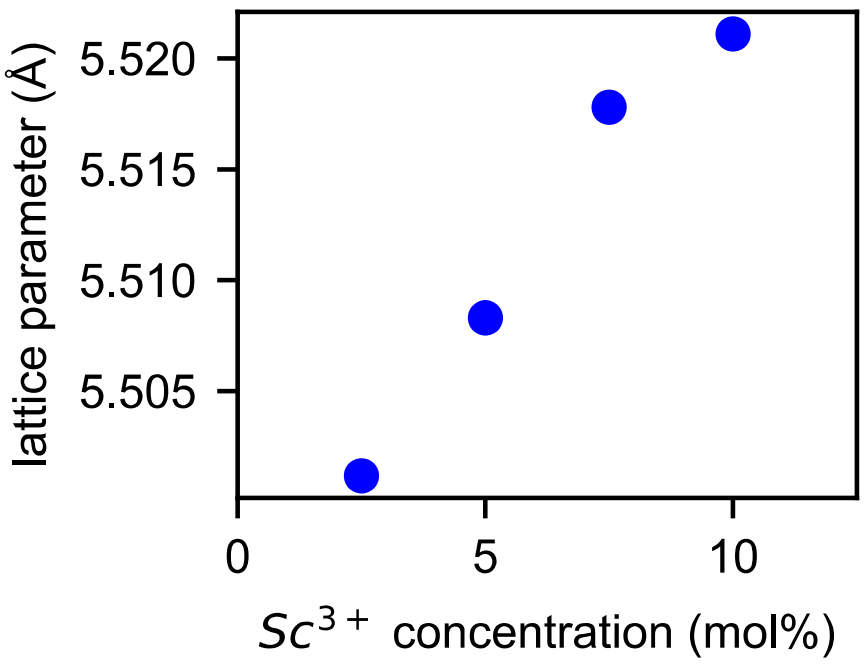

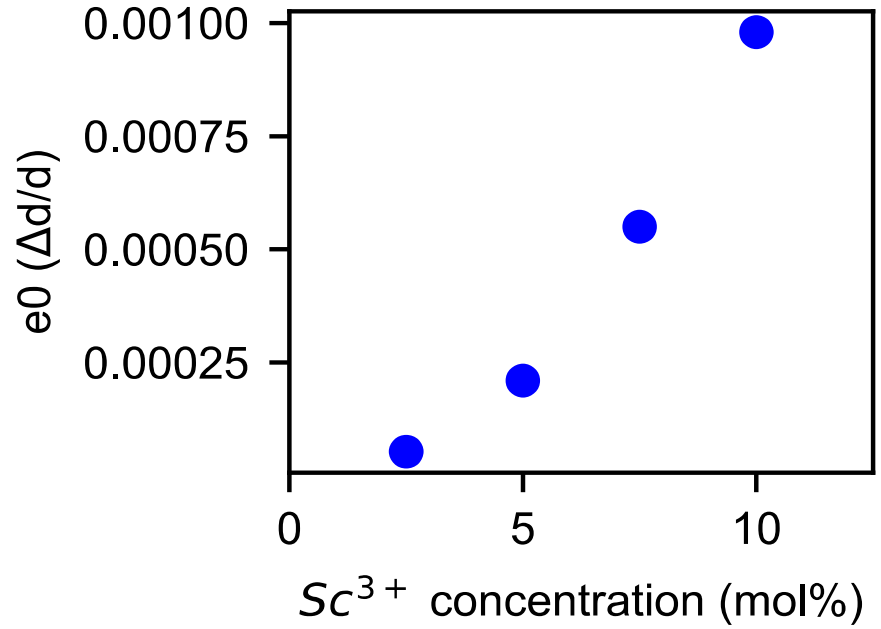

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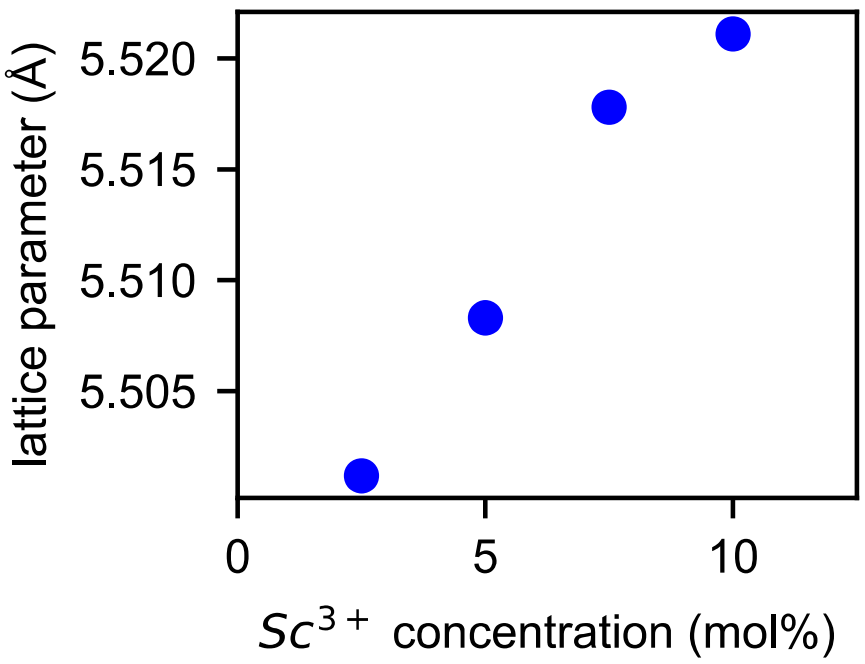

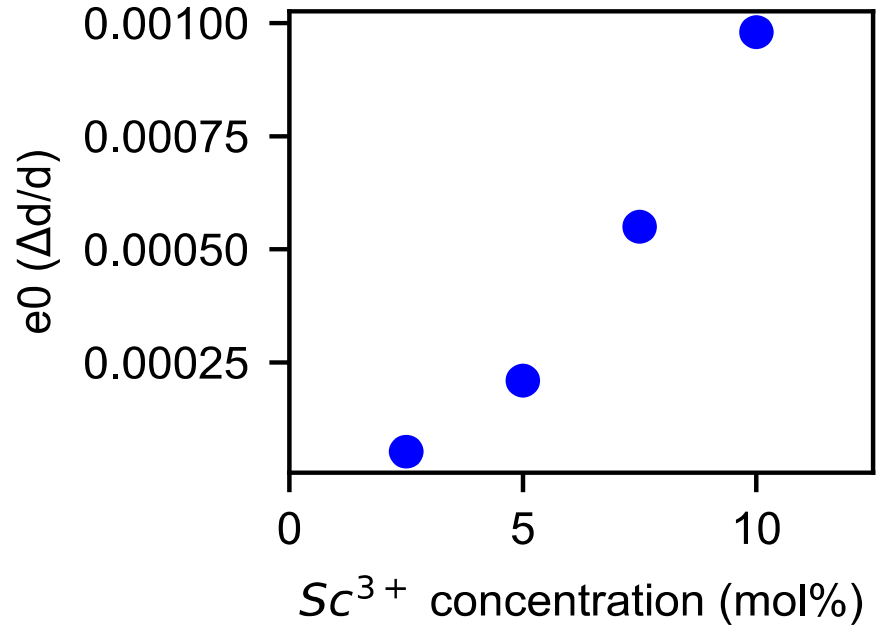

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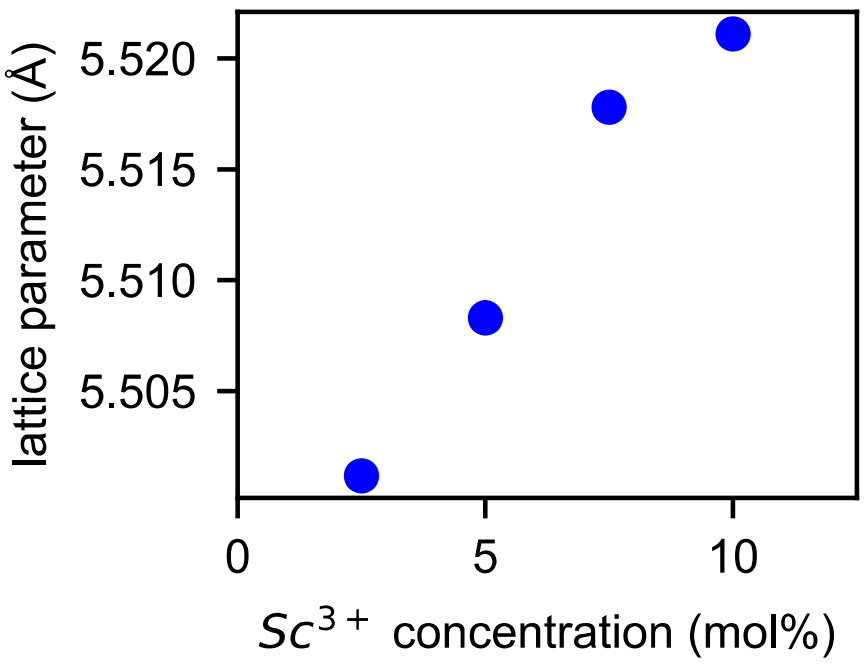

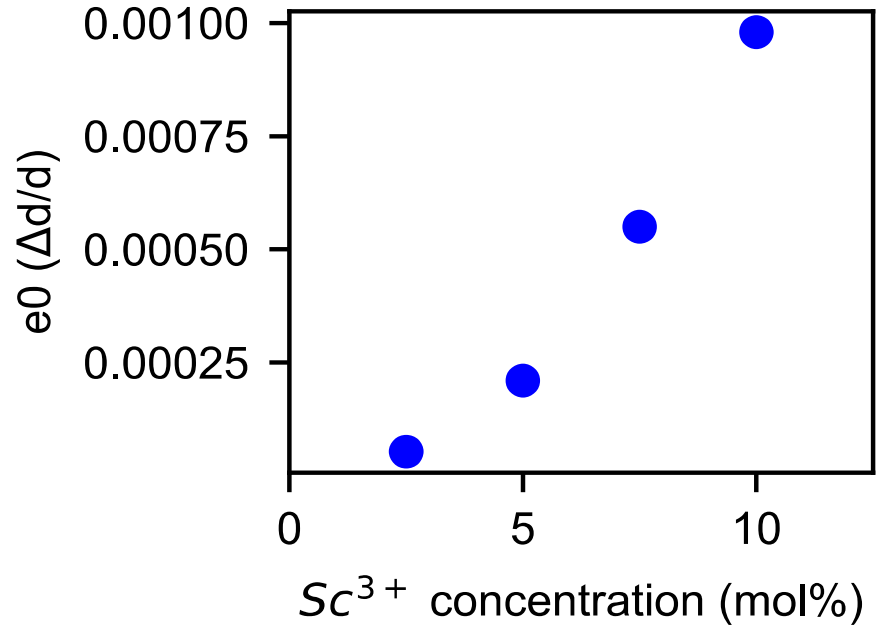

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STA suggested a reversible order-disorder transition of the oxide ion sublattice

Future work

Brookhaven National Laboratory

X-ray absorption spectroscopy (NSLS-II beamline 6-BM)

Ambient and variable temperature synchrotron powder X-ray diffraction and pair distribution function (NSLS-II beamline 28-ID-1)

Future work

Brookhaven National Laboratory

X-ray absorption spectroscopy (NSLS-II beamline 6-BM)

Ambient and variable temperature synchrotron powder X-ray diffraction and pair distribution function (NSLS-II beamline 28-ID-1)

Ambient and variable temperature Raman spectroscopy

Variable temperature electrochemical impedance spectroscopy

Variable temperature powder X-ray diffraction of aged materials

Acknowledgements

science & innovation
Department:
Science and Innovation
REPUBLIC OF SOUTH AFRICA

NRF

DSI-NRF CENTRE OF EXCELLENCE IN STRONG MATERIALS

School of CHEMISTRY

Brookhaven National Laboratory

ENERGY MATERIALS RESEARCH GROUP
UNIVERSITY OF THE WITWATERSRAND

Thank you!

Any questions?

1046999@students.wits.ac.za