

Partial melting of the charge order in the mixed-valent homometallic ludwigite $\text{Co}_2^{2+}\text{Co}^{3+}\text{BO}_5$

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C. B. Pinheiro⁶, G. M. Azevedo⁷, E. Granado¹

APS March Meeting 2021

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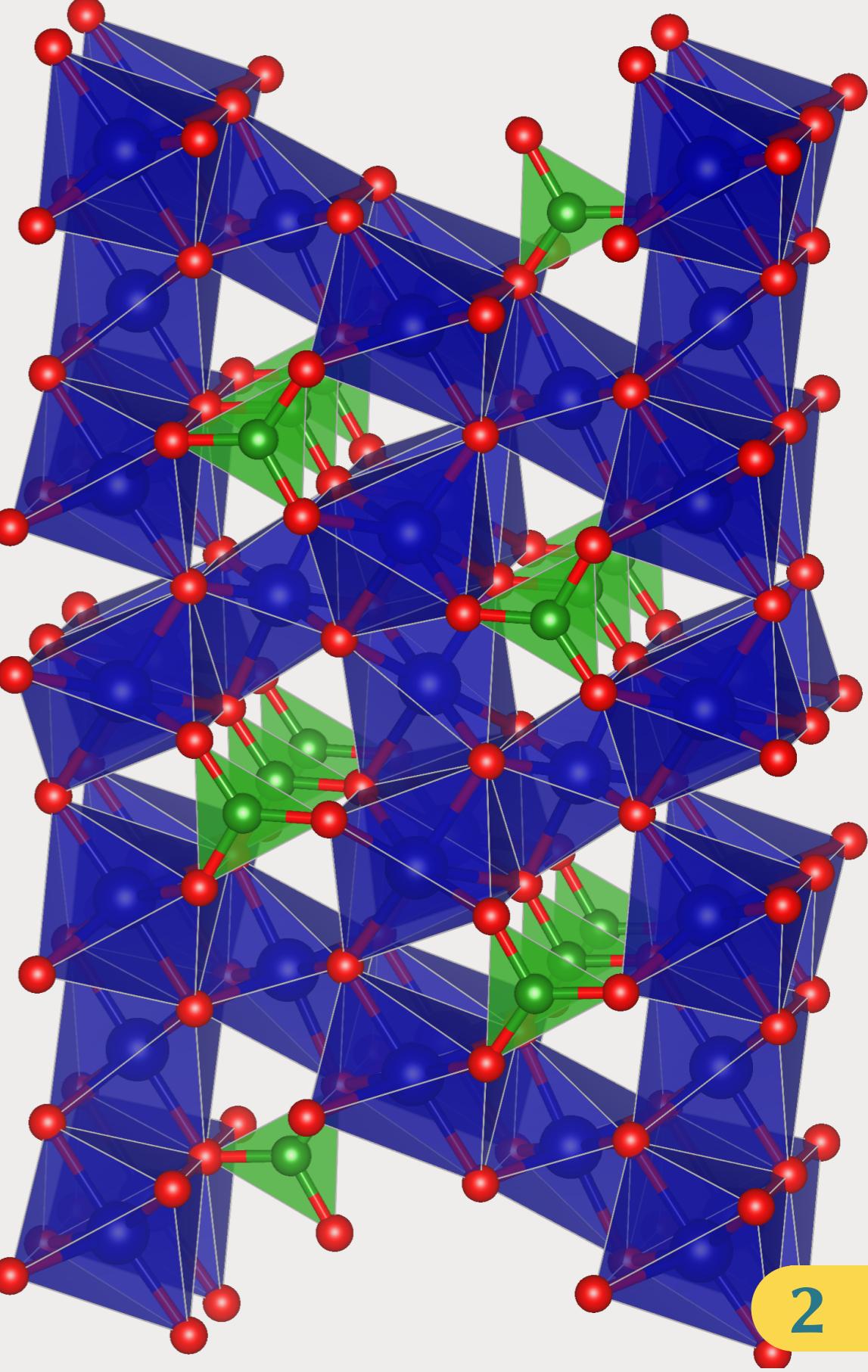
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⁵Institut Néel/CNRS-UJF, Grenoble, France

⁶Universidade Federal de Minas Gerais (UFMG), Belo Horizonte – MG, Brazil

⁷Universidade Federal do Rio Grande do Sul (UFRGS), Porto Alegre – RS, Brazil

Ludwigites

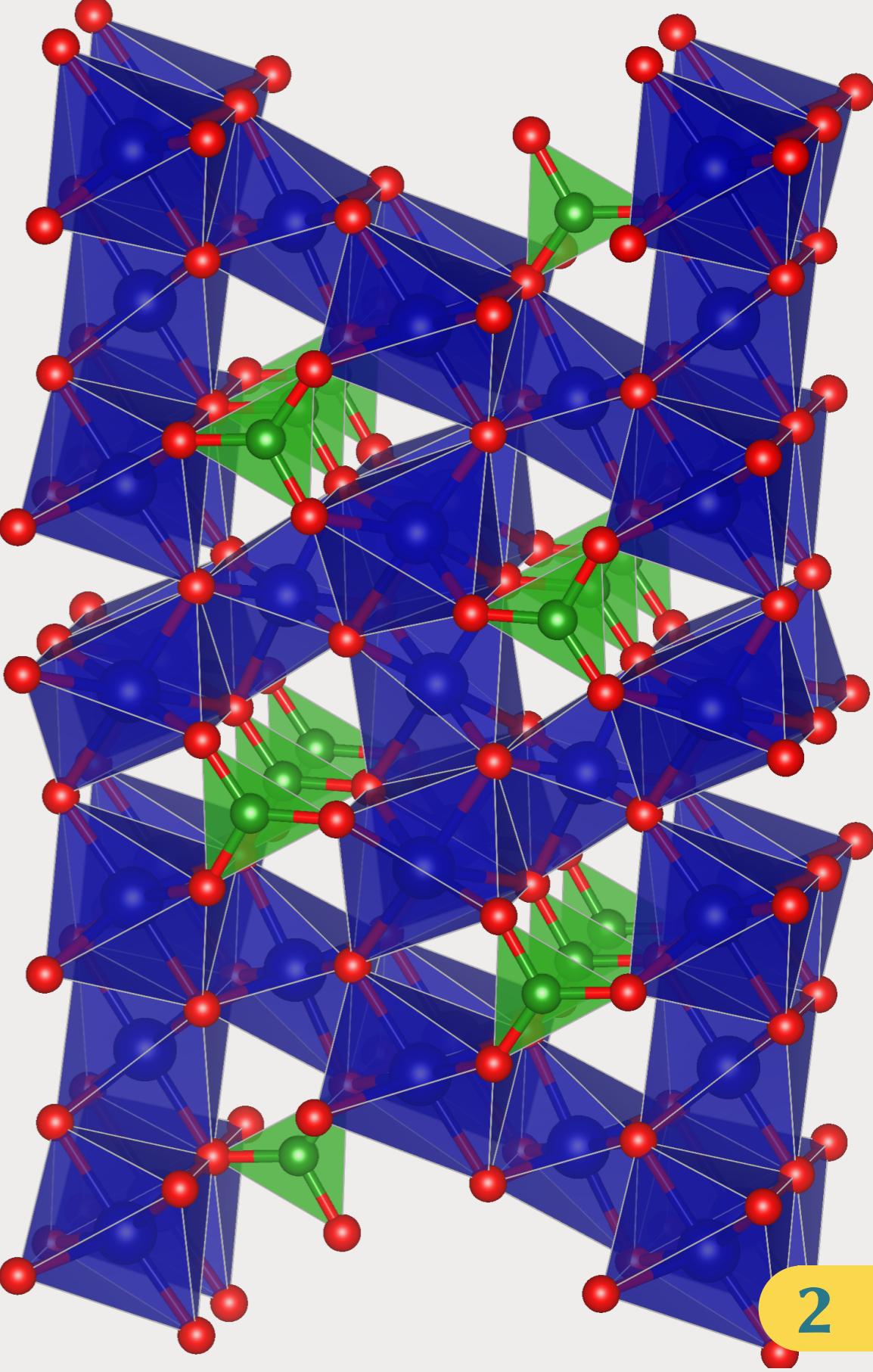


Ludwigites



- CDW ordering
- Charge-ordering transitions
- Spin-state transitions
- OER catalyst

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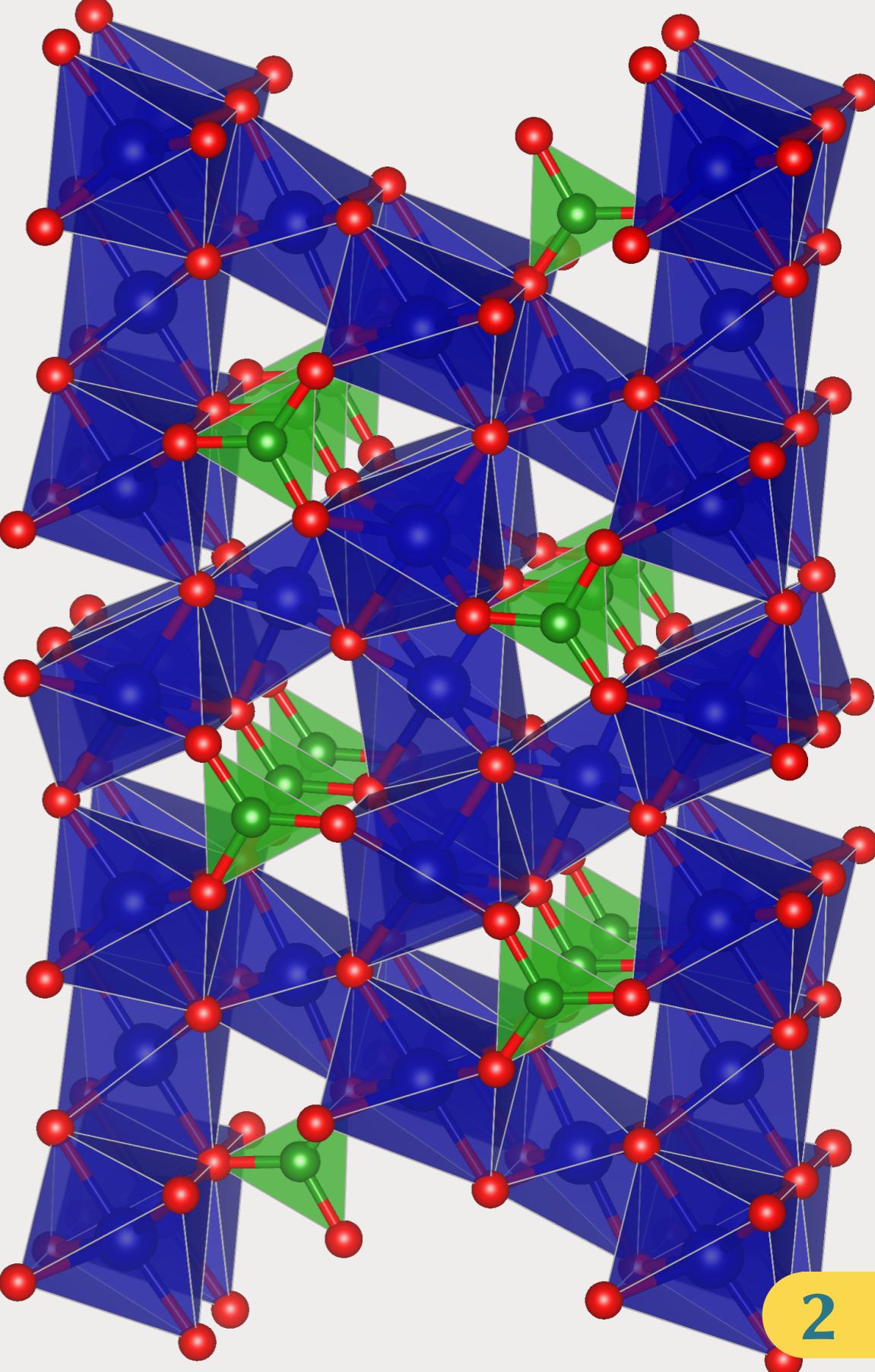


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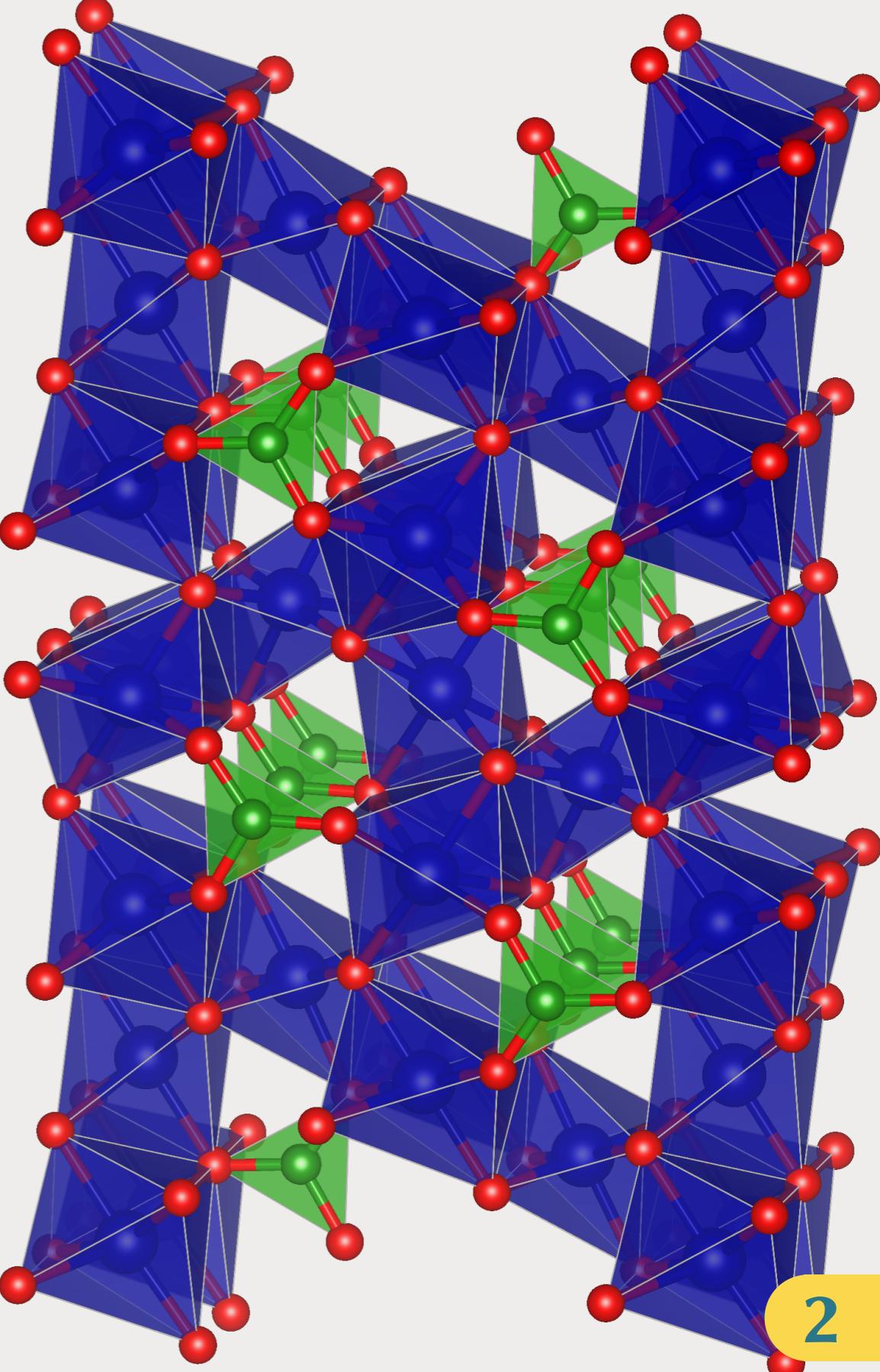


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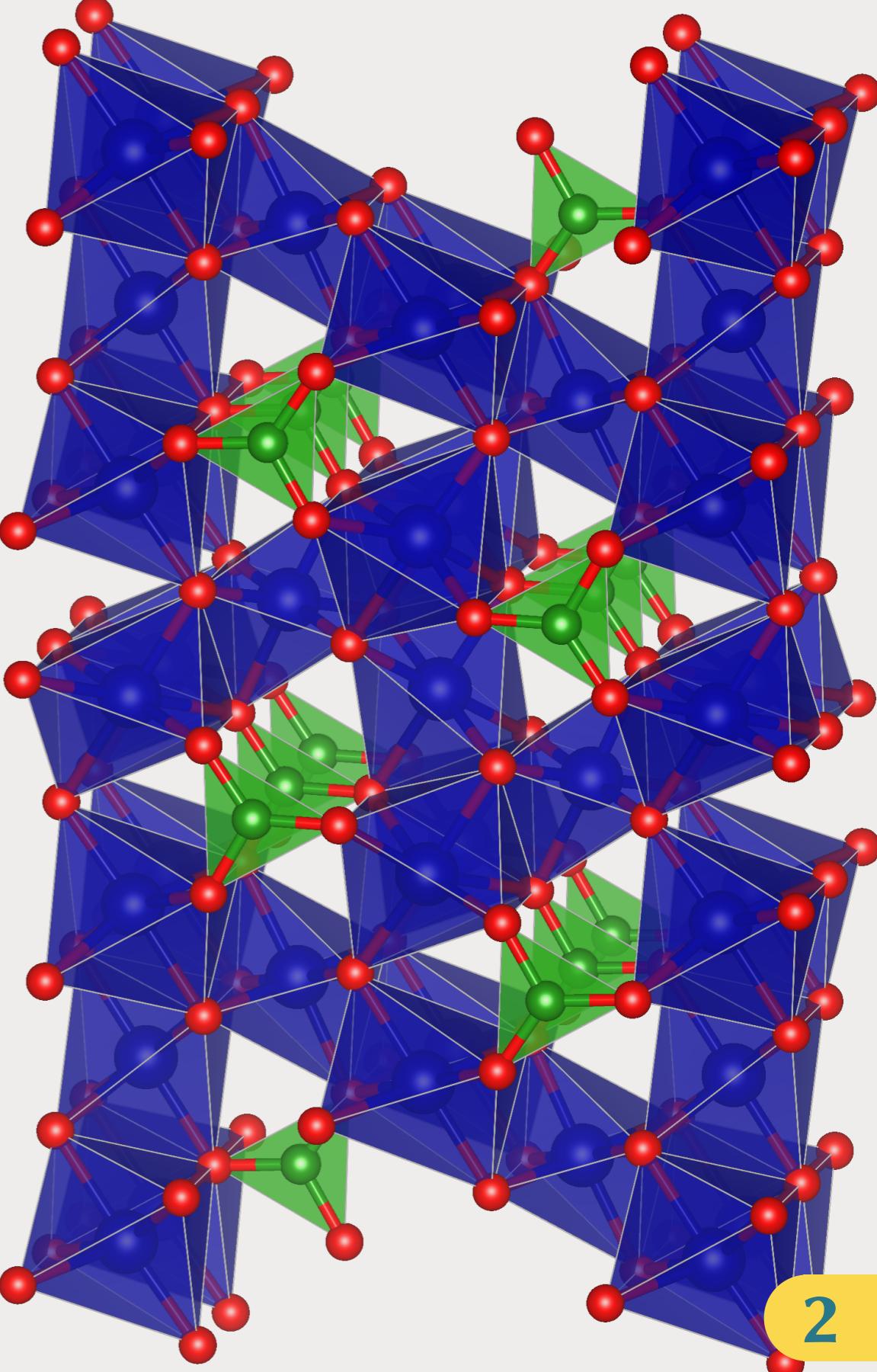


Ludwigites

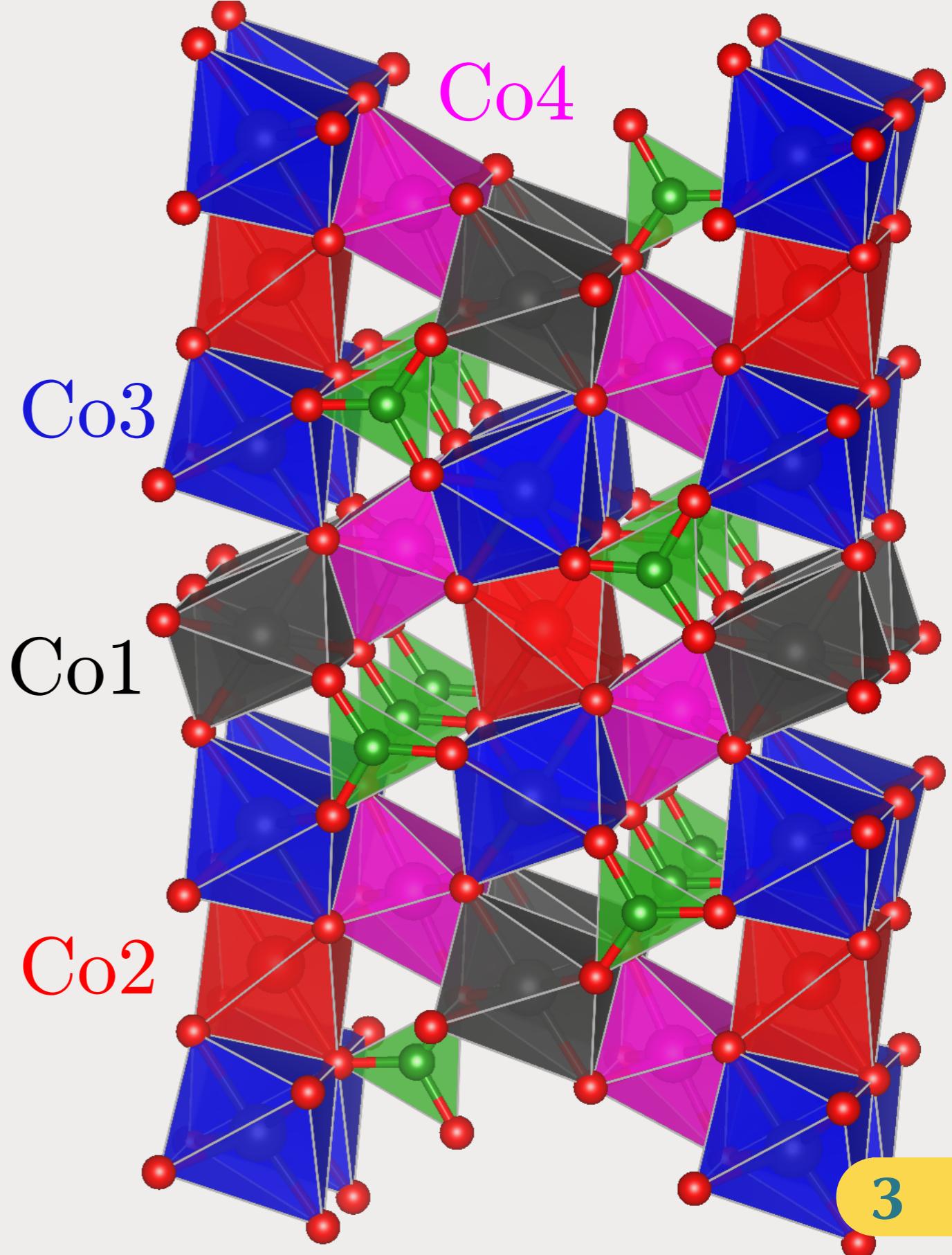


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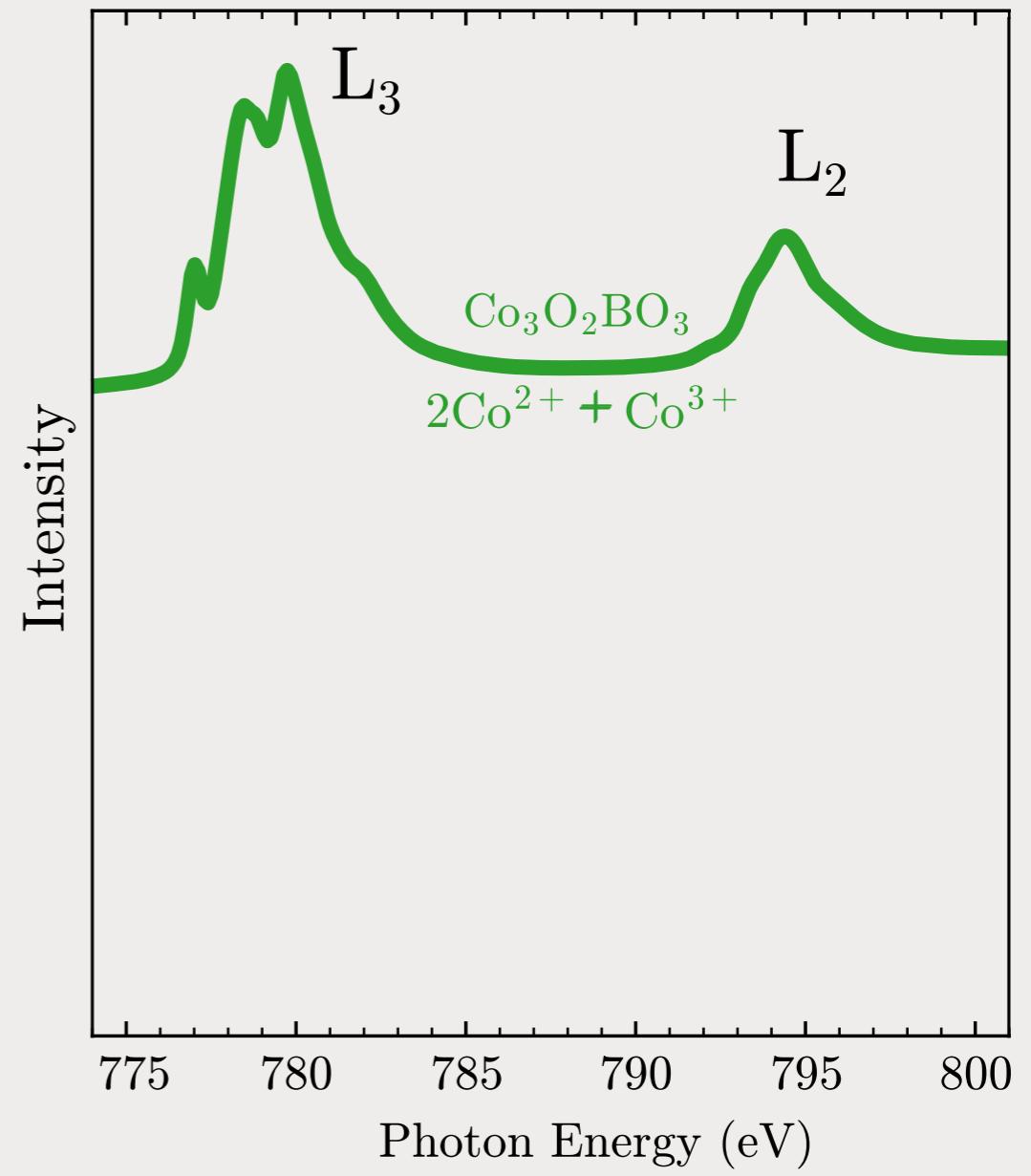


Ludwigites



X-ray absorption spectroscopy

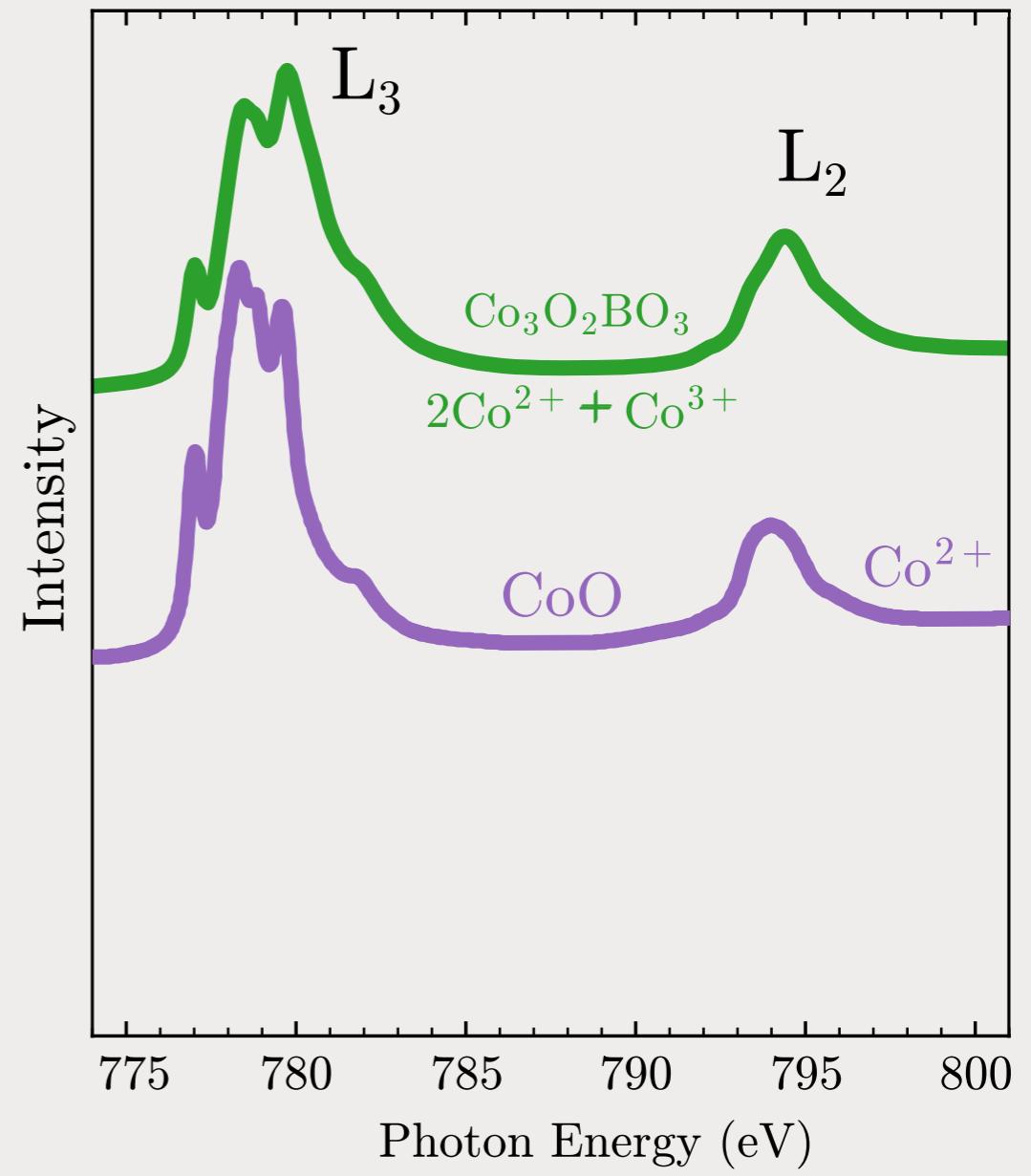
Co L_{2,3} edges



Galdino et al. Phys. Rev. B 100, 165138 (2019)

X-ray absorption spectroscopy

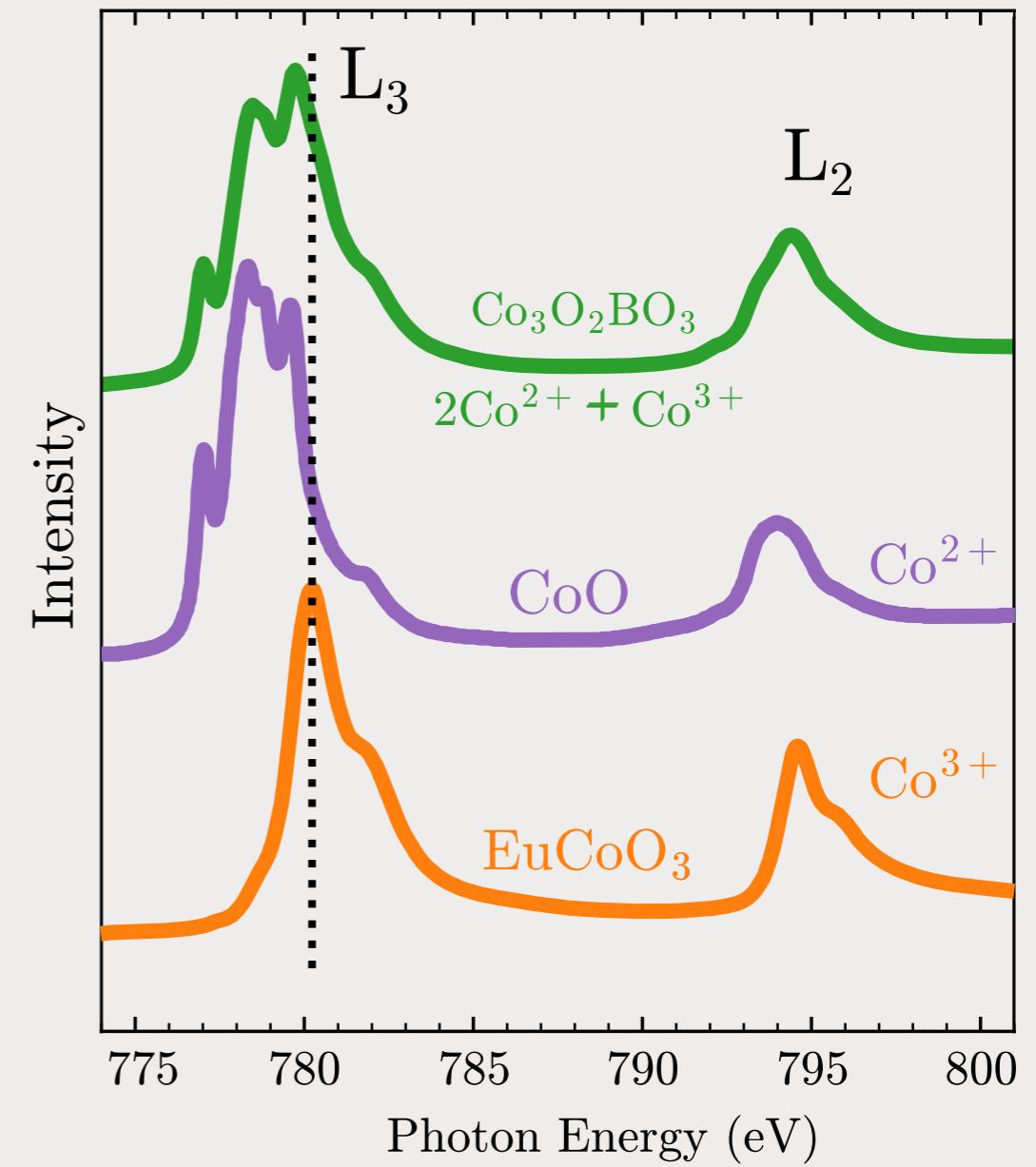
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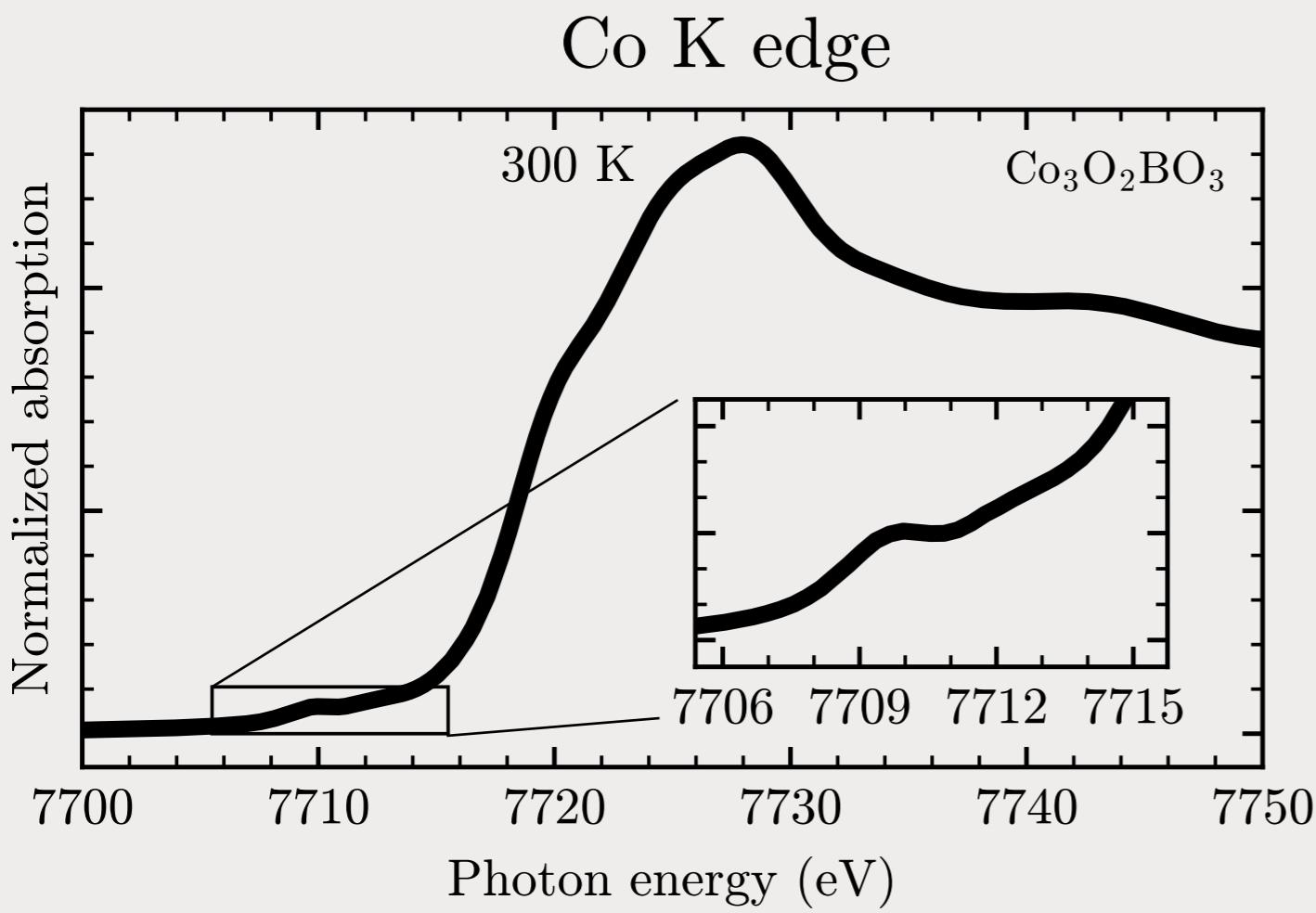
X-ray absorption spectroscopy

Co L_{2,3} edges



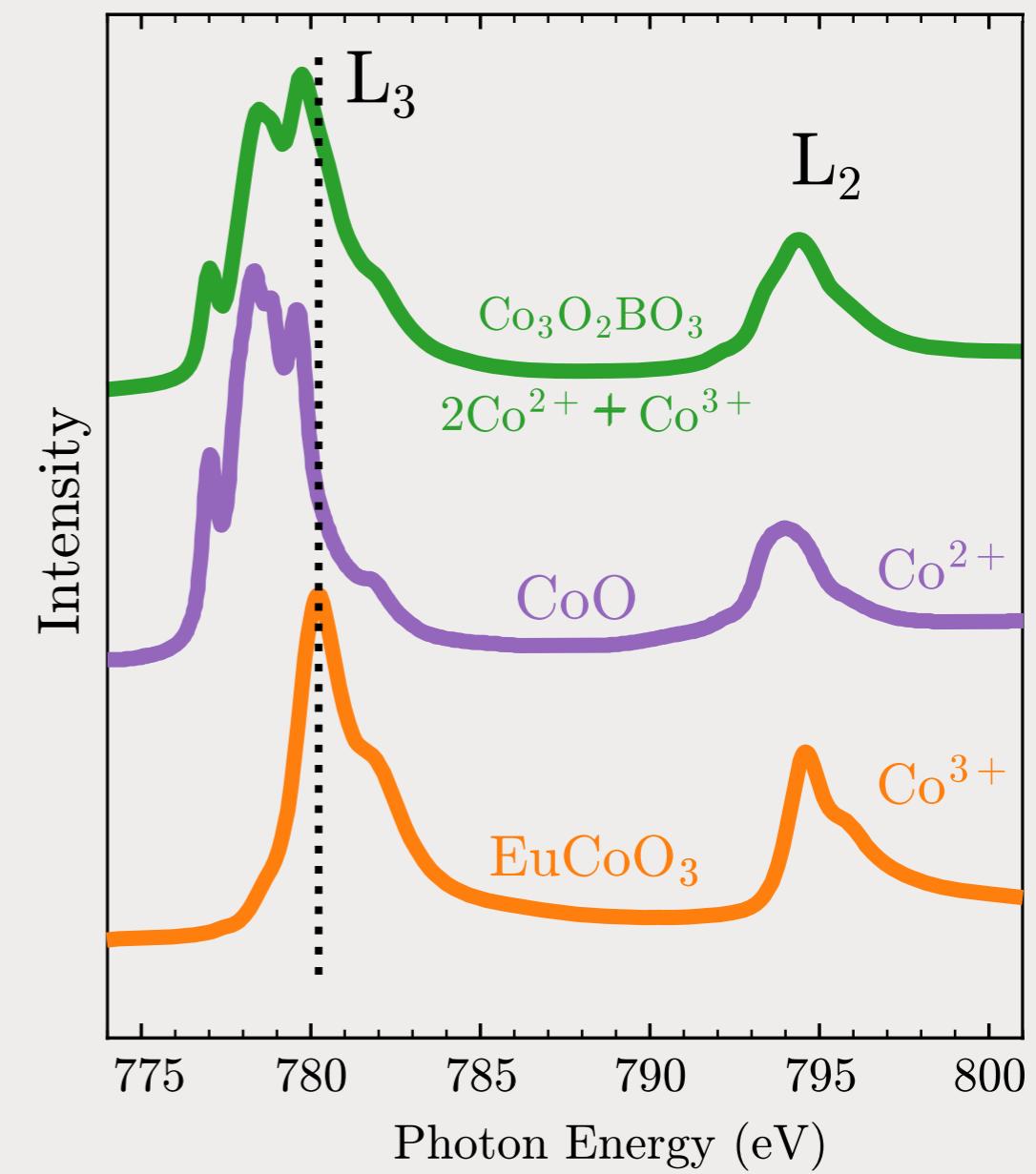
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X-ray absorption spectroscopy



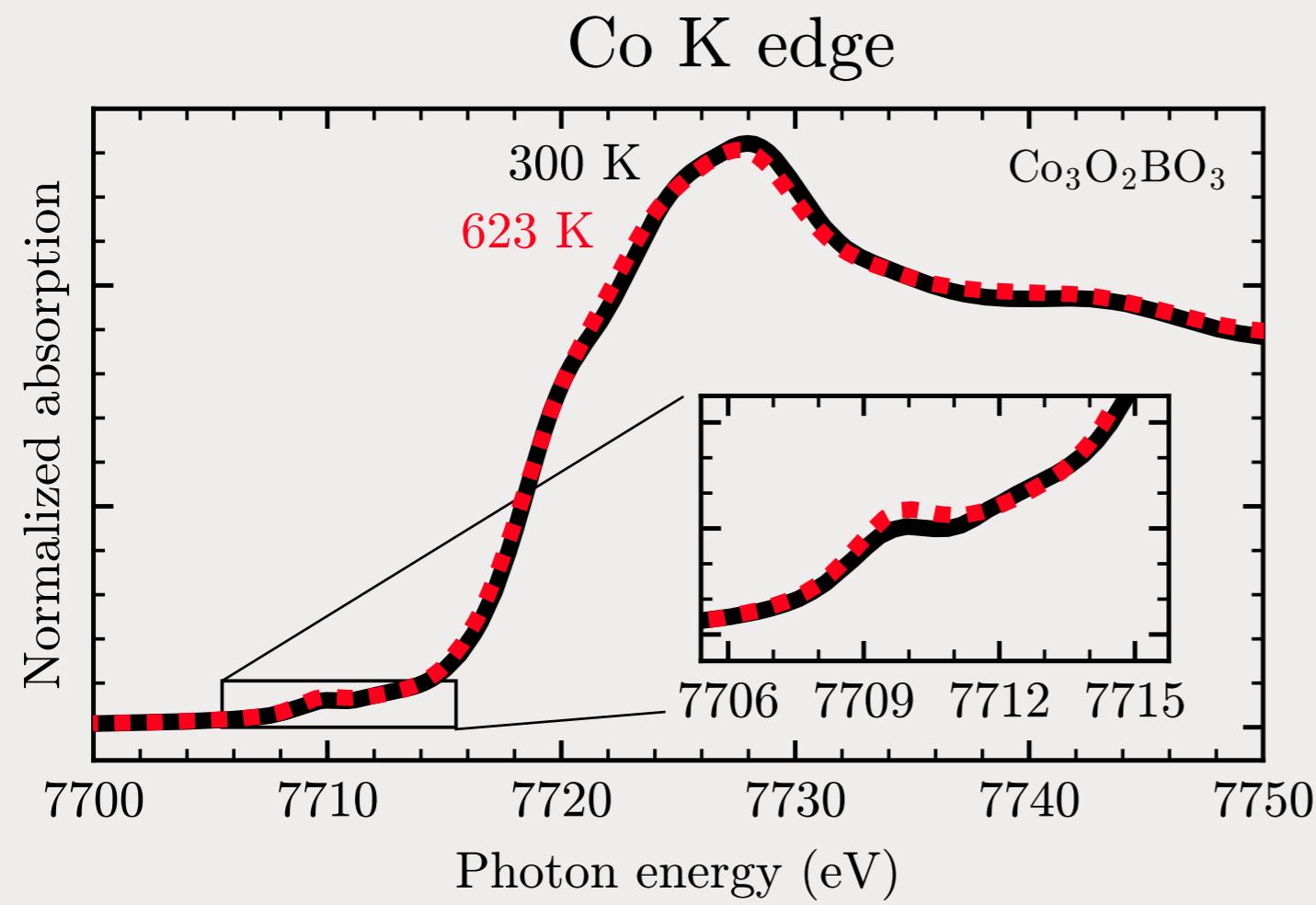
Galdino et al. In preparation

Co L_{2,3} edges



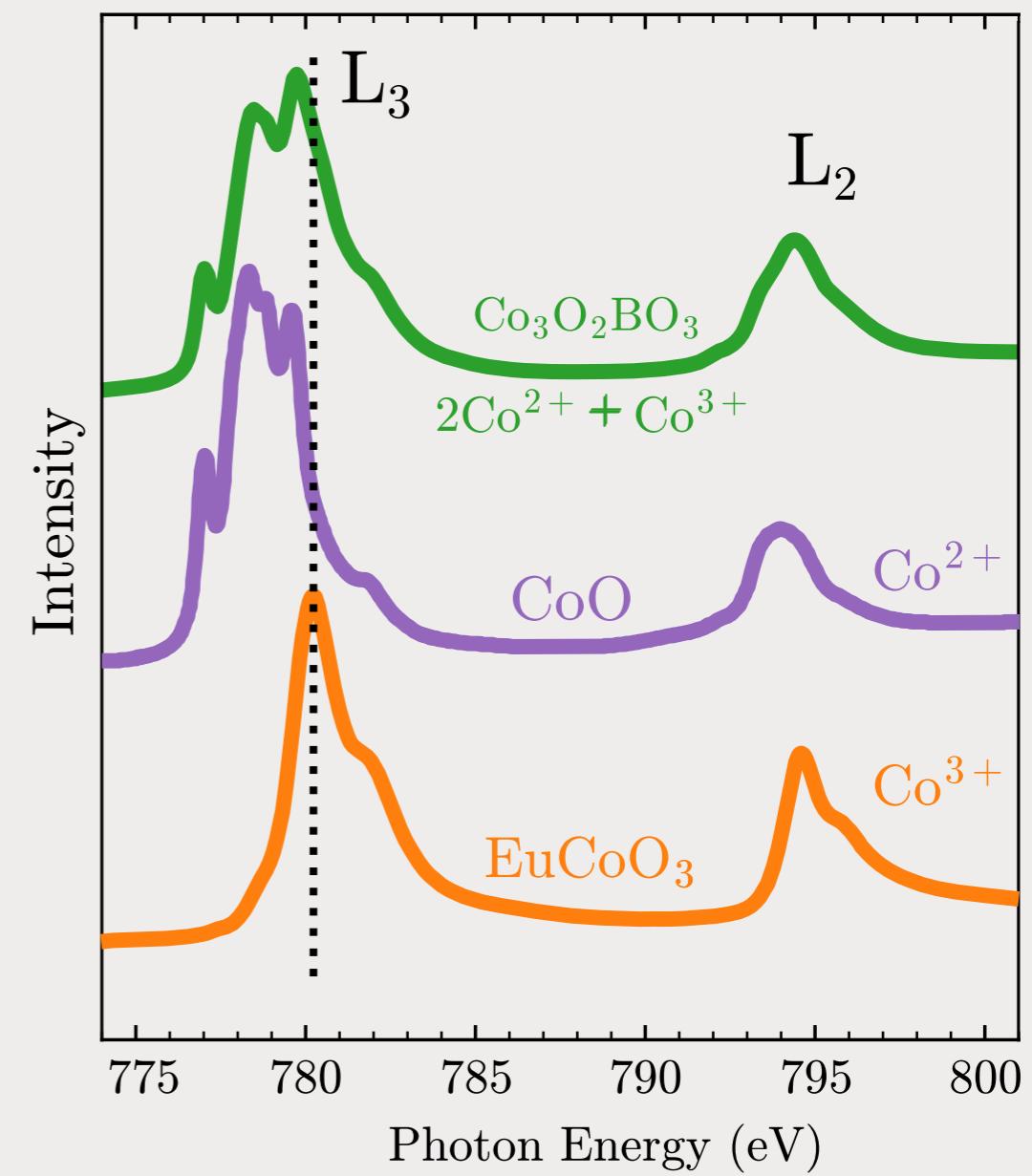
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X-ray absorption spectroscopy



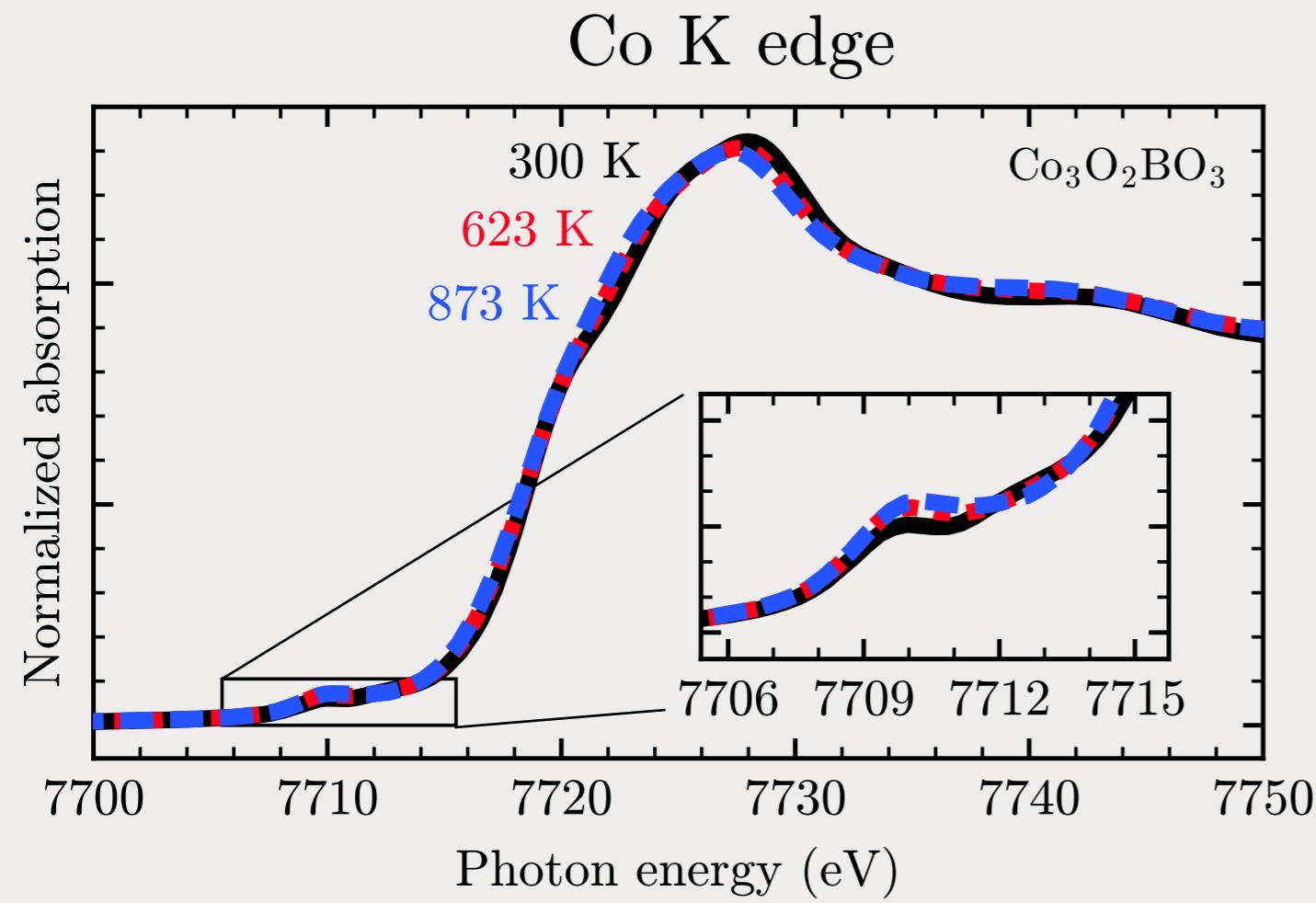
Galdino et al. In preparation

Co L_{2,3} edges



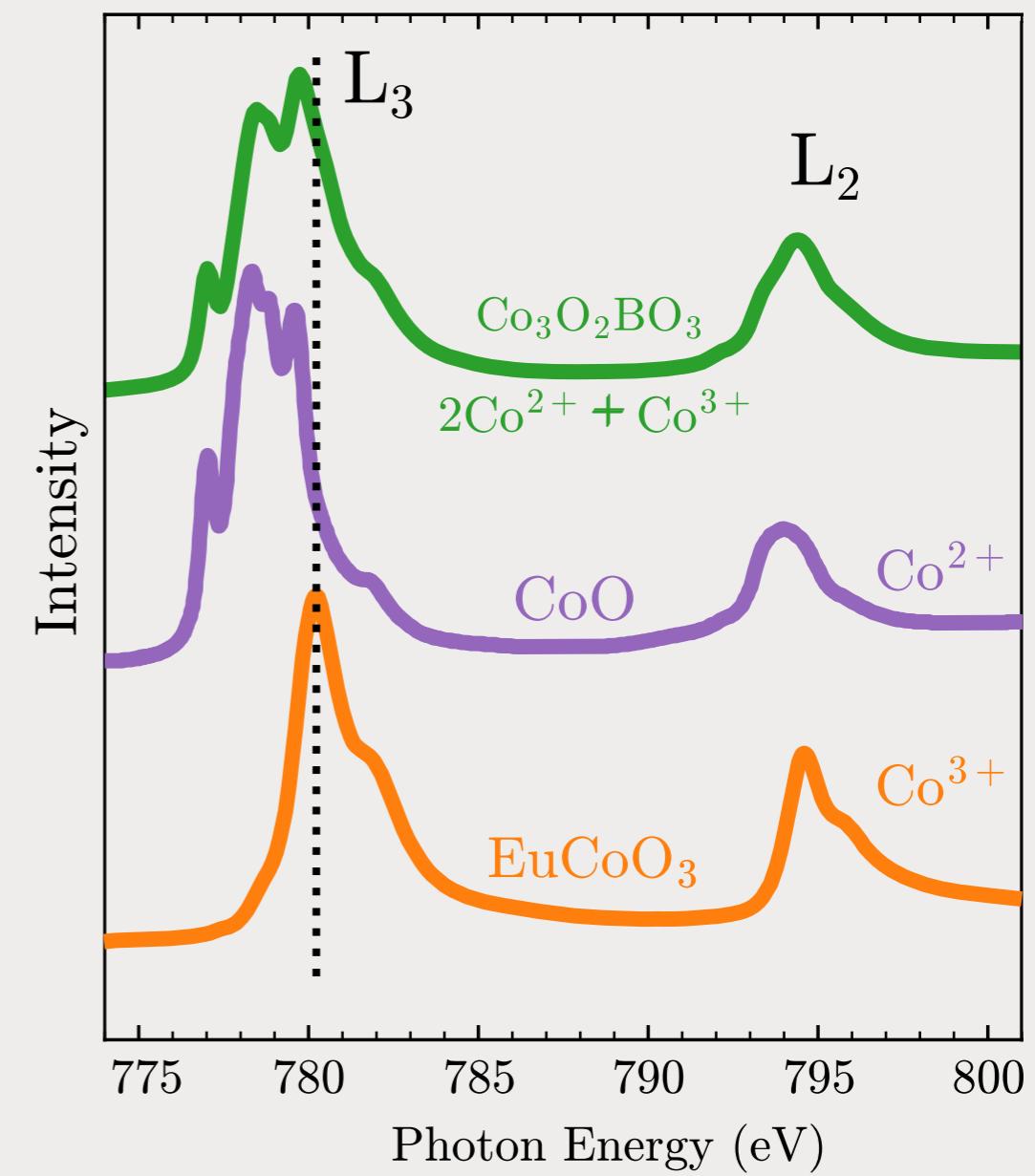
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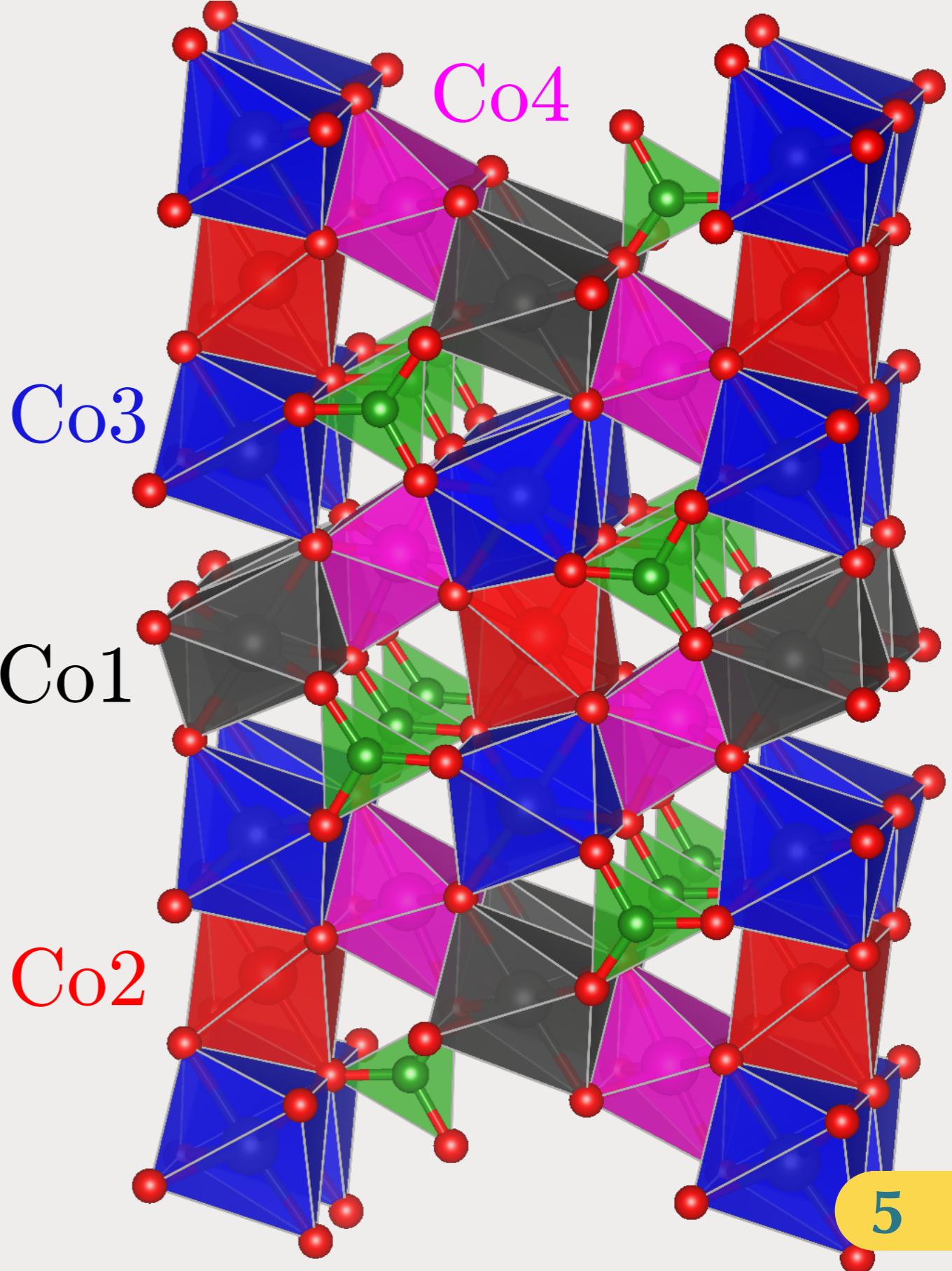
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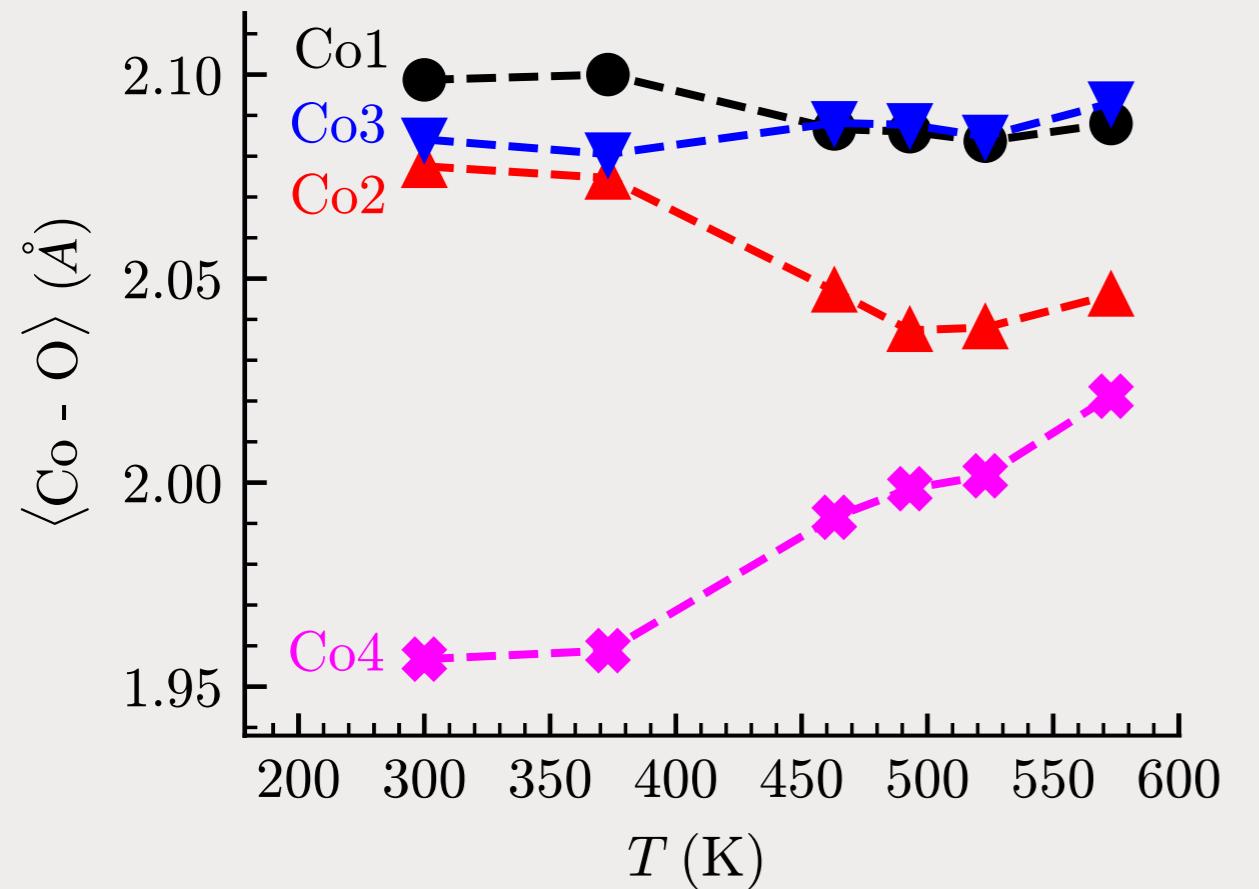


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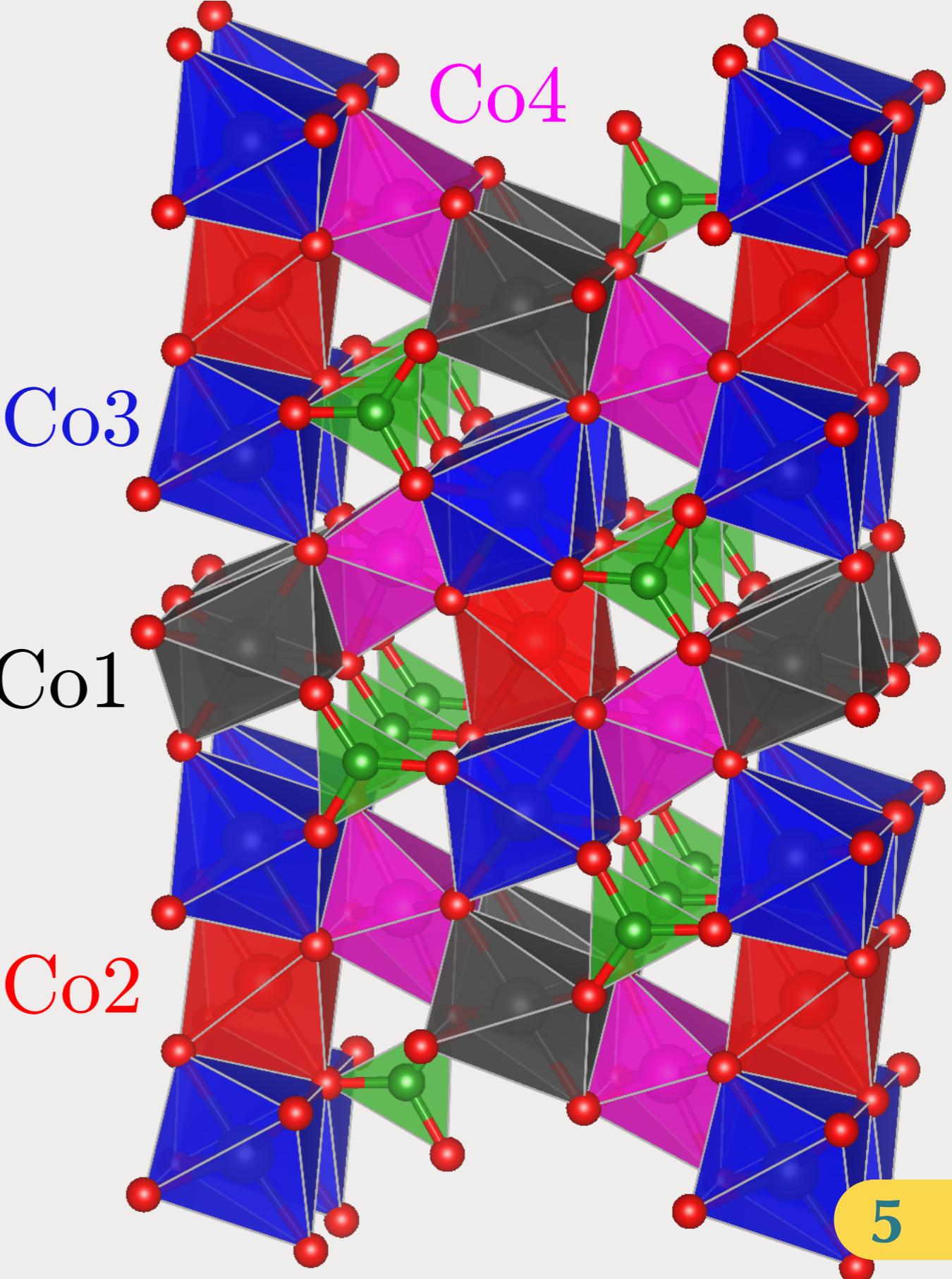
X-ray diffraction (Charge-order)



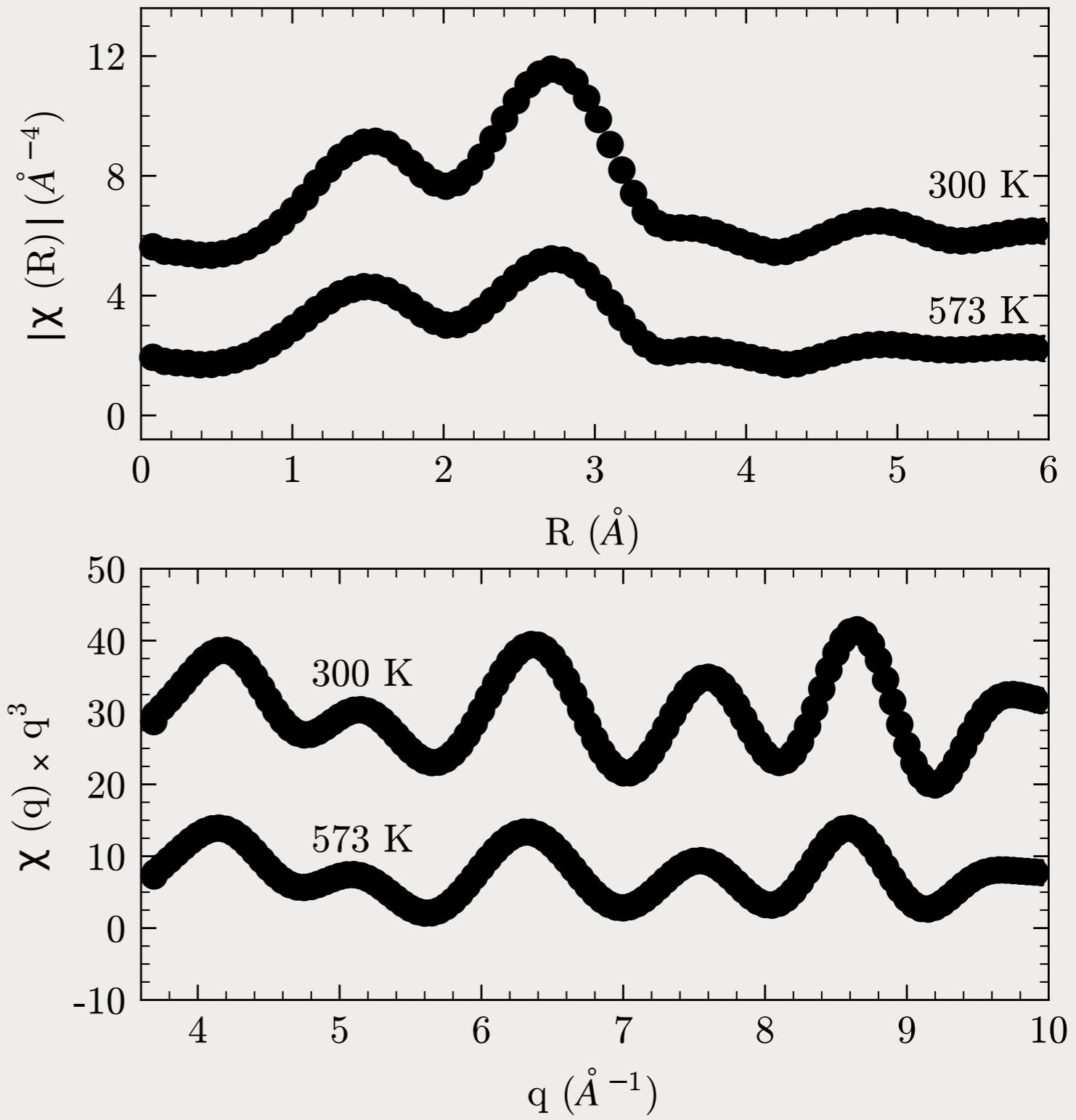
X-ray diffraction (Charge-order)



Galdino et al. In preparation



EXAFS (Local environment)



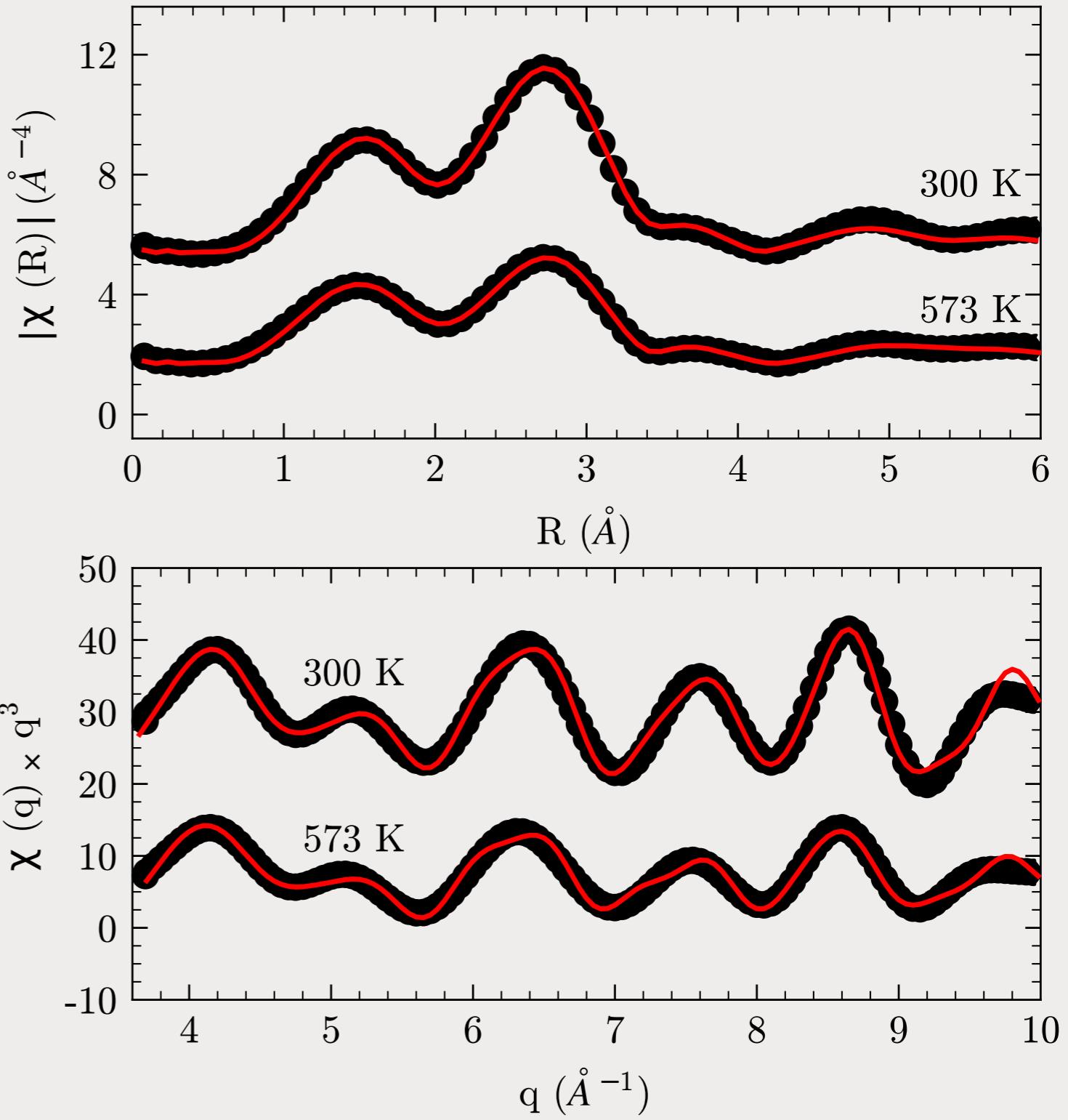
EXAFS (Local environment)

Reverse Monte Carlo

+

Genetic Algorithm

Timoshenki et al. JPCM 26, 55401 (2014)



Local environment (EXAFS)

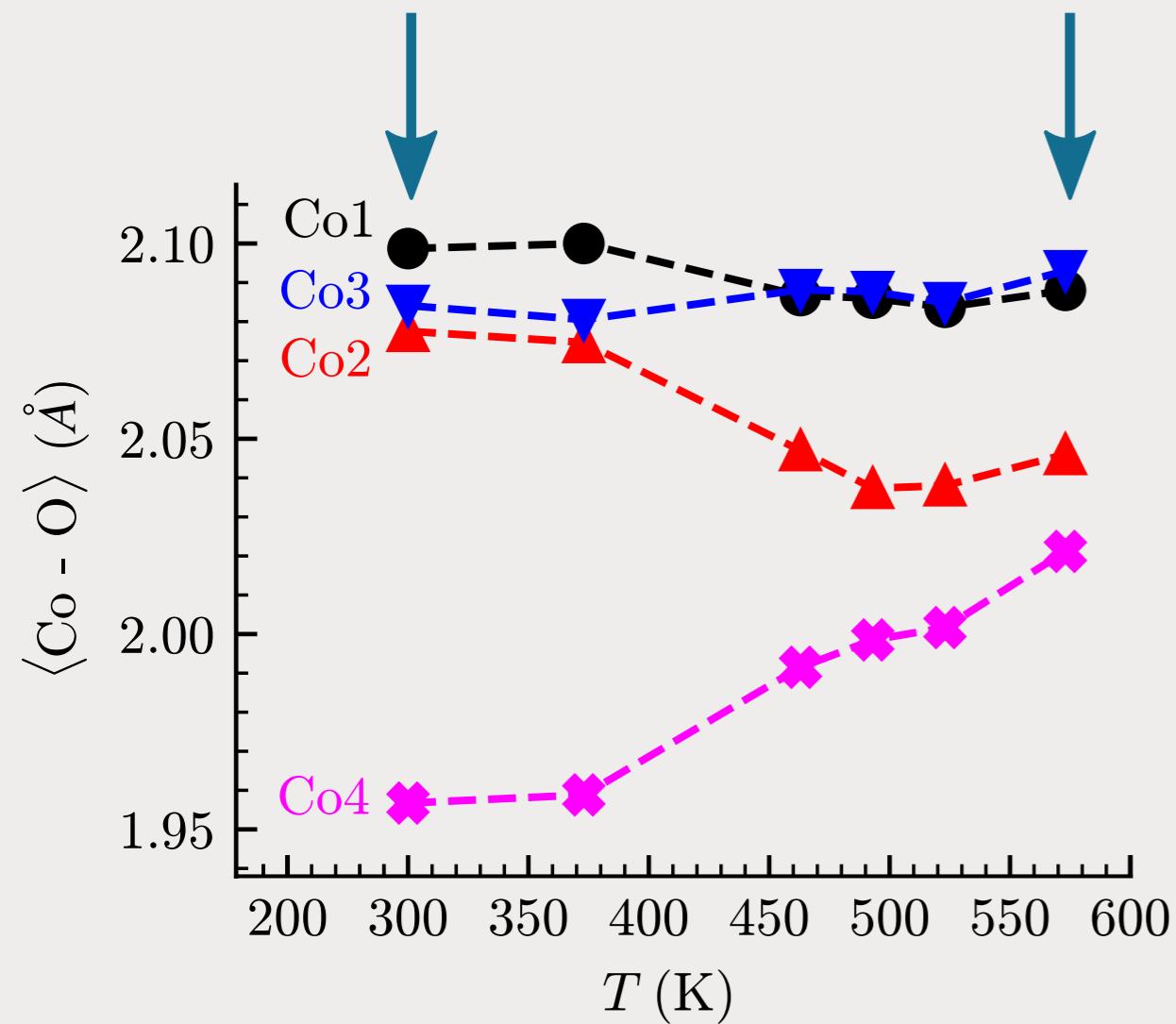
x

Long range order (XRD)

Local environment (EXAFS)

x

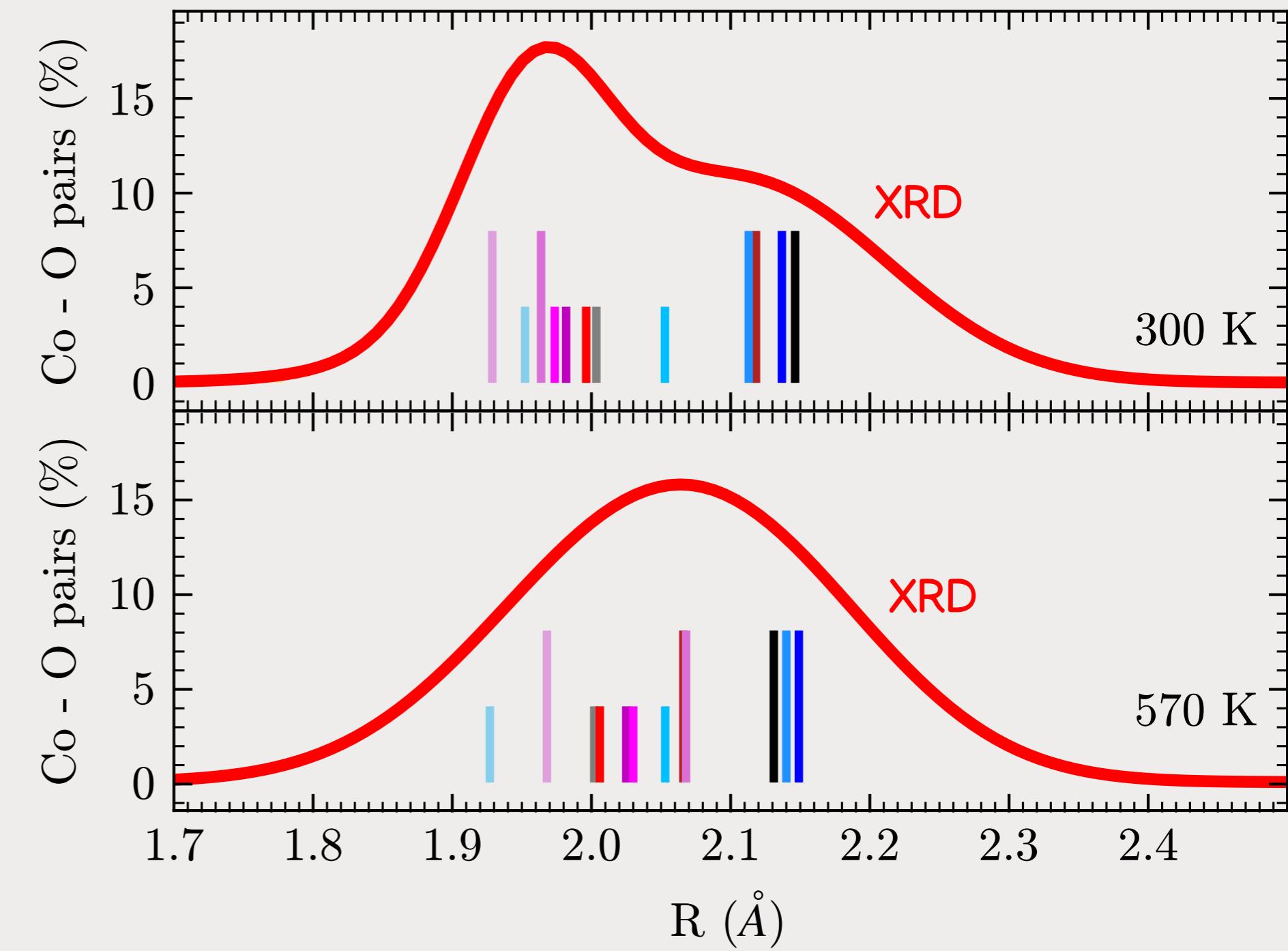
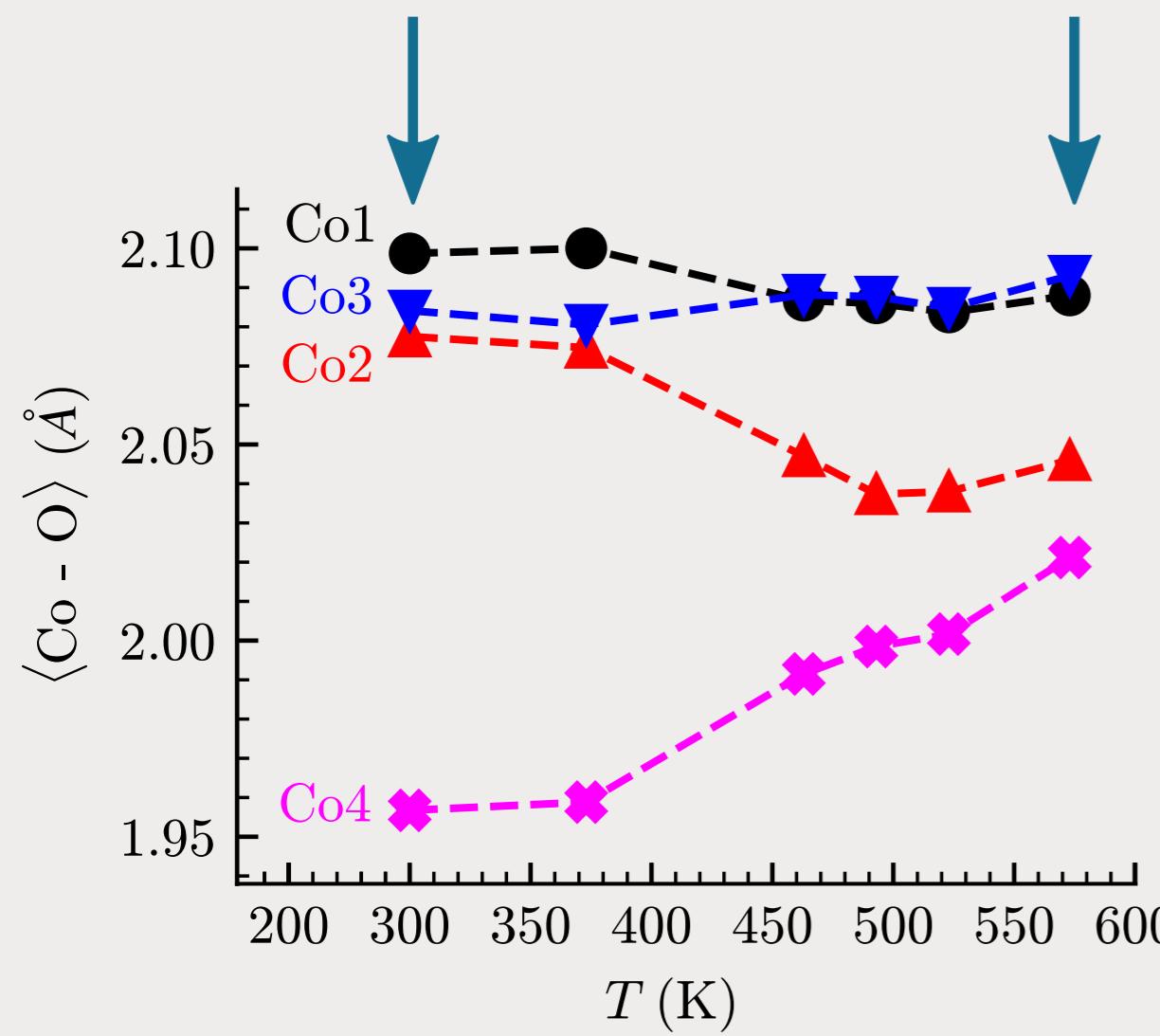
Long range order (XRD)



Local environment (EXAFS)

X

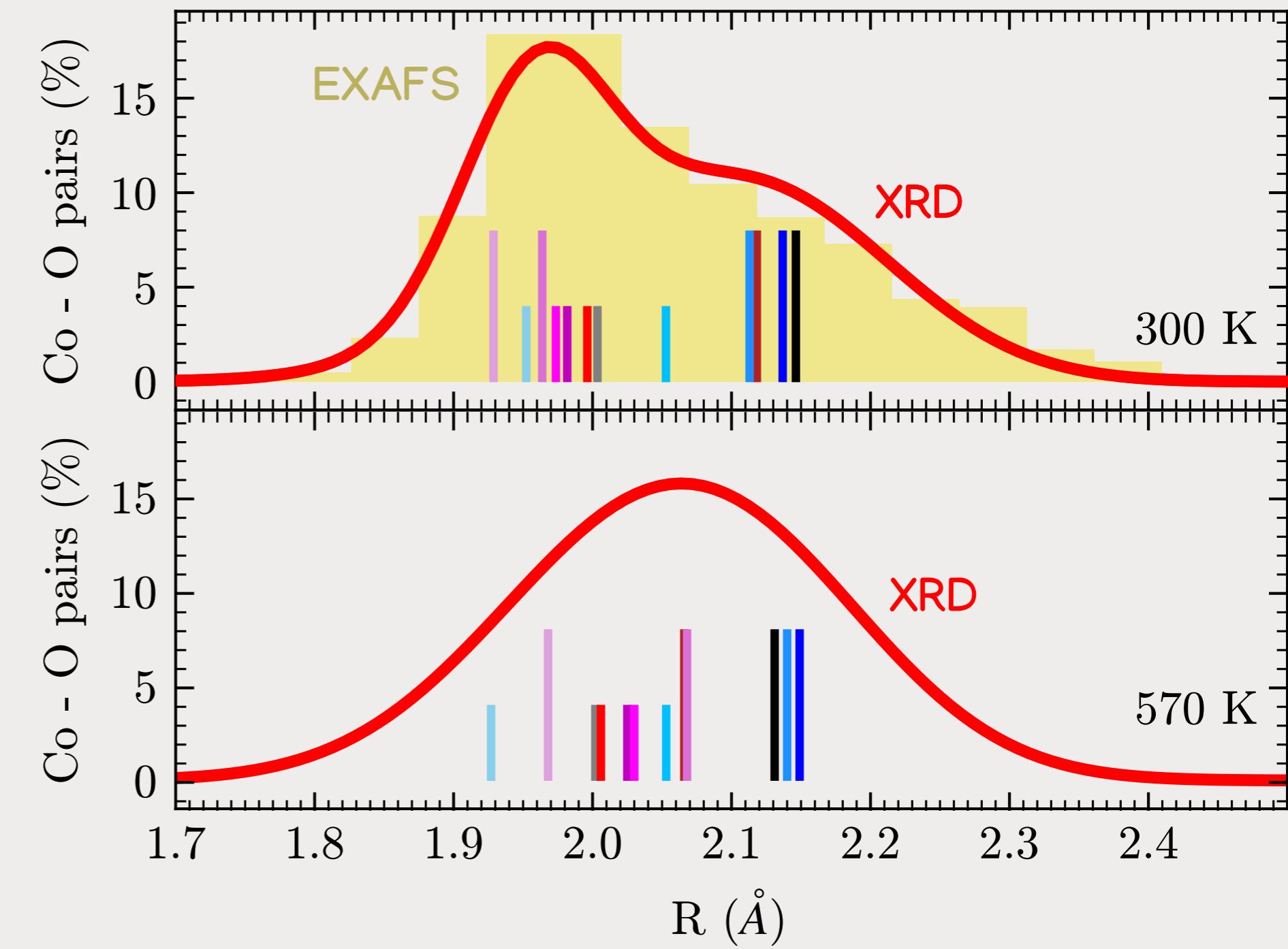
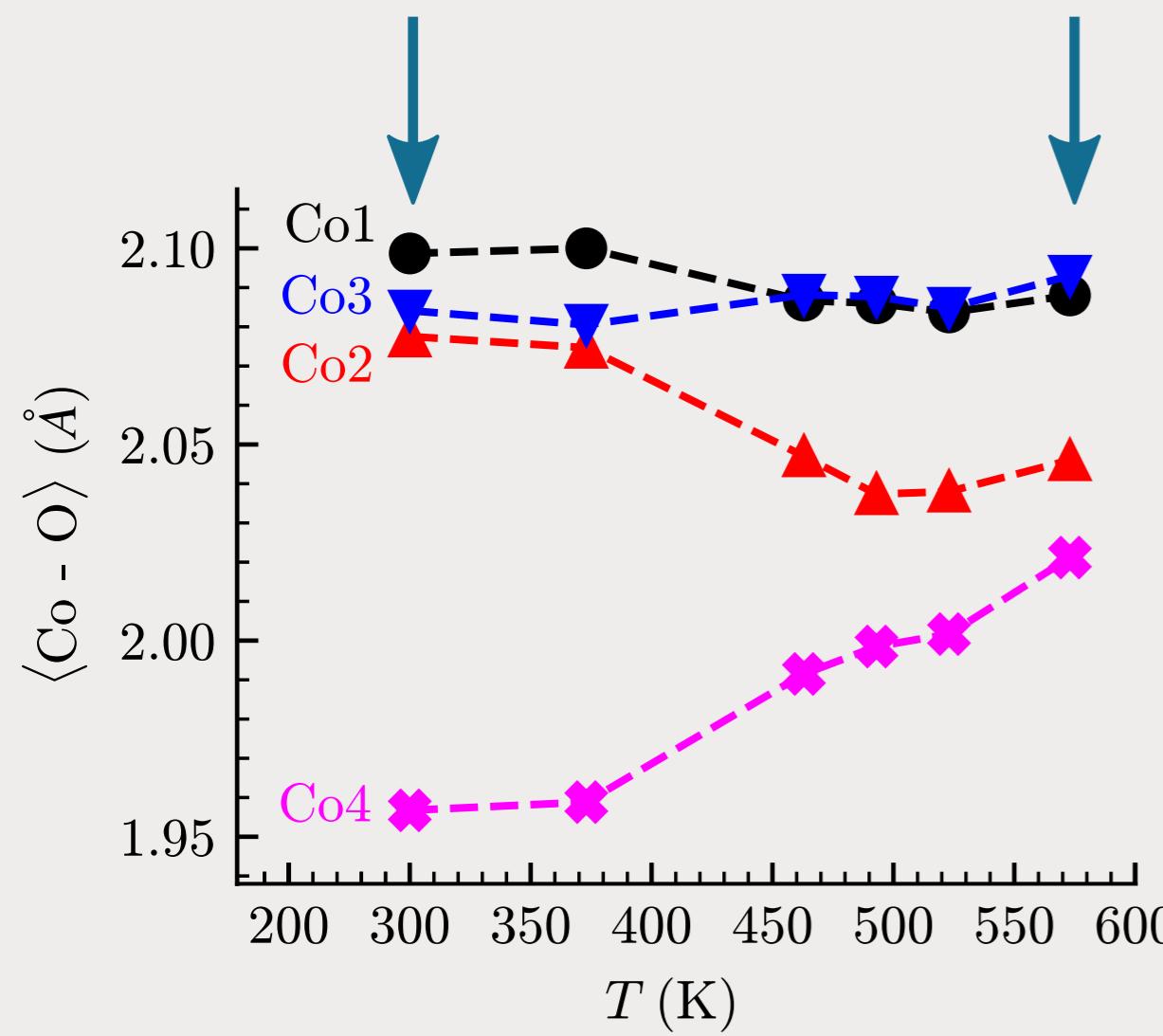
Long range order (XRD)



Local environment (EXAFS)

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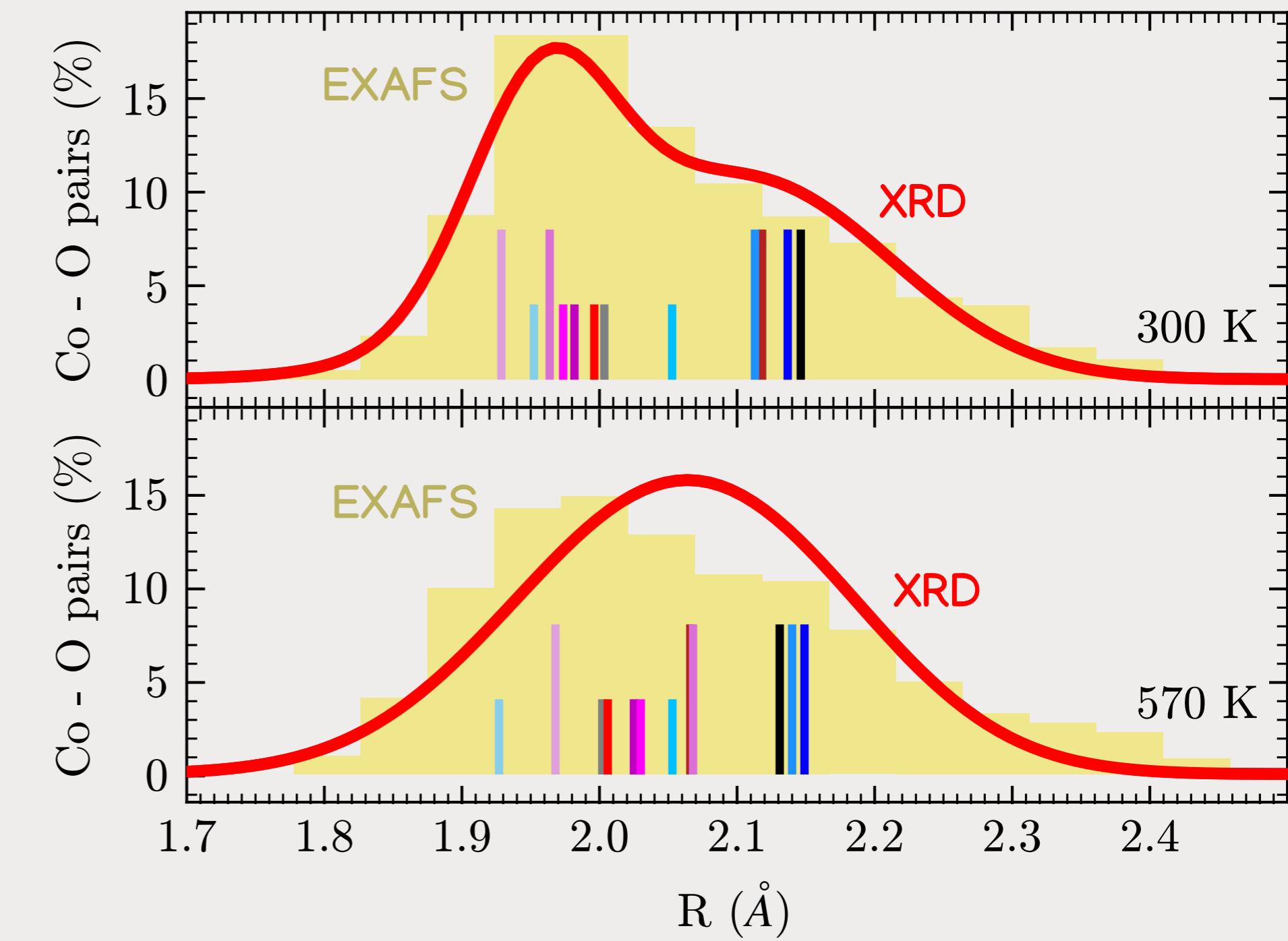
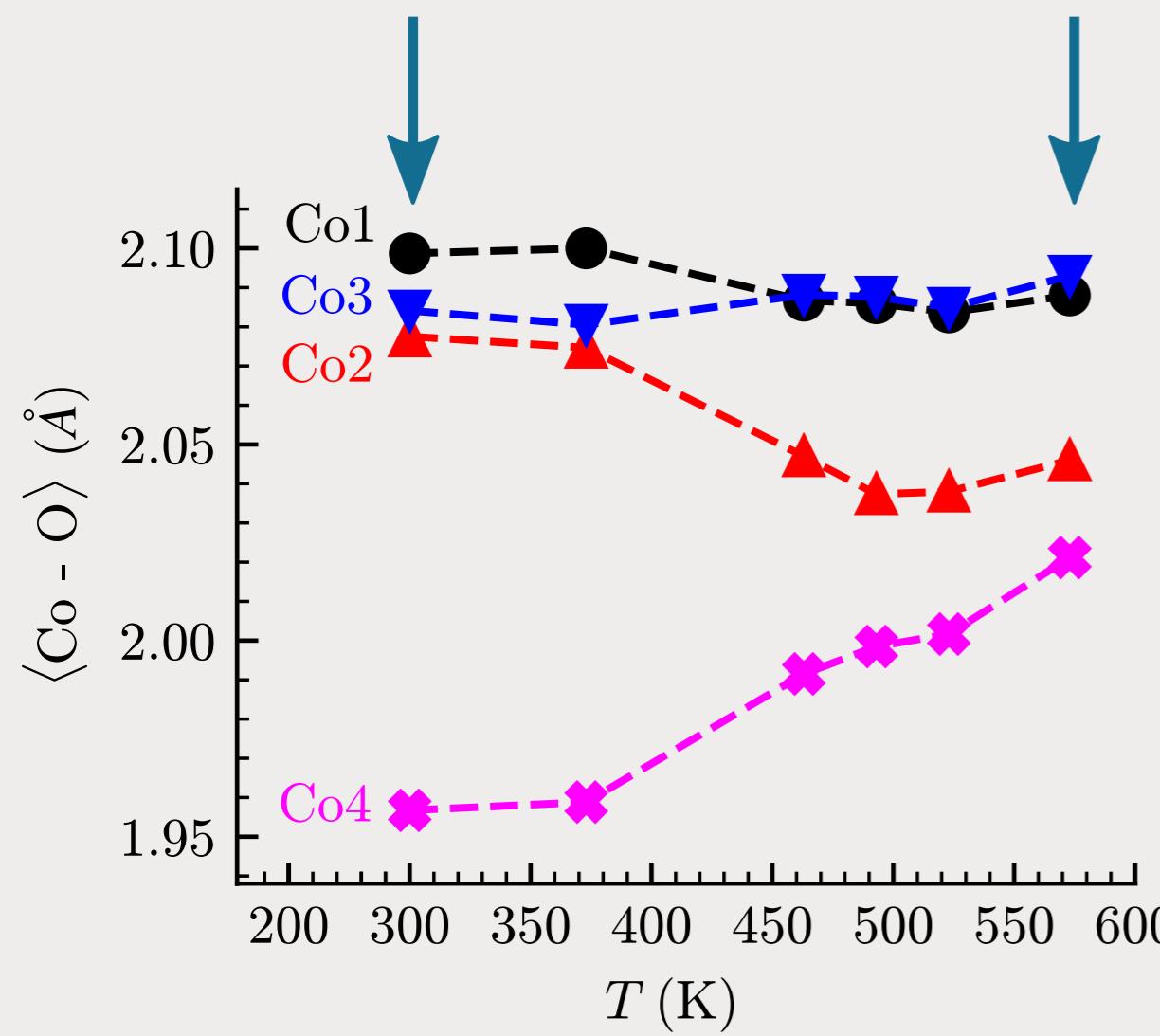
Long range order (XRD)



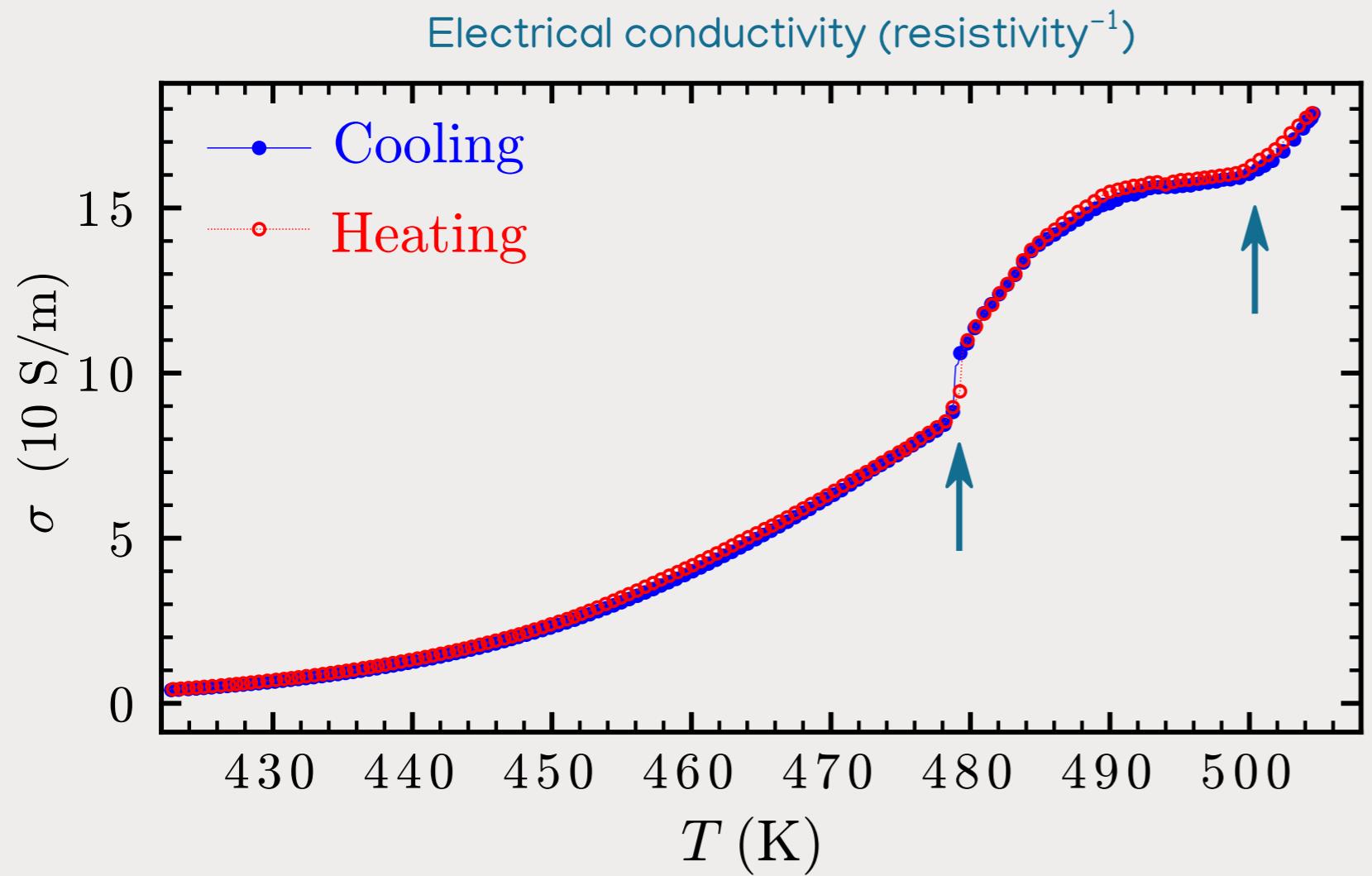
Local environment (EXAFS)

X

Long range order (XRD)

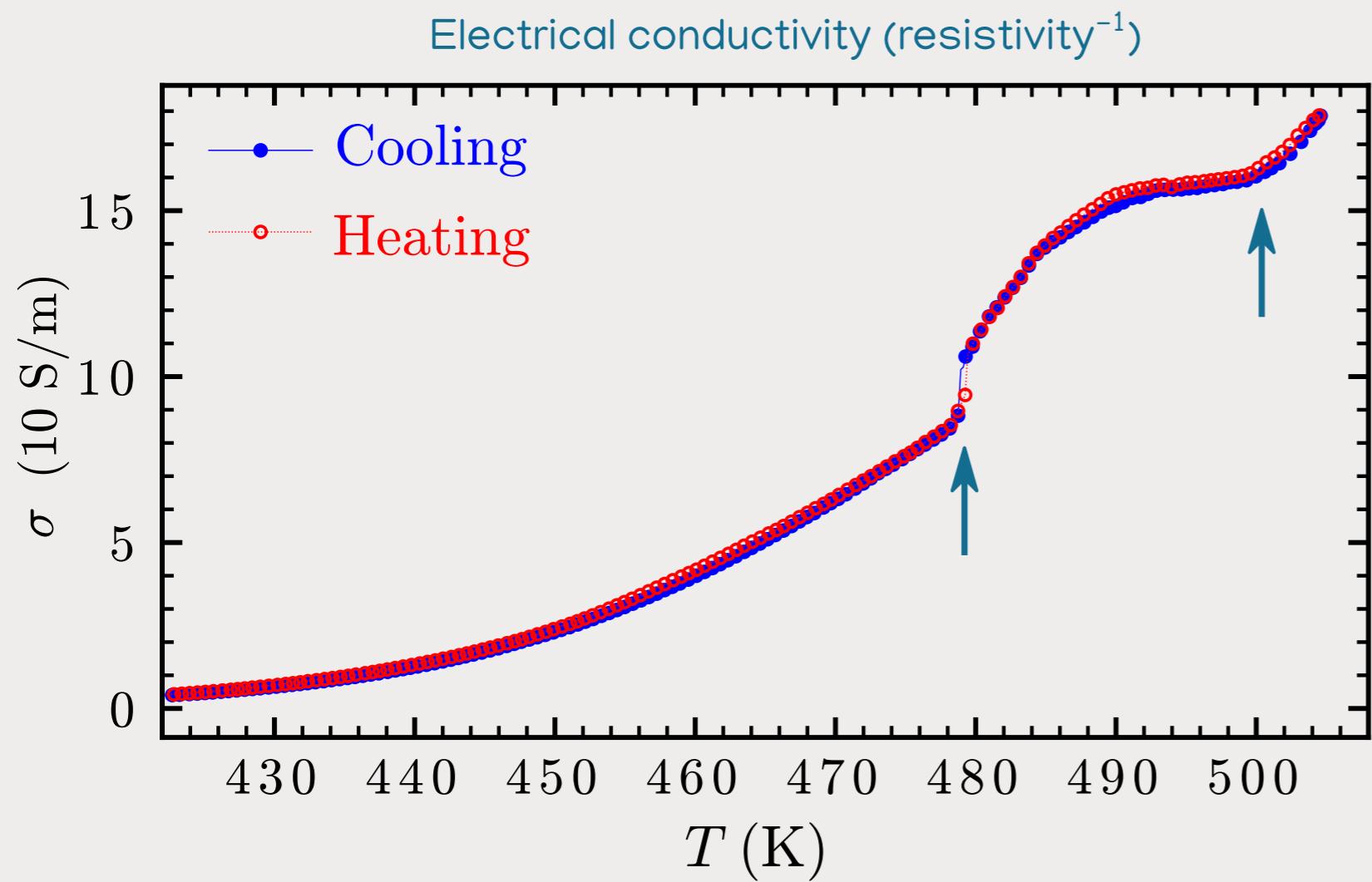


Macroscopic quantities



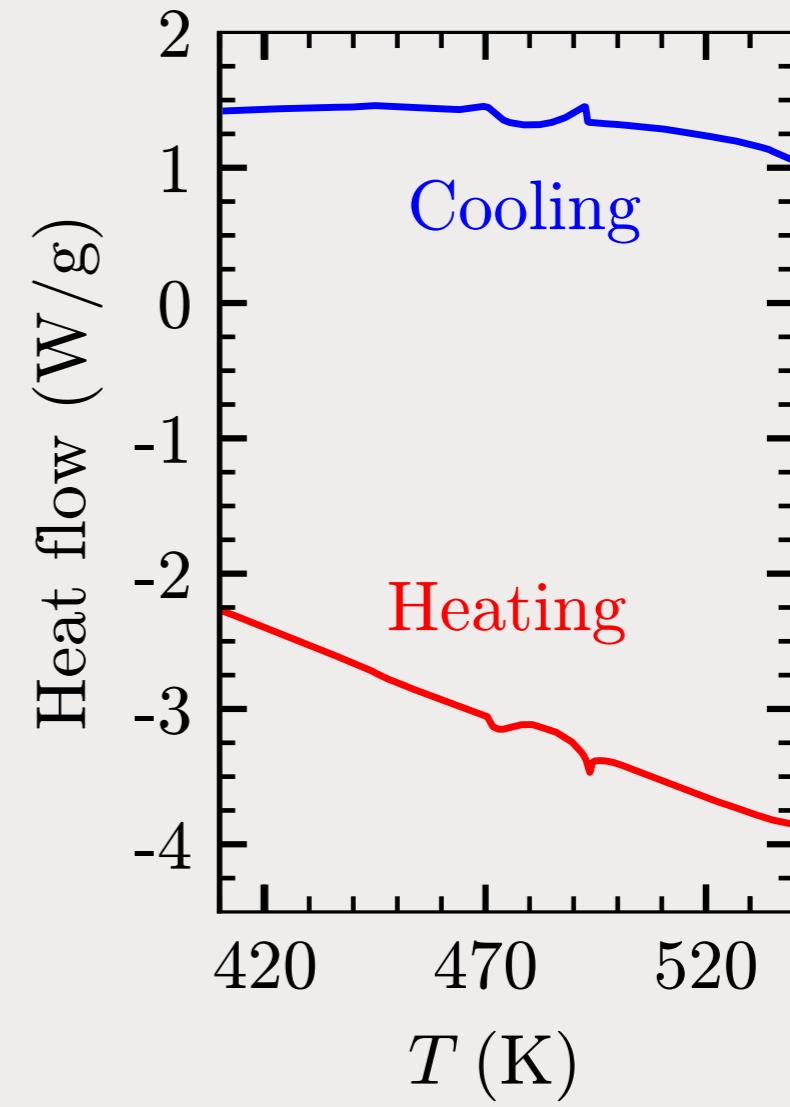
Galdino et al. Phys. Rev. B 100, 165138 (2019)

Macroscopic quantities



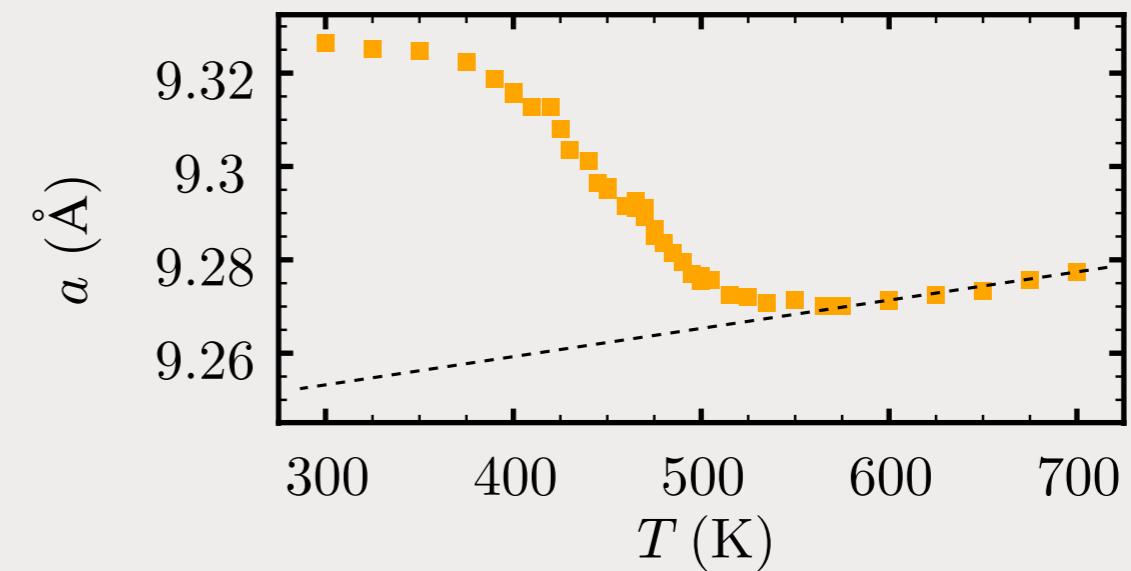
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Differential scanning calorimetry (DSC)

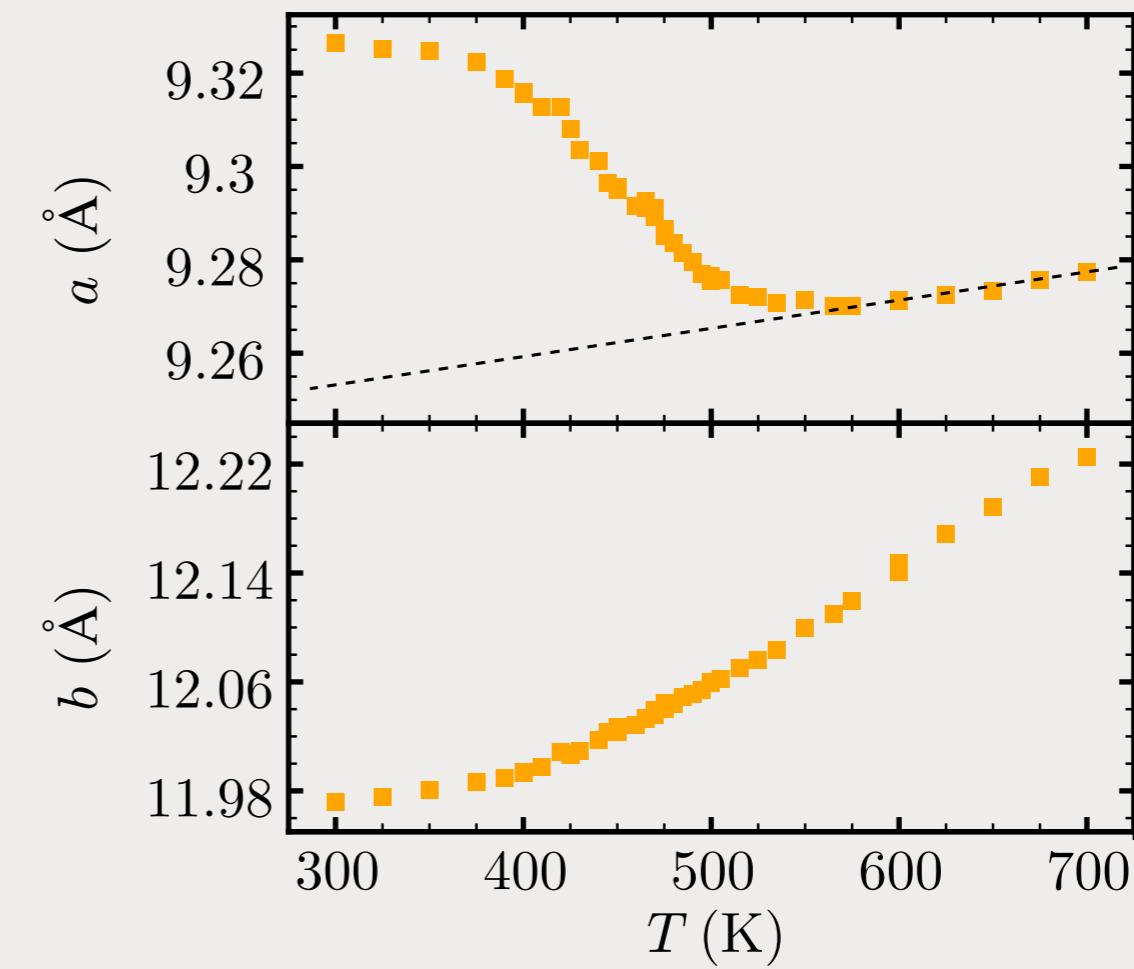


Galdino et al. Phys. Rev. B 100, 165138 (2019)

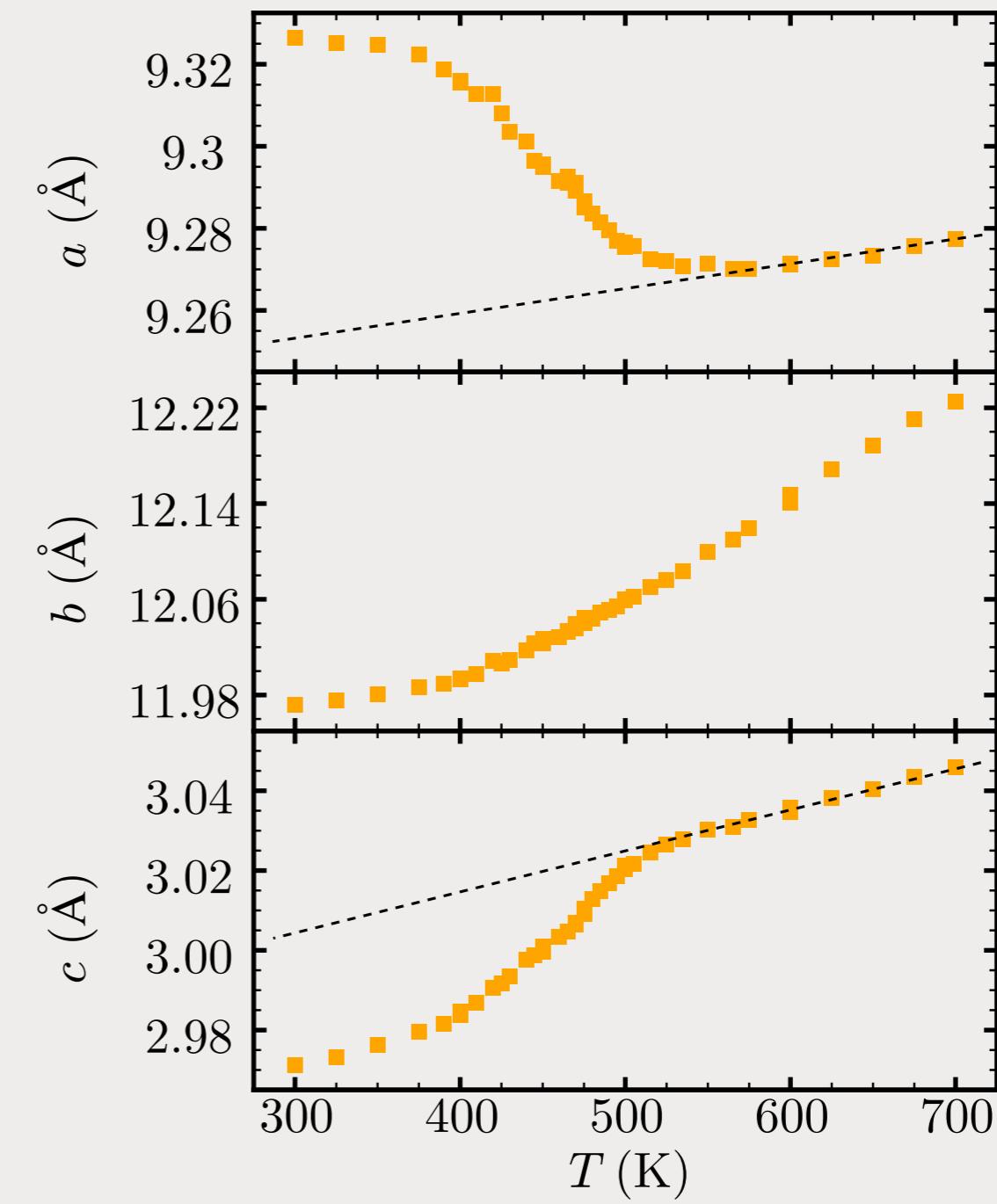
X-ray powder diffraction



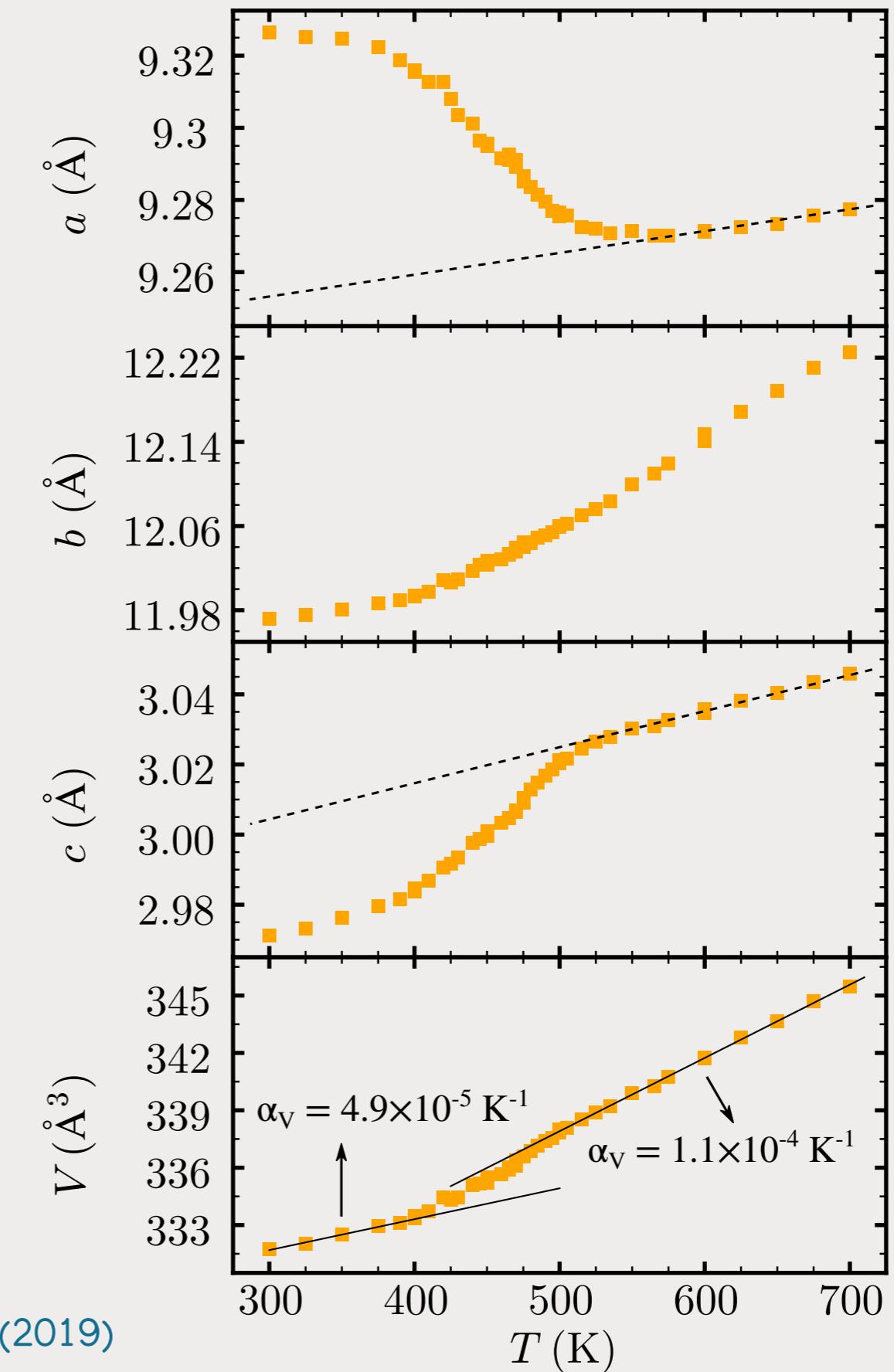
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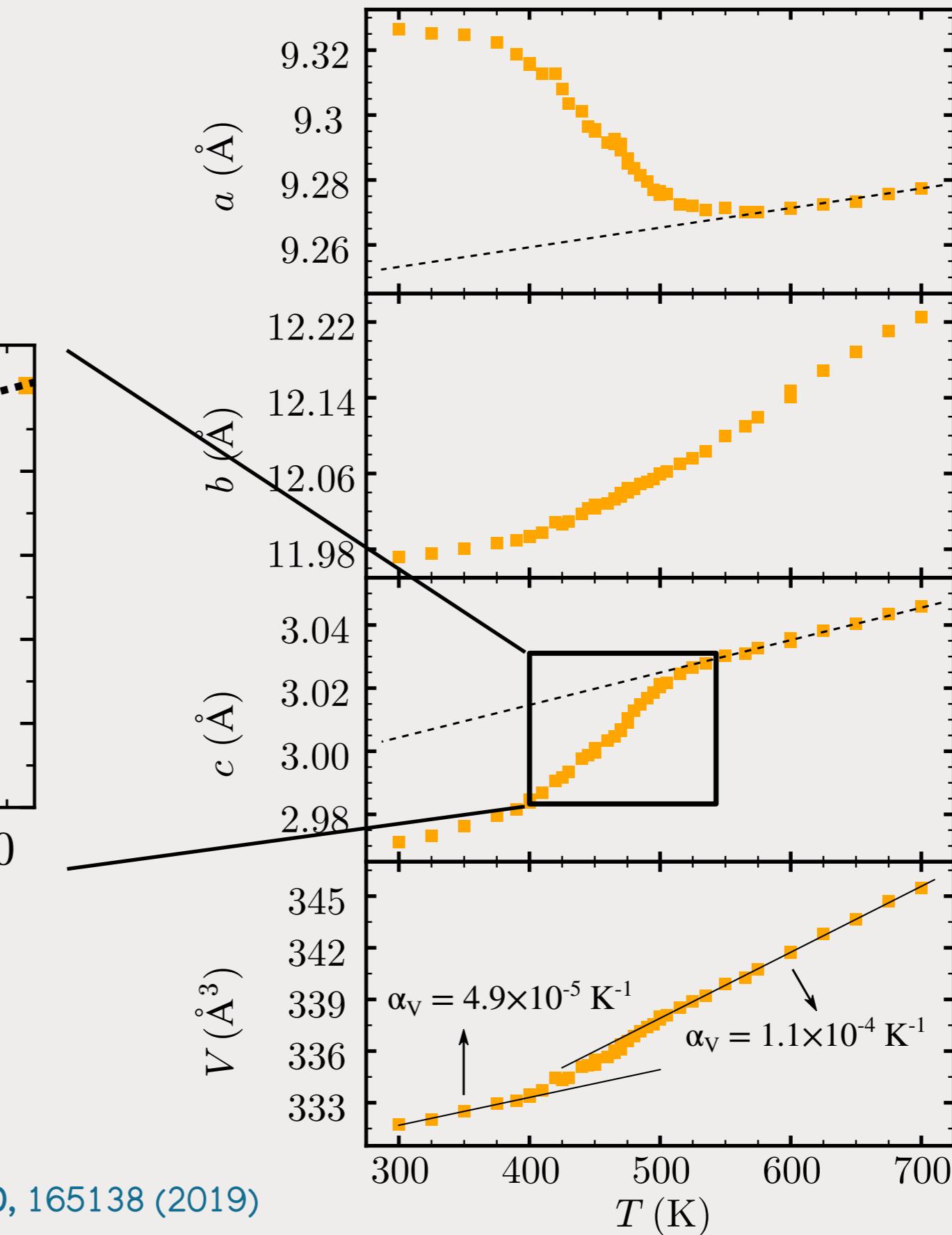
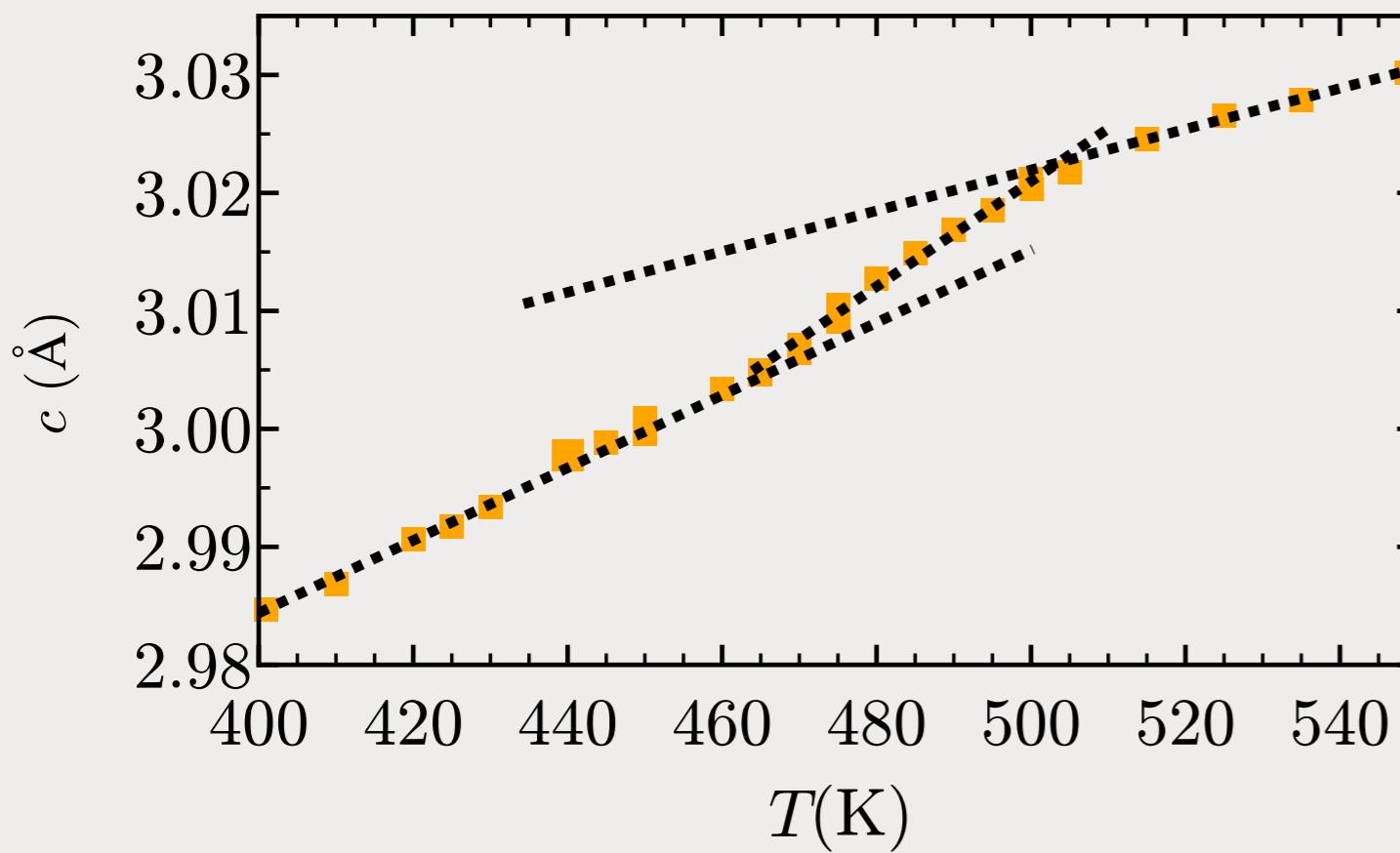
X-ray powder diffraction



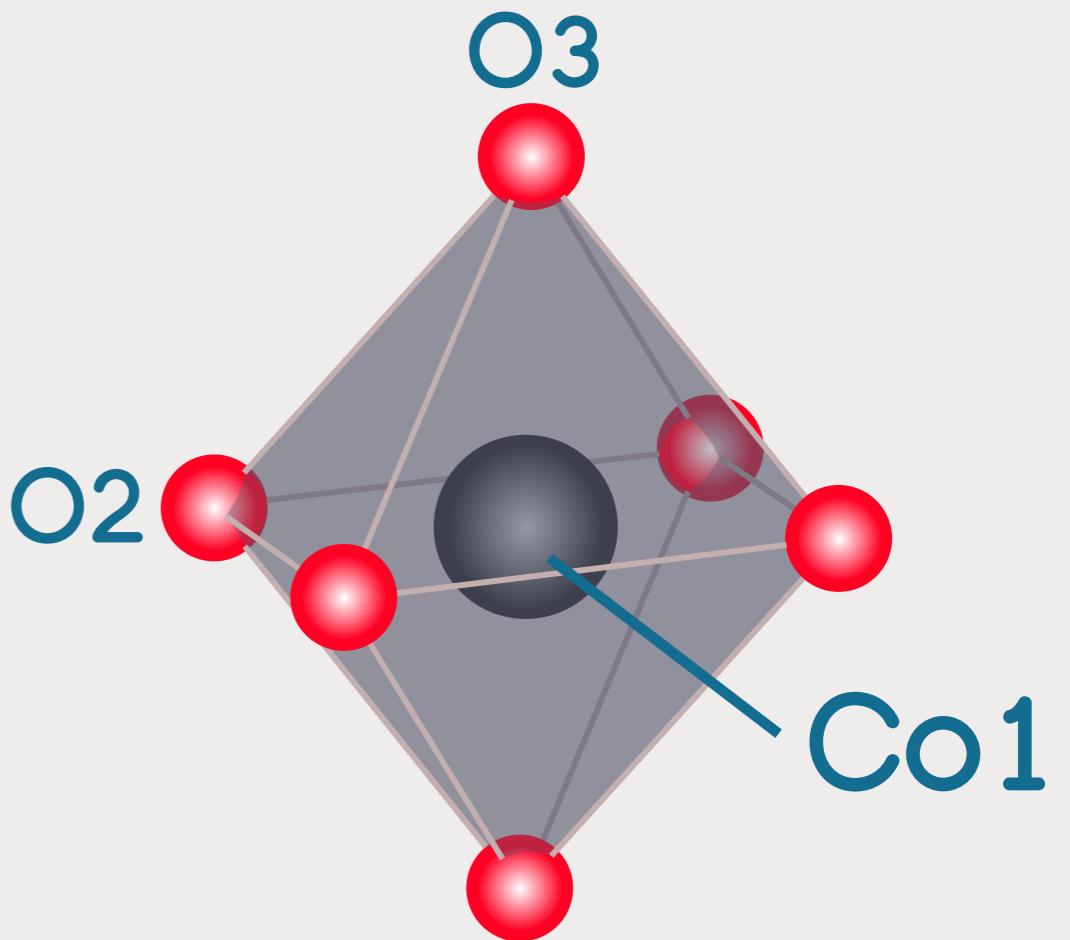
X-ray powder diffraction



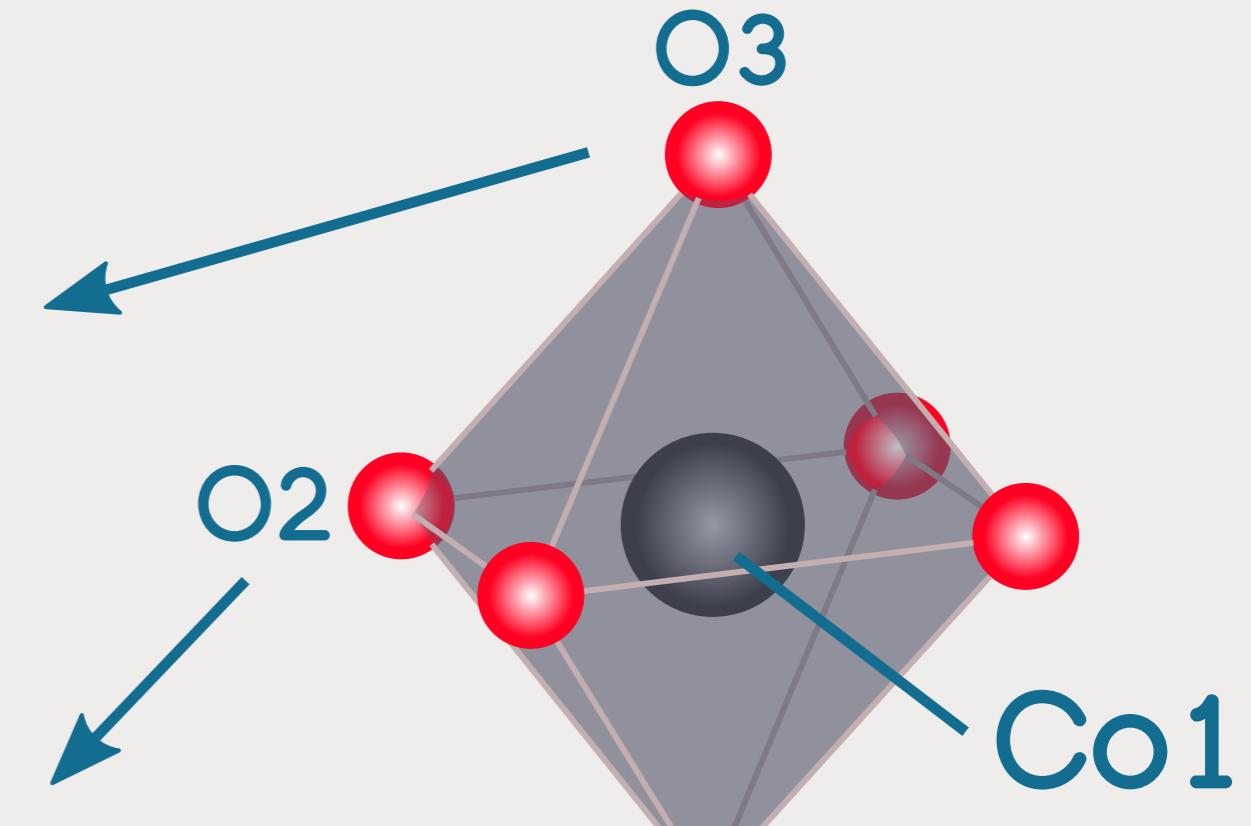
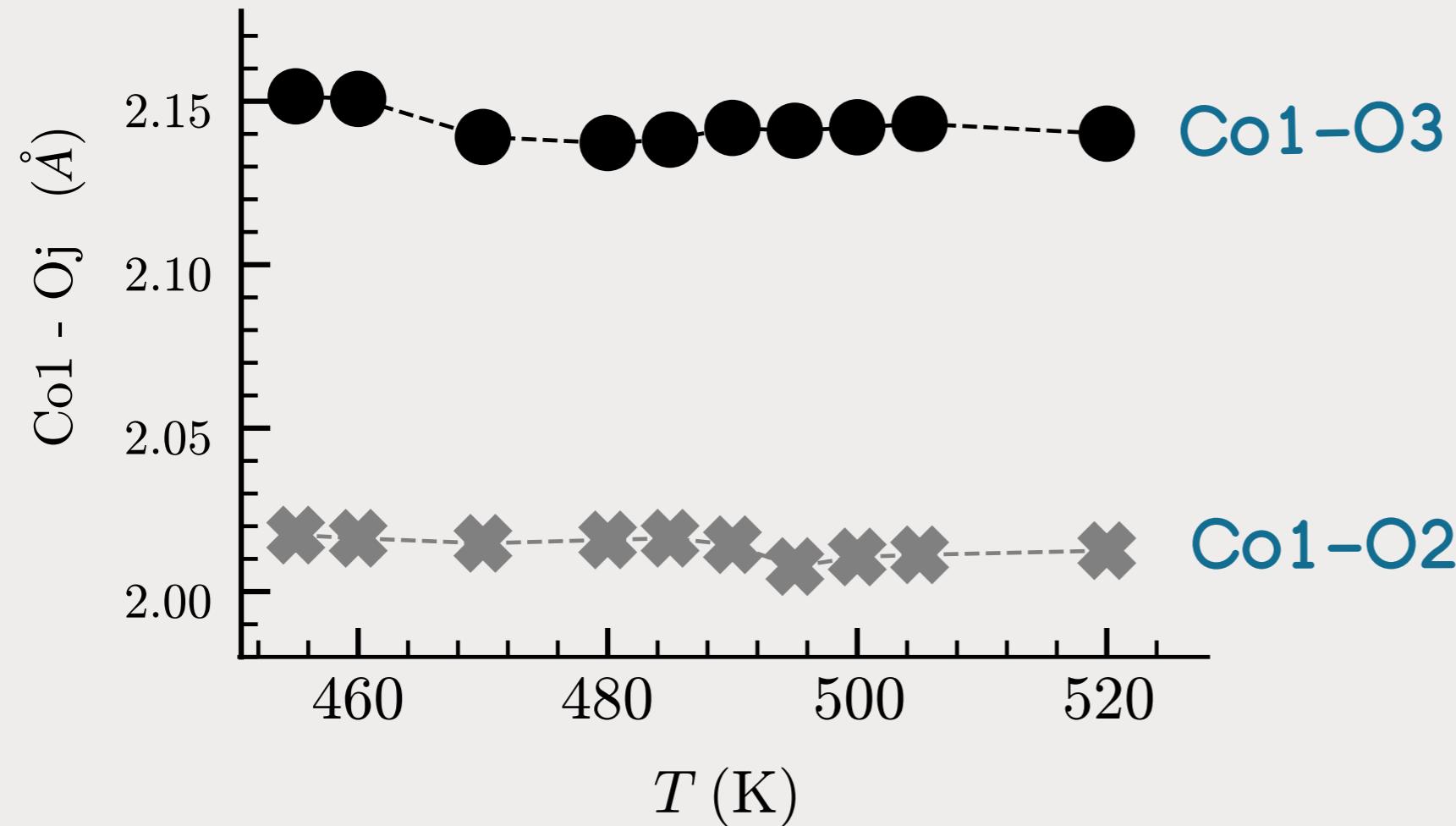
X-ray powder diffraction



Neutron powder diffraction

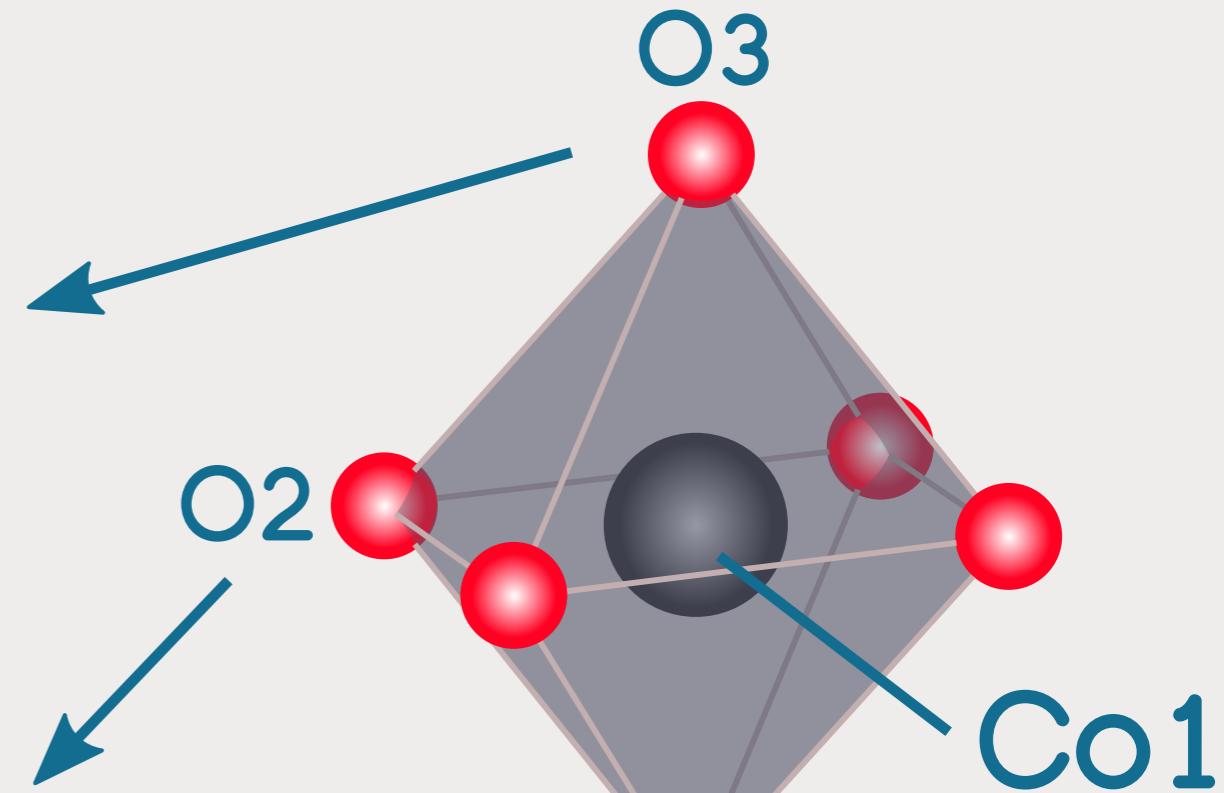
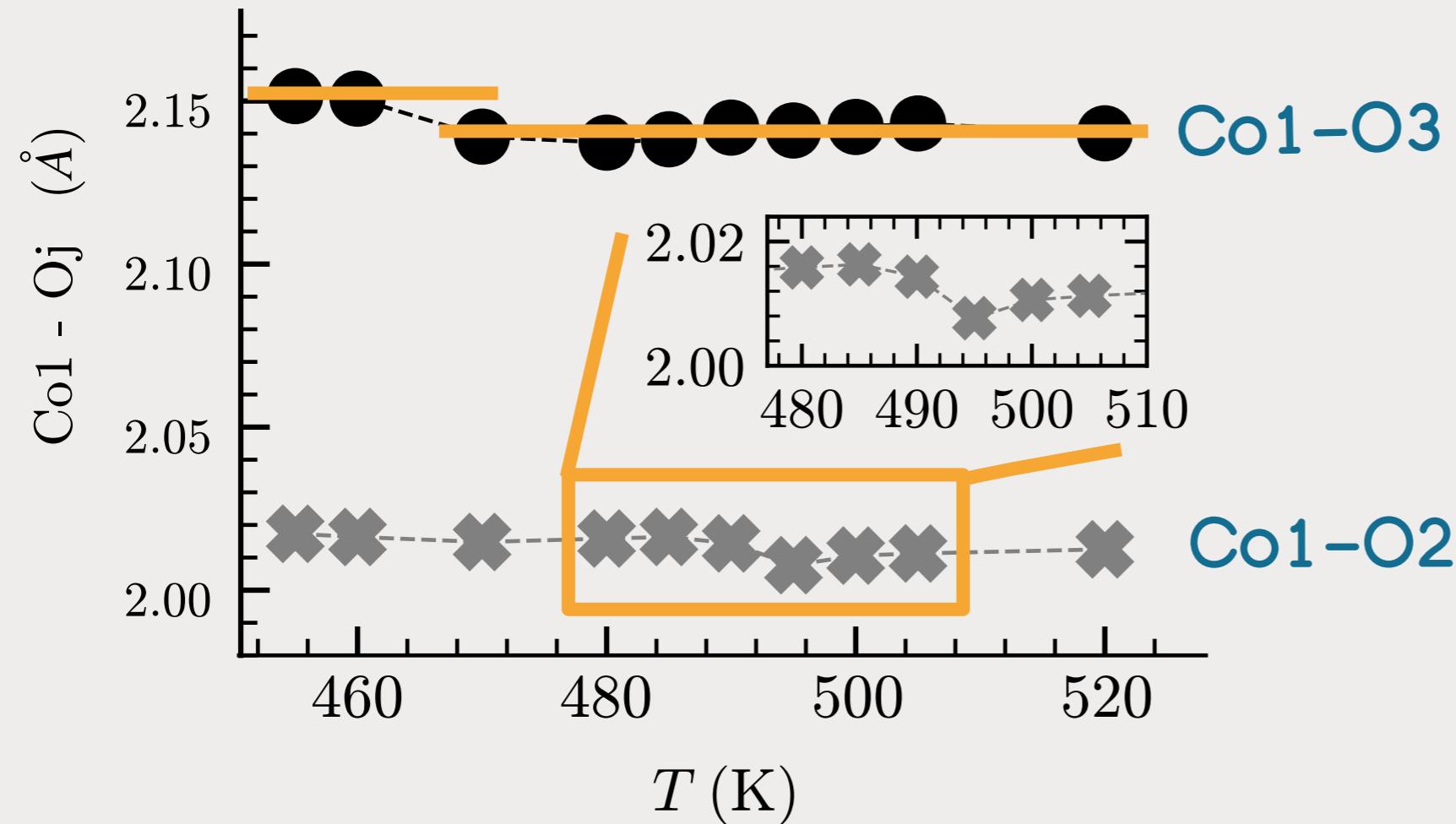


Neutron powder diffraction



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Neutron powder diffraction



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- Gradual charge sharing between specific sites
- Sharp phase transitions between charge-ordered states
- EXAFS x XRD

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- Sharp phase transitions between charge-ordered states
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