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French CRG XAS beamlines Handbook

Hester Blommaert, Mohamed Redhouane Boudjehem, Abdallah Nassereddine, Antonio Aguilar-Tapia, Robin Arnaud, D Borschneck, Perrine Chaurand, Julio Cesar da Silva, Jean-Louis F Hazemann, Zoltan Hubert, et al.

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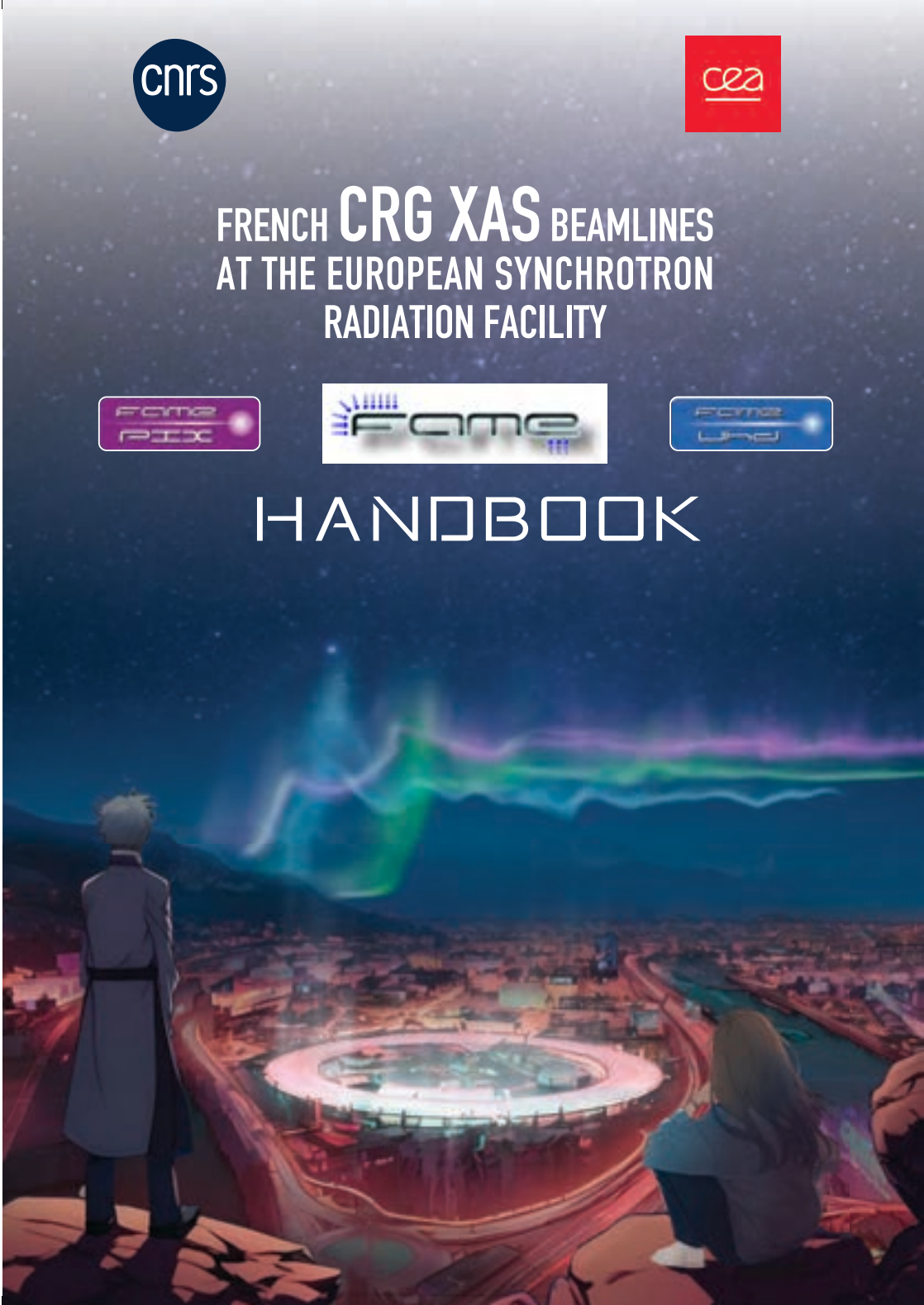
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FRENCH **CRG XAS** BEAMLINES AT THE EUROPEAN SYNCHROTRON RADIATION FACILITY

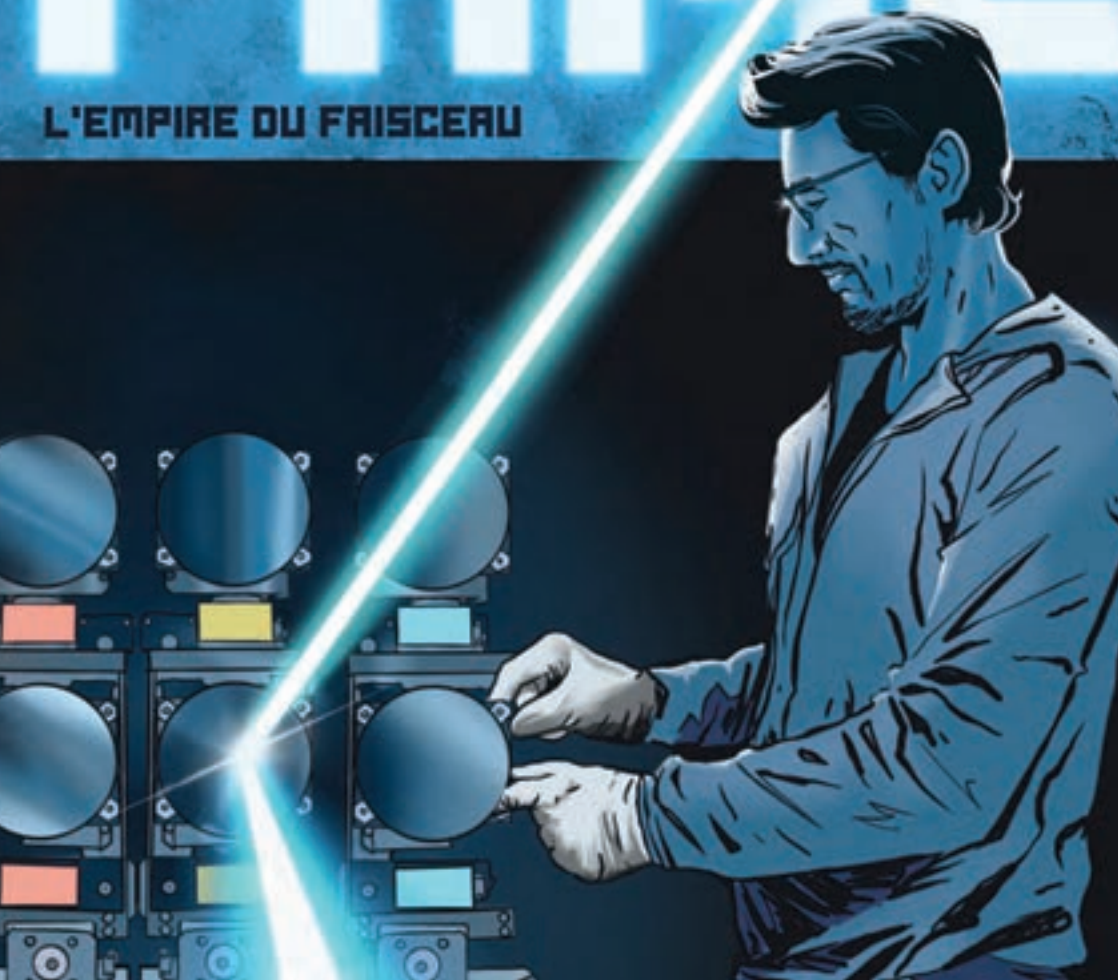


HANDBOOK



FRANCE

L'EMPIRE DU FAISCEAU



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Version 1 - 2025

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The beamlines

FAME gathers two instruments dedicated to X-ray absorption spectroscopy. FAME-PIX is the French Absorption spectroscopy beamline in Material and Environmental science - Ptychography Imaging with X-ray. FAME-UHD is the French Absorption spectroscopy beamline in Material and Environmental sciences at Ultra-High Dilution.

<https://www.esrf.fr/home/UsersAndScience/Experiments/CRG/BM30.html>

<https://www.esrf.fr/home/UsersAndScience/Experiments/CRG/BM16.html>

Both instruments are French Collaborating Research Group beamlines at the European Synchrotron Radiation Facility.

FAME-PIX and FAME-UHD projects are financially supported by the French “grand emprunt” EquipEx (MAGNIFIX, ANR-21-ESRE-0011), the French “Programmes et équipements prioritaires de recherche” (DIADEM), the CEA-CNRS CRG consortium and the INSU CNRS institute.

ASTER'X

A thematic school, ASTER'X, is organized each year in Grenoble since 2021. This school focuses on training scientists using X-ray absorption techniques, X-ray emission spectroscopy, and X-ray imaging (tomography and ptychography), with lectures, tutorials and practicals. Speakers of the last sessions were Antonio Aguilar Tapia¹, Daniel Borschneck², Redhouane Boudjehem³, Perrine Chaurand², Julio Cesar Da Silva³, Jean-Louis Hazemann³, Yves Joly³, Isabelle Kieffer⁴, Anico Kulow³, Eric Lahera⁴, Manuel Muñoz⁵, Olivier Proux⁴, Mauro Rovezzi⁴, Denis Testemale³, Vladimir Vidal², with the support of Françoise Mollier-Sabet³ & Florence Fernandez³ for the management and communication, and Caroline Scatigno⁶ for the pedagogical organization.

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Introduction

This handbook aims at gathering information needed during a XAS experiment, or to prepare it, starting by a general description of a XAS beamline and a checklist (do I have all the needed information at the end of my experiment?), followed by several sheets on the XAS subject.

This handbook also gathers characteristic data of the elements in their pure state (such as the metallic state for most of the elements):

- absorption edge energies (or electron binding energies),
- natural width of these edges,
- X-ray fluorescence line energies,
- X-ray fluorescence line natural width.

Several databases are available, scientists are still working on the subject to improve the precision of the values. We tried to compare the different values, not to determine which is the best one but to show the necessity to always cite which database is used.

Used literature is in the bibliography, but one has to cite here two essential sources:

X-ray Data Booklet: <https://xdb.lbl.gov/>
<https://xraydb.xrayabsorption.org/>

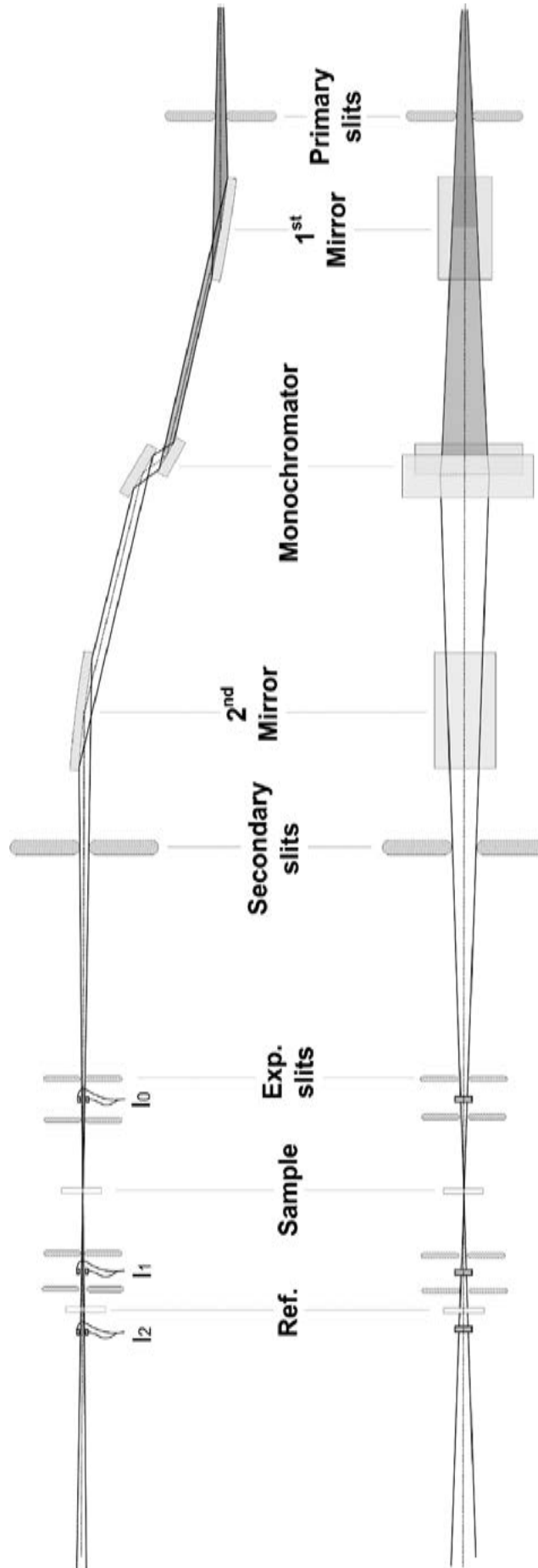
Finally, this handbook presents a compilation from the literature of the emission line shifts for the transition metals and a selection of XAS spectra of several model compounds.

Beamline optical constituents

Main constituents of FAME-PIX and FAME-UHD beamlines are the following:

- Primary slits. Delimitation of the X-ray fan delivered by the source in the storage ring. Adaptation of the vertical and horizontal divergences to the optical acceptances in both directions. The slits are cooled down with water as they are illuminated by the white-beam.
- 1st mirror. Collimation of the white-beam in the vertical direction. Harmonic rejection. After the mirror we have the so-called pink-beam.
- Monochromator. Monochromatization of the beam. Horizontal (sagittal) focusing on the sample.
- 2nd mirror. Focusing of the beam on the sample in the vertical direction. Harmonic rejection
- Secondary and experimental slits. “Cleaning” of the beam by removing all the spurious photons (scattered by the optical element edges).
- X-ray monitors. Measurement of the X-ray photons intensities (using Si photodiodes): I_0 , I_1 and I_2

Beamline optical constituents



Mandatory information to describe an experiment

The mandatory technical information necessary to describe X-ray Absorption Spectroscopy (in conventional or High Energy Resolved Fluorescence Detected mode) and X-ray Emission Spectroscopy measurements are the following (with typical details as examples):

Optical systems:

- 1) monochromator crystals (“2-crystal variable-exit monochromator equipped with Si220 crystals”),
- 2) mirrors surrounding the monochromator (“Si mirrors covered by a Rh layer at a n mrad incidence angle”),
- 3) beam-size on the sample (“200x100 μ m Full-Width at Half Maximum”)

X-ray detection systems:

- 1) Incident and transmitted X-ray intensities (“ I_0 and I_1 were measured using Si diodes collecting photons scattered by a kapton foil”)
- 2) Fluorescence detectors:
 - a. Ge Solid-State Detector or Silicon-Drift Detector: number of elements, typical energy bandwidth
 - b. Crystal Analyzer Spectrometer: nature of the crystals, radius of curvature, geometry (Johann-Johansson, Von Hamos...)

Optimization of the experiment

- 1) Incident energy calibration (“Energy was calibrated by setting the 1st inflexion point / 1st derivative 1st maximum of the metallic foil reference spectrum to ...”),
- 2) Solid-State Detector or Silicon-Drift Detector: selected emission line (“the SSD was optimized to select the $K\alpha$ emission line of...”)
- 3) Crystal Analyzer Spectrometer:
 - a. selected emission line (“the CAS was optimized in order to select the $K\alpha_1$ emission line of...”),
 - b. emission energy can vary depending on the chemical state of the probed element: it must be mentioned whether the emission

Mandatory information to provide

energy was kept constant or changed to stay on the maximum intensity during the measurement sets,

- c. energy bandwidth (“energy bandwidth was estimated to X eV by measuring the elastic peak”)
- d. calibration mode (if the calibration is linked to the monochromator calibration indicate the energy of the emission line for the metallic reference or a model compounds)
- e. Energy of the incident beam if X-ray Emission Spectroscopy measurements are performed

Additional useful information

- 1) Typical photon flux on the sample
- 2) Storage ring parameters (current, mode of injection...)
- 3) Use of a reference sample in double transmission to check the calibration for each spectrum

Acronyms

List of acronyms

XAS: X-ray Absorption Spectroscopy

EXAFS: Extended X-Ray Absorption Fine Structure

XANES: X-ray Absorption Near Edge Structure

HERFD: High Energy Resolution Fluorescence Detected

TFY: Total Fluorescence Yield

PFY: Partial Fluorescence Yield

RIXS: Resonant Inelastic X-ray Scattering

XES: X-ray Emission Spectroscopy

XRF: X-ray Fluorescence

See here for a complete list with descriptions:

<https://xafs.xrayabsorption.org/acronyms.html>

BM : Bending Magnet

ID: Insertion Device

DCM: Double-Crystal Monochromator

SSD: Solid-State Detector

SDD: Silicon Drift Detector

DXP: Digital X-ray Processor

CAS: Crystal Analyzer Spectrometer

Selected formula

Selected general formula

Bragg's law

$$\lambda = 2d \cdot \sin \theta$$

where λ is the wavelength of the radiation,

d the interplanar distance,

θ the incidence angle

Energy to wavelength conversion

$$E(\text{keV}) \approx \frac{12.3984191}{\lambda(\text{\AA})}$$

Wave-vector to photo-electron energy conversion

$$E - E_0 = \frac{\hbar^2 k^2}{2m_e}$$

Photo-electron energy to wave-vector conversion

$$k = \sqrt{\frac{2m_e}{\hbar^2} (E - E_0)}$$

where E_0 is the absorption edge energy,

m_e the electron mass ($9.109\ 3826(16) \times 10^{-31}$ kg)

\hbar the reduced Planck constant ($6.582\ 119\ 15(56) \times 10^{-16}$ eV.s)

EXAFS equation

The EXAFS signal can be theoretically described by this formula:

$$\chi(k) = \sum_j S_i(k) \frac{N_j}{kR_j^2} e^{-2k^2\sigma_j^2} e^{-2R_j/\lambda(k)} f_j(k) \times \sin[2kR_j + \delta_{ij}(k)]$$

The summation is performed on each coordination shell j , constituted of identical neighbouring (scattering) atoms at the same bond length from the central (absorbing) atom i

$S_i(k)$ is a scale factor characteristic of the absorbing atom,

N_j is the coordination number,

R_j is the bond length,

σ_j^2 is the mean-square displacement of the bond length,

$f_j(k)$ is the scattering amplitude,

$\delta_{ij}(k)$ is the scattering phase induced both by the central and neighbouring atoms,

$\lambda(k)$ is the mean-free-path of the photo-electron.

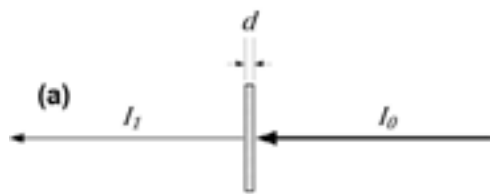
The approximations made to establish the formula are

- the bond length distribution is Gaussian (harmonic approximation), so limited to small disorder
- only 1 electron is considered during the absorption process (monoelectronic approximation)
- central atom potential is spherical
- spherical outgoing photo-electron wave-function is considered as a plane-wave close to the scattering atoms
- only backscattering (or single scattering) is considered

The formula can be written to take into account polarization effect, large or asymmetric bond length distribution function, multiple-scattering effects...

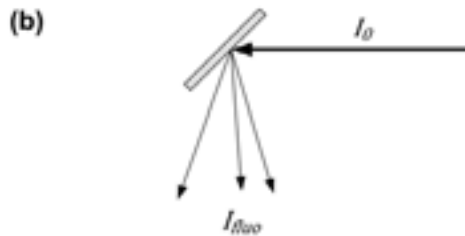
XAS mode of detection

XAS signal, $\mu(E)$, can be measured directly by quantifying the absorption induced by the sample, in transmission mode (a). The absorption (excitation) process is associated to two decay processes (des-excitation), radiative (fluorescence emission) and non-radiative (Auger electron). Measurements of the intensity of these decay (or secondary signals induced by these decays) is another way to measure $\mu(E)$:



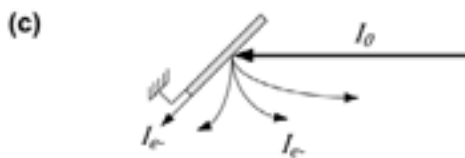
Transmission (Beer-Lambert's law)

$$\mu(E).d = \ln(I_0/I_1)$$



Fluorescence

$$\mu(E) \propto \frac{I_{fluor}}{I_0}$$



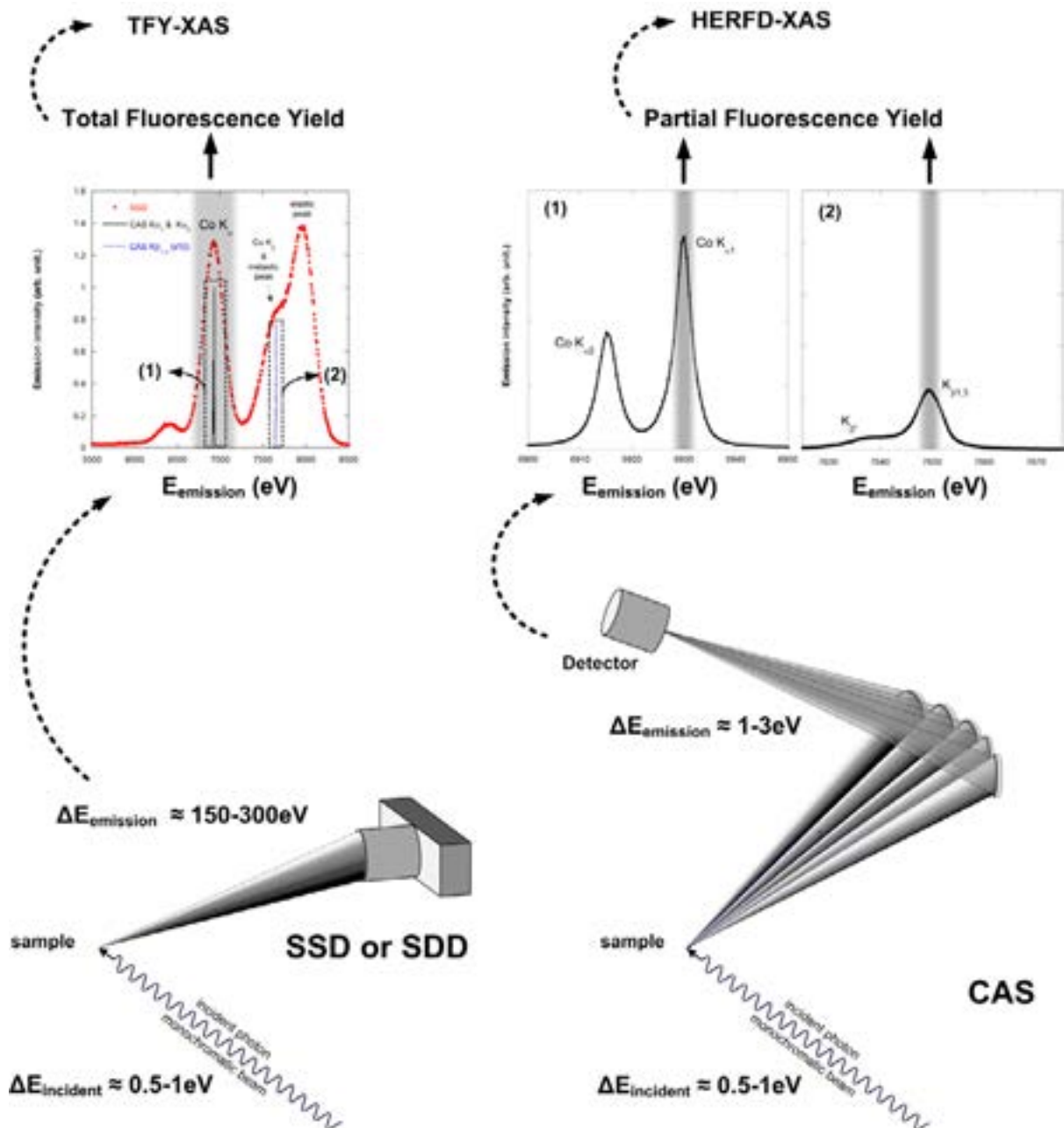
Auger

$$\mu(E) \propto \frac{I_{e-}}{I_0}$$

(b) Fluorescence measurements can be performed by collecting all the photons emitted by the sample, but the signal of interest will be then superimposed with other contributions such as the elastic and inelastic signals, the emission lines of the other constituents... It is therefore almost mandatory to use an energy resolved detector to select only the appropriate emission line, a Solid-State Detector (SSD) or Silicon Drift Detector (SDD), both with an energy bandwidth around 150-300eV, or a Crystal Analyzer Spectrometer (CAS), around 1-3eV.

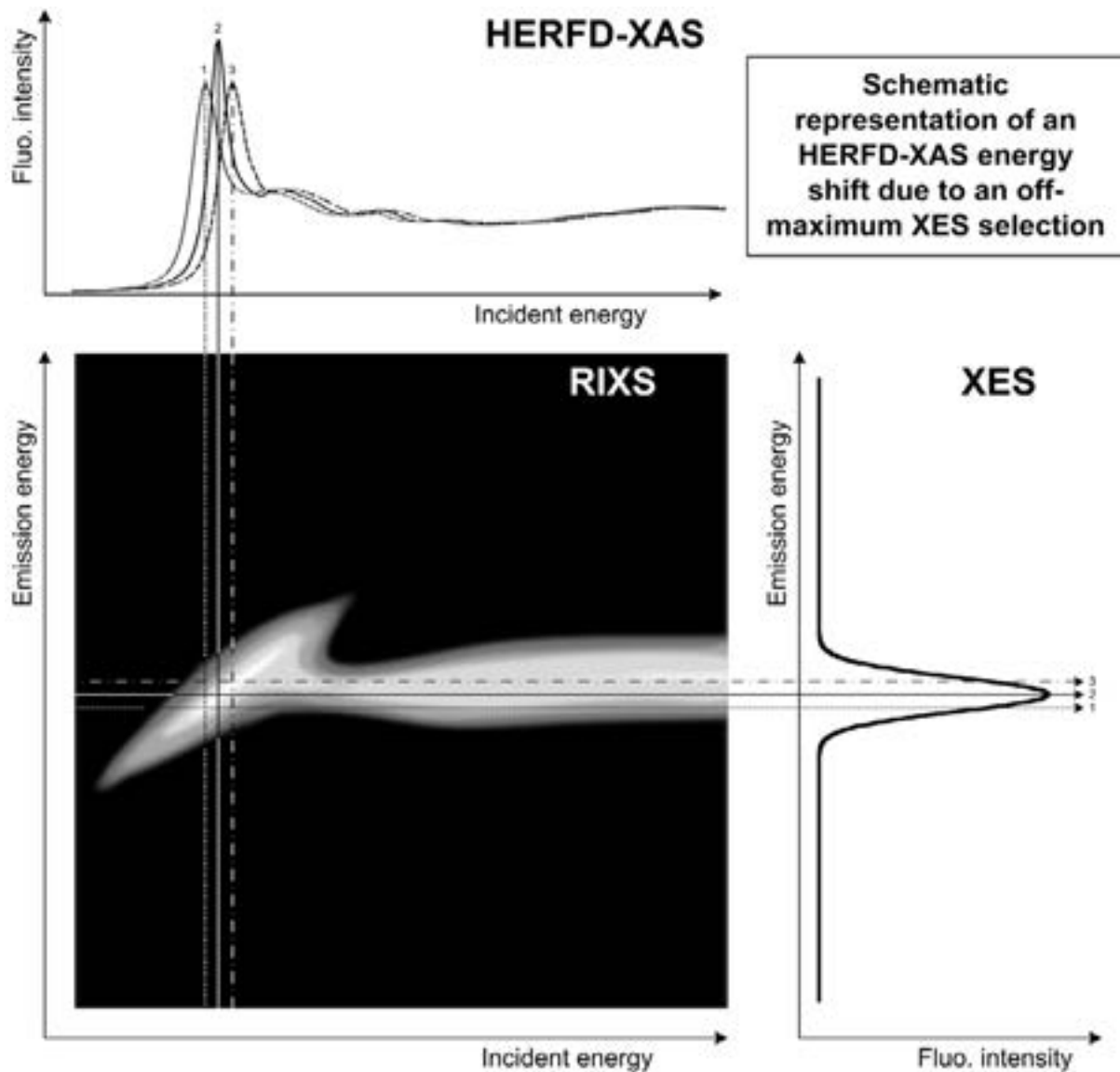
- With a SSD (or SDD), the acquisition will be performed by integrating the entire fluorescence signals due to both $K_{\alpha 1}$ and $K_{\alpha 2}$ lines (K-edge) or $L_{\alpha 1}$ (L_3 -edge), in Total Fluorescence Yield
- With a CAS, acquisitions will be performed by integrating a fraction of the $K_{\alpha 1}$ or $K_{\alpha 2}$ lines (K-edge), $L_{\alpha 1}$ (L_3 -edge) emission line, in Partial Fluorescence Yield. The resulting XAS spectrum will be an HERFD-XAS spectrum.

XAS mode of detection



When performing the acquisition using a CAS, in Partial Fluorescence Yield mode, the optimization of the CAS is done at the maximum of the emission line. An energy shift of the selected emission energy in the XES spectrum can induce an energy shift of the so-obtained HERFD-XAS spectra (e.g. Nehzati et al. [Nehzati 2021] for Se K-edge). Be careful, position of such maximum can change depending on the samples (valence, chemical environment... of the probed element), as shown on § “X-ray Emission Spectroscopy: energy shifts and chemical bonding” for the transition metals.

XAS mode of detection



(c) Auger measurements are sensitive to the very near surface (ca. few tenths of Å), limited by the Auger electron mean-free path. This kind of measurement is then (almost) limited to the study of samples prepared *in situ* and studied under vacuum. Collection of all the electron emitted by the sample (Auger and secondary electrons) is less surface sensitive, ca. few hundred of Å, in Total Electron Yield (TEY, [Schroeder 1995]) or in Conversion Electron Yield (CEY, [Girardeau 1992], [Proux 2001]) modes. In TEY mode, sample is under vacuum and the electrons are directly collected using a polarized anode, the sample being at the ground. CEY mode is similar except that sample is under a gas atmosphere (typically He): electrons ionize the gas which act as an amplifier, and the current between the polarized anode and the sample is in fact an ionization current.

Self-Absorption effects in Fluorescence mode

XAS measurements in fluorescence mode is the optimum way to measure XAS signal of a diluted element. Reversingly such kind of detection can lead to signal distortion when the concentration of the target element is too high. That's the self-absorption effect, which has been formalized by several authors (e.g. [Tröger 1992], [Pfalzer 1999]) leading to correction algorithms implemented in most of the XAS analysis softwares.

To explain the origin of the self-absorption let's describe step-by-step the different processes leading to the quantification of the fluorescence signal:

- Incident photons: intensity $I_0(E)$, angle Φ
- Absorption event occurs after a given path in the sample (depth x): the photon flux is reduced by a factor $\exp\left(-\mu_{tot}(E) \cdot \frac{x}{\sin \Phi}\right)$
- Probability of absorption: $\mu_{elt,edge}(E)$
- Fluorescence process characterized by its yield ($\omega_{elt,edge}$), energy (E_f) and angle (θ)
- Fluorescence flux attenuation by a factor $\exp\left(-\mu_{tot}(E_f) \cdot \frac{x}{\sin \theta}\right)$

Integrating x from 0 to d , for a detector area A at a distance r from the sample yields to a total fluorescence intensity:

$$I_f(E) \propto \frac{A}{r^2} \omega_{elt,edge} \frac{\mu_{elt,edge}(E)}{\mu_{tot}(E) + \mu_{tot}(E_f) \frac{\sin \Phi}{\sin \theta}} \times \left\{ 1 - \exp\left[-\left(\frac{\mu_{tot}(E)}{\sin \Phi} + \frac{\mu_{tot}(E_f)}{\sin \theta}\right) d\right] \right\}$$

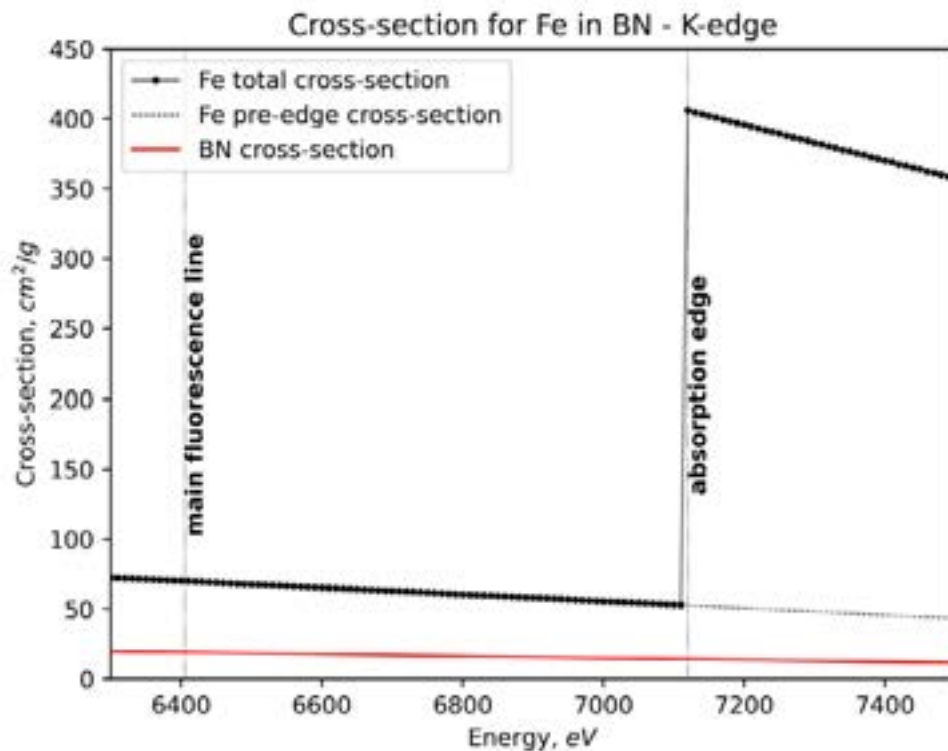
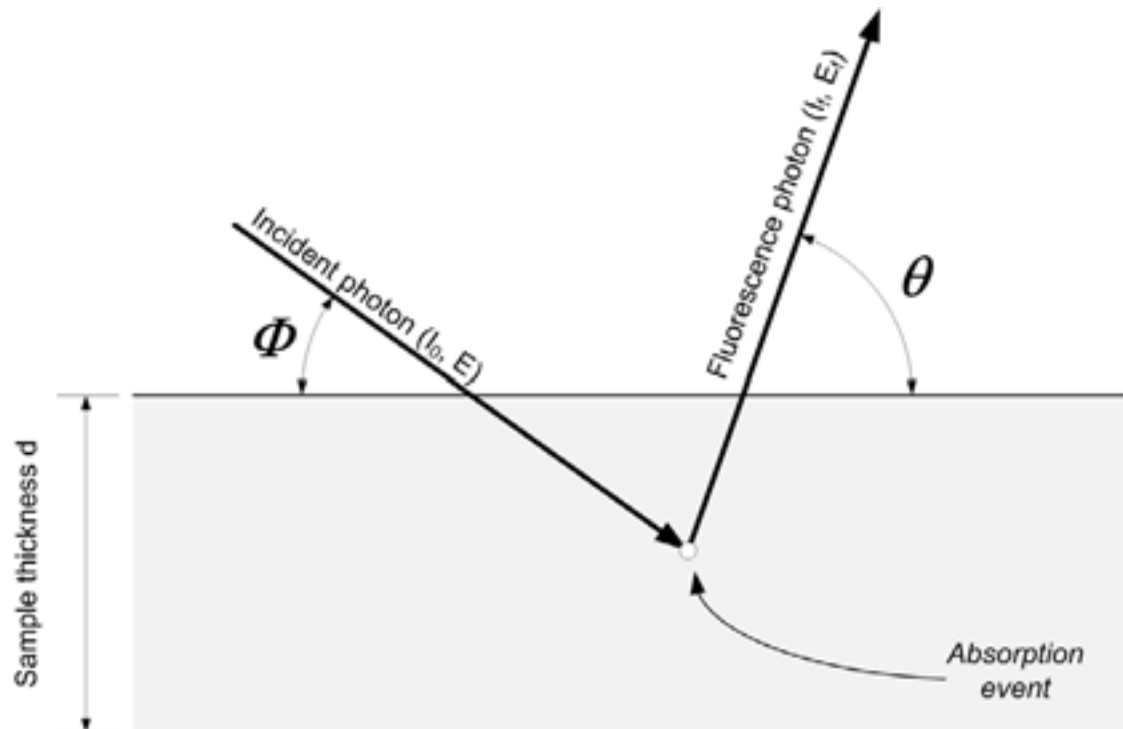
For a sample thickness much higher than the absorption length one has

$$I_f(E) \propto \frac{A}{r^2} \omega_{elt,edge} \frac{\mu_{elt,edge}(E)}{\mu_{tot}(E) + \mu_{tot}(E_f) \times \frac{\sin \Phi}{\sin \theta}}$$

The correction factor and the self-absorption rate can be expressed as :

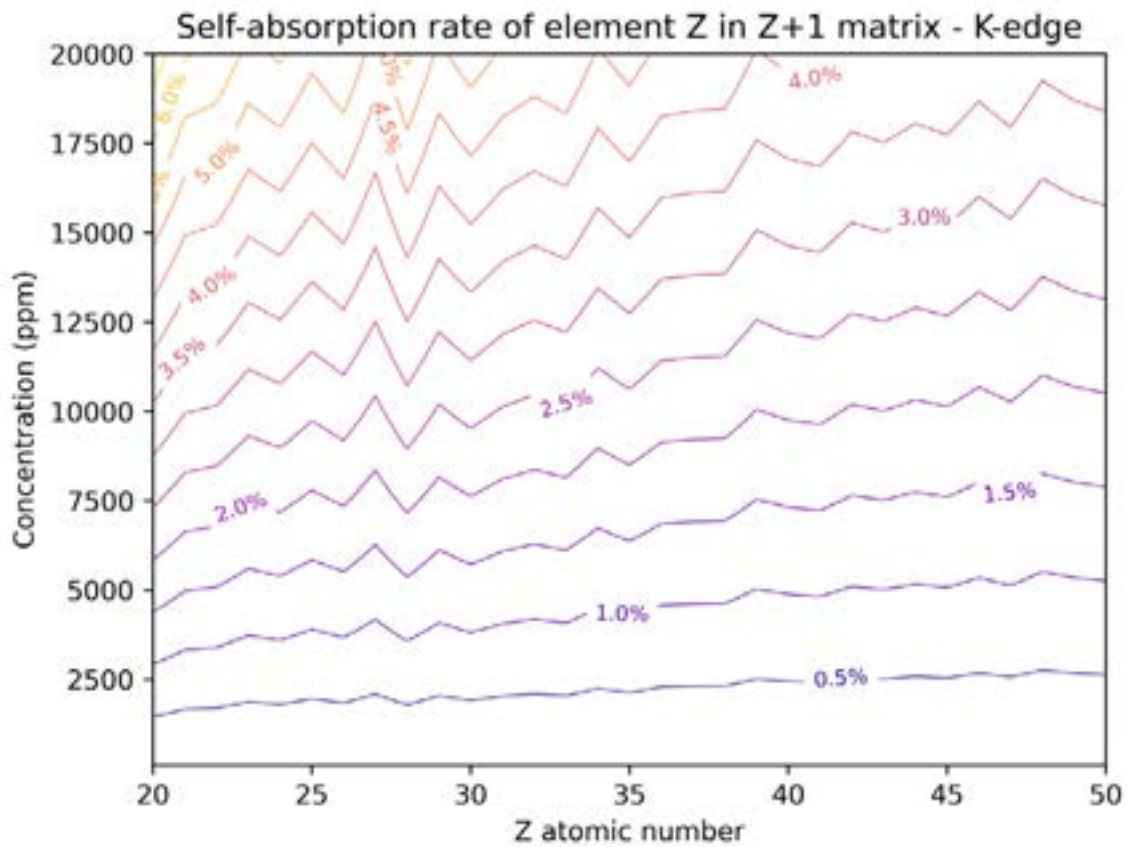
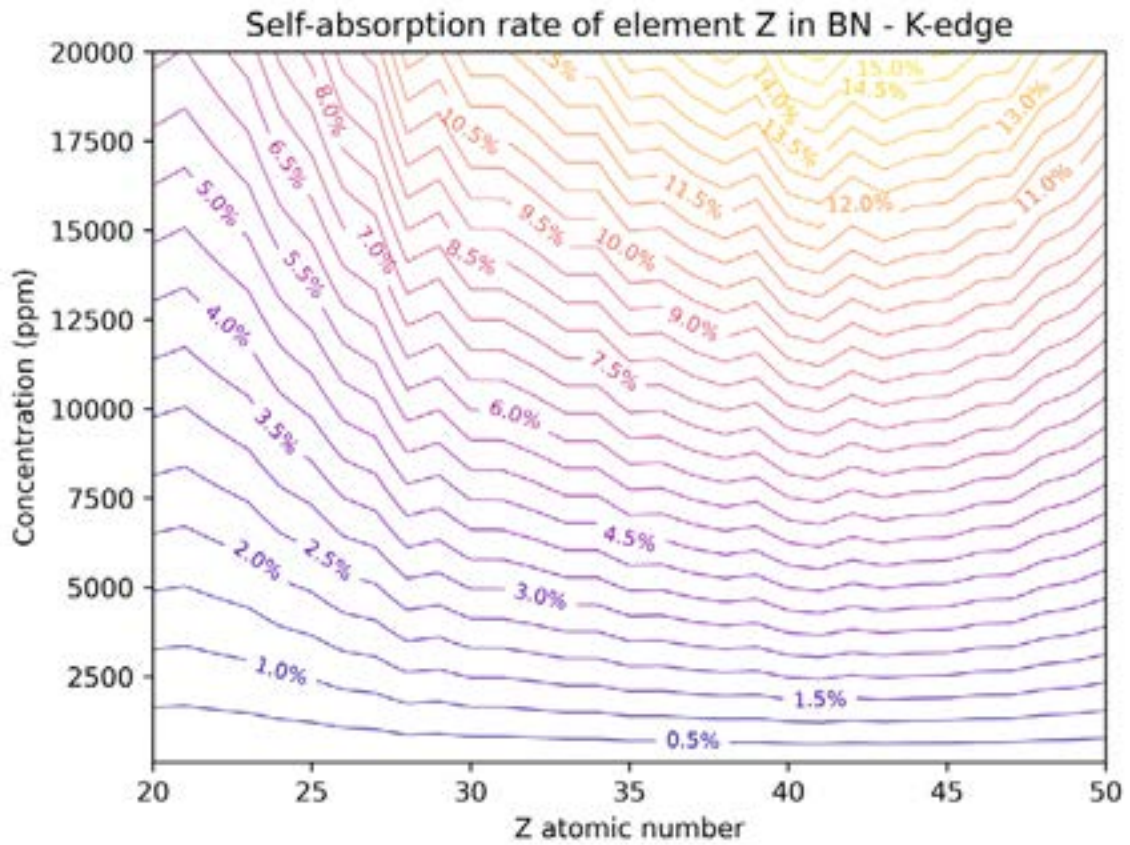
$$correction = \left[1 - \frac{\bar{\mu}_{elt,edge}(E)}{\bar{\mu}_{tot}(E) + \bar{\mu}_{tot}(E_f) \times \frac{\sin \Phi}{\sin \theta}} \right]^{-1} \text{ and } SA \text{ rate} = 1 - correction$$

Self-Absorption effects in Fluorescence mode



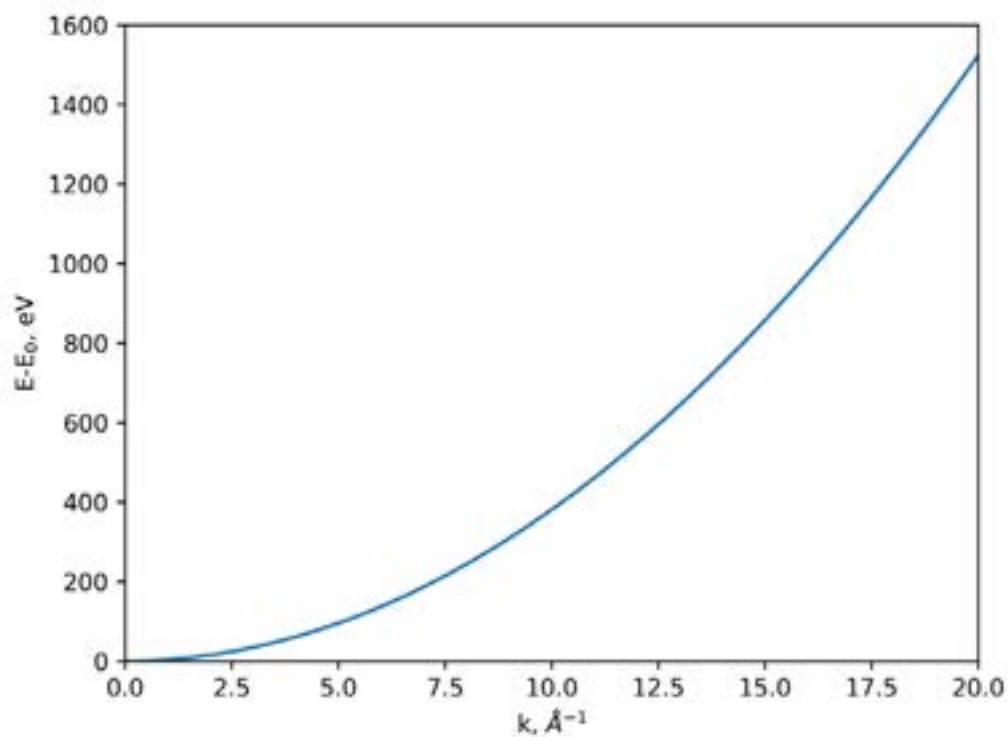
In order to choose the optimum conditions and concentrations between, transmission and fluorescence measurements, calculations have been performed for $\theta = \Phi = 45^\circ$, for different elements (characterized by the atomic number Z), in 2 different matrices, for K-edge absorption. Results are shown on figures below.

Self-Absorption effects in Fluorescence mode



Correspondence between wave-vector and photoelectron energy

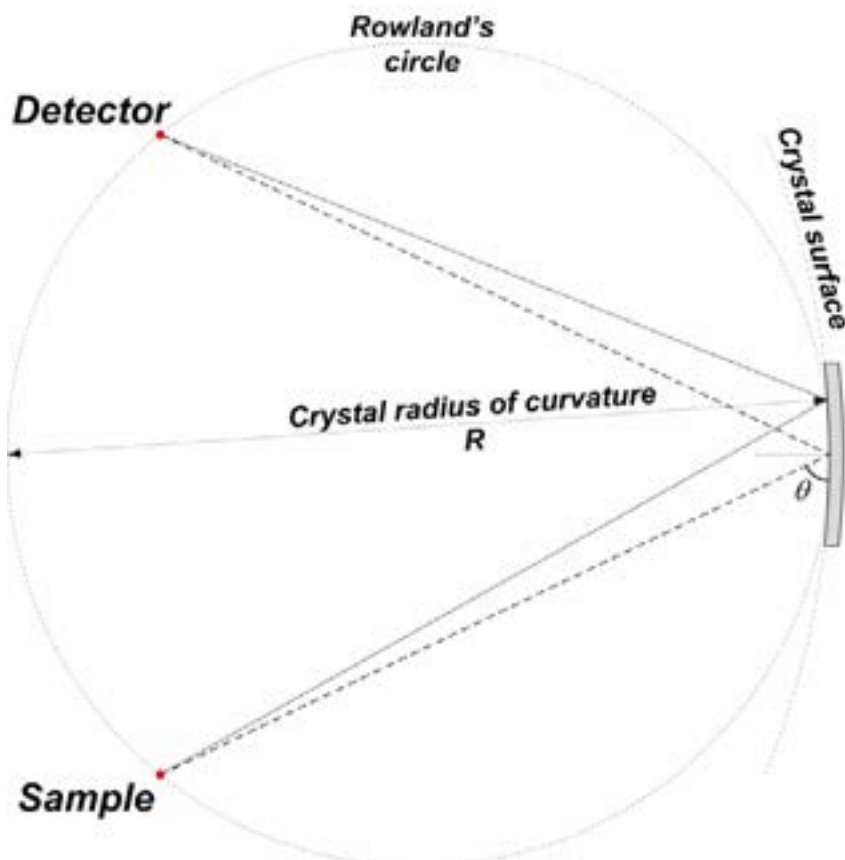
k (\AA^{-1})	$(E - E_0)$ (eV)	k (\AA^{-1})	$(E - E_0)$ (eV)
3.5	47	12	549
4	61	12.5	595
4.5	77	13	644
5	95	13.5	694
5.5	115	14	747
6	137	14.5	801
6.5	161	15	857
7	187	15.5	915
7.5	214	16	975
8	244	16.5	1037
8.5	275	17	1101
9	309	17.5	1167
9.5	344	18	1234
10	381	18.5	1304
10.5	420	19	1375
11	461	19.5	1449
11.5	504	20	1524



Crystal Analyzer Spectrometer – choice of the crystals

A Crystal Analyzer Spectrometer in Johann-Johansson geometry is equipped with spherically bent crystals (with a radius of curvature R) positioned as well as the sample and the detector on a virtual circle (the Rowland's circle, radius $R/2$). In Johann geometry only the centre of the crystal is on Rowland's circle. This geometry allows to probe with a given crystal a quite large emission energy range, with an optimum when the Bragg angle θ is close to 90° . When θ decreases, Johann's error increase giving rise to an increase of the energy bandwidth. If the typical required energy bandwidth is around 1eV, with a 1m radius of curvature R , θ ranges from around 90° to $\sim 75^\circ$.

The nature of the crystals has to be chosen to fulfil this requirement, taking also into account the availability of the crystals on the instrument.



Crystal Analyzer Spectrometer – choice of the crystals

Table 1. Choice of the crystals: $K\alpha_1$ and $K\beta_1$ emission lines

element		$K\alpha_1$			$K\beta_1$		
name	Z	E (keV)	θ (°)	Crystal	E (keV)	θ (°)	Crystal
Ti	22	4 512.2	76.3	Ge400	4 933.4	75.5	Ge331
V	23	4 952.9	74.6	Ge331	5 427.8	81.5	Ge422
Cr	24	5 414.9	82.4	Ge422	5 946.8	85.8	Si333
Mn	25	5 900.3	74.9	Ge333	6 491.8	84.1	Si440
Fe	26	6 405.2	75.4	Ge440	7 059.3	79.0	Ge620
Co	27	6 930.9	88.9	Ge620	7 649.1	83.0	Ge444
Ni	28	7 480.3	74.8	Si620	8 266.8	80.4	Si551
Cu	29	8 046.3	79.4	Si444	8 903.9	79.9	Ge800
Zn	30	8 637.2	81.5	Si642	9 570.4	82.5	Ge555
Ga	31	9 250.6	80.8	Si800	10 267	74.3	Si555
Ge	32	9 886.0	78.4	Si660	10 982	77.8	Ge844
As	33	10 543	69.7	Si555	11 726	72.5	Si844
Se	34	11 224	85.2	Si844	12 497	82.7	Ge880
Br	35	11 924	82.0	Si951	13 292	76.3	Si880
Kr	36	12 647	78.6	Ge880	14 112	78.7	Si777
Rb	37	13 396	82.7	Ge777	14 961	86.1	Si993
Sr	38	14 165	77.7	Si777	15 835	87.2	Si888
Y	39	14 958	86.3	Si993	16 739	74.7	Si 10 10 0
Zr	40	15 775	79.2	Ge 10 10 0	17 668	75.2	Ge999
Nb	41	16 615	76.3	Si 10 10 0	18 625	87.0	Si 11 11 11
Mo	42	17 480	77.8	Ge999	19 606	71.5	Ge 12 12 0

Crystal Analyzer Spectrometer – choice of the crystals

Table 2. Choice of the crystals: $L\alpha_1$ and $L\beta_1$ emission lines

element		$L\alpha_1$			$L\beta_1$		
name	Z	E (keV)	θ (°)	Crystal	E (keV)	θ (°)	Crystal
Cs	55	4 286.0	62.05	Si311	4 619.0	81.3	Si400
Ba	56	4 466.5	78.9	Ge400	4 828.3	81.6	Ge331
La	57	4 647.0	79.3	Si400	5 038.0	81.0	Si331
Ce	58	4 839.2	80.7	Ge331	5 261.6	71.0	Si331
Pr	59	5 035.2	81.2	Si331	5 491.7	77.8	Ge422
Nd	60	5 227.6	72.1	Si331	5 718.7	84.6	Ge333
Pm	61	5 432.0	81.2	Ge422	5 961.0	84.3	Si333
Sm	62	5 632.6	83.1	Si422	6 201.1	88.3	Ge440
Eu	63	5 849.5	76.7	Ge333	6 458.4	89.1	Si440
Gd	64	6 053.4	78.5	Si333	6 708.1	74.3	Si440
Tb	65	6 272.9	81.1	Ge440	6 975.1	83.5	Ge620
Dy	66	6 498	83.6	Si440	7 248	84.9	Si620
Ho	67	6 720	74.7	Si531	7 526	84.0 73.6	Si533 Si620
Er	68	6 949	85.7	Ge620	7 811	76.4	Ge444
Tm	69	7 180	74.8	Ge620	8 102	77.4	Si444
Yb	70	7 416	76.8	Si620	8 402	76.0	Si551
Lu	71	7 655	82.6	Ge444	8 710	69.4	Si551
Hf	72	7 899	74.0	Ge444	9 023	83.7 76.3	Ge733 Ge800
Ta	73	8 146	76.1	Si444	9 343	84.3	Ge660
W	74	8 398	76.1	Si551	9 672	78.8	Ge555

Crystal Analyzer Spectrometer – choice of the crystals

Table 2. Choice of the crystals: $L\alpha_1$ and $L\beta_1$ emission lines (continued)

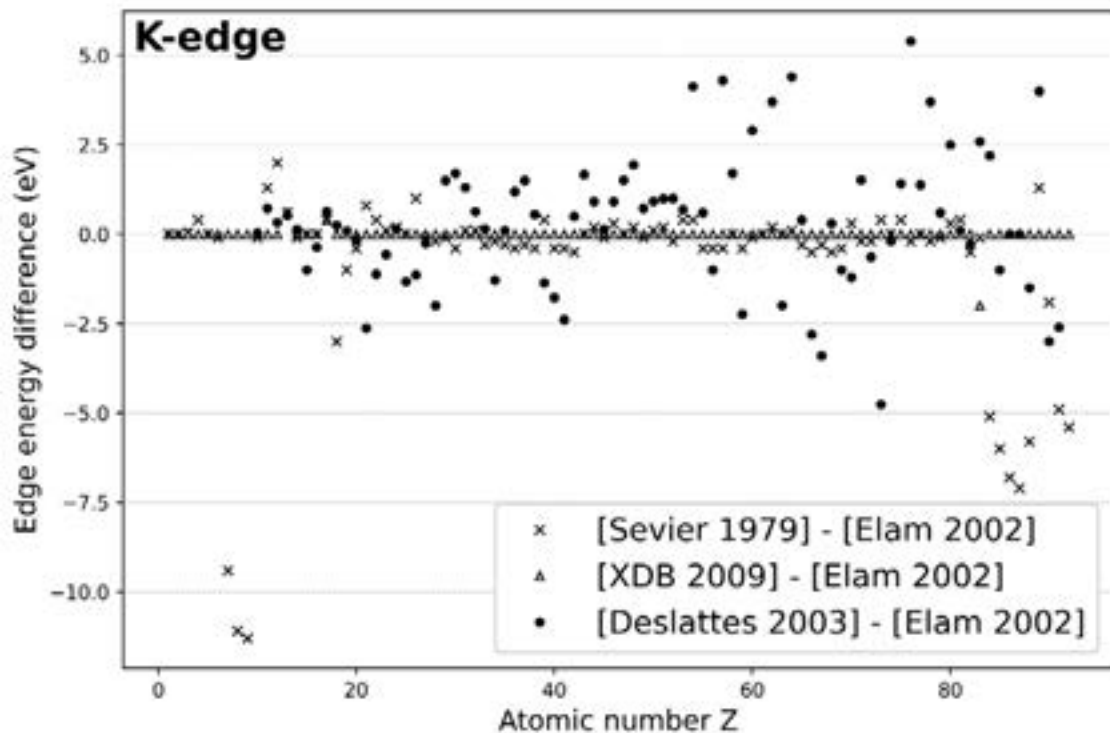
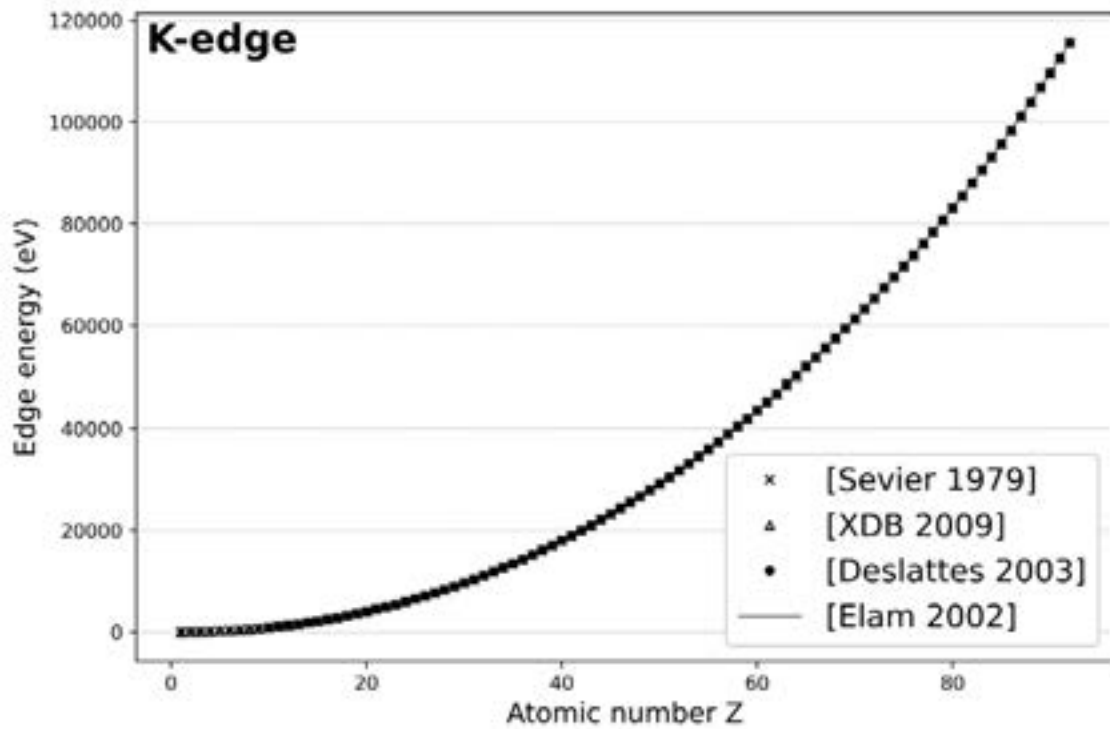
element		$L\alpha_1$			$L\beta_1$		
name	Z	E (keV)	θ (°)	Crystal	E (keV)	θ (°)	Crystal
Re	75	8 652	80.9	Si642	10 010	85.7	Ge753
						80.9	Si555
Os	76	8 911	79.6	Ge800	10 354	83.1	Ge664
						72.7	Si555
Ir	77	9 175	84.4	Si800	10 708	77.4	Ge931
						67.4	Si555
Pt	78	9 442	80.0	Ge660	11 071	79.6	Si931
						75.9	Ge844
Au	79	9 713	85.7	Si660	11 443	83.0	Si755
						77.8	Si844
Hg	80	9 989	81.7	Si555	11 824	87.0	Si951
Tl	81	10 269	74.3	Si555	12 213	84.3	Ge775
						75.2	Si951
Pb	82	10 551	69.5	Si555	12 614	79.3	Ge880
Bi	83	10 839	82.1	Ge844	13 023	82.6	Si880
Po	84	11 131	74.7	Ge844	13 446	81.1	Ge777
At	85	11 427	83.7	Si933	13 876	85.9	Si777
Rn	86	11 727	72.5	Si844	14 315	75.2	Si777
Fr	87	12 031	68.4	Si845	14 771	75.9	Ge993
Ra	88	12 339	73.1	Si951	15 236	85.2	Ge888
Ac	89	12 652	78.5	Ge880	15 713	80.5	Ge 10 10 0
Th	90	12 968	84.8	Si880	16 202	85.1	Si 10 10 0
Pa	91	13 291	88.2	Ge777	16 703	75.1	Si 10 10 0
U	92	13 614	77.4	Ge777	17 220	82.7	Ge999

Data

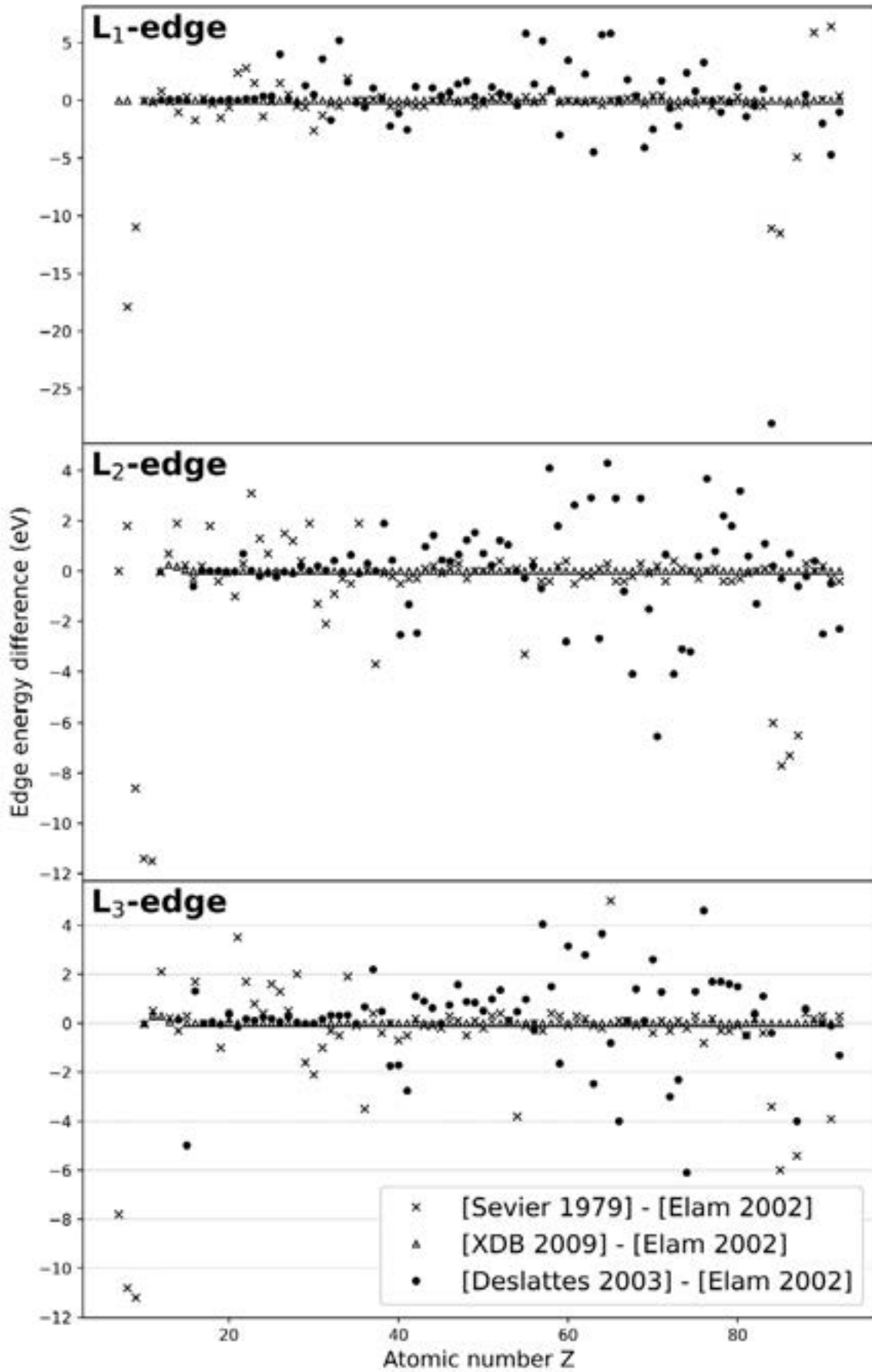
X-ray Absorption edge energies

X-ray Absorption edge energies

Comparison of different databases



X-ray Absorption edge energies



X-ray Absorption edge energies

Table 3. Electron binding energies, in eV, from [Elam 2002]

element	Z	K-edge	L₁-edge	L₂-edge	L₃-edge
H	1	13.60			
He	2	24.6			
Li	3	54.7	5.3		
Be	4	111.5	8	3	3
B	5	188	12.6	4.7	4.7
C	6	284.2	18	7.2	7.2
N	7	409.9	37.3	17.5	17.5
O	8	543.1	41.6	18.2	18.2
F	9	696.7	45	19.9	19.9
Ne	10	870.2	48.5	21.7	21.6
Na	11	1 070.8	63.5	30.4	30.5
Mg	12	1 303	88.6	49.6	49.2
Al	13	1 559	117.8	72.9	72.5
Si	14	1 839	149.7	99.8	99.2
P	15	2 145.5	189	136	135
S	16	2 472	230.9	163.6	162.5
Cl	17	2 822	270	202	200
Ar	18	3 205.9	326.3	250.6	248.4
K	19	3 608.4	378.6	297.3	294.6
Ca	20	4 038.5	438.4	349.7	346.2
Sc	21	4 492	498	403.6	398.7
Ti	22	4 966	560.9	460.2	453.8
V	23	5 465	626.7	519.8	512.1
Cr	24	5 989	696	583.8	574.1

X-ray Absorption edge energies

Table 3. Electron binding energies, in eV, from [Elam 2002] (continued)

element	Z	K-edge	L₁-edge	L₂-edge	L₃-edge
Mn	25	6 539	769.1	649.9	638.7
Fe	26	7 112	844.6	719.9	706.8
Co	27	7 709	925.1	793.2	778.1
Ni	28	8 333	1 008.6	870	852.7
Cu	29	8 979	1 096.7	952.3	932.7
Zn	30	9 659	1 196.2	1 044.9	1 021.8
Ga	31	10 367	1 299	1 143.2	1 116.4
Ge	32	11 103	1 414.6	1 248.1	1 217
As	33	11 867	1 527	1 359.1	1 323.6
Se	34	12 658	1 652	1 474.3	1 433.9
Br	35	13 474	1 782	1 596	1 550
Kr	36	14 326	1 921	1 730.9	1 678.4
Rb	37	15 200	2 065	1 864	1 804
Sr	38	16 105	2 216	2 007	1 940
Y	39	17 038	2 373	2 156	2 080
Zr	40	17 998	2 532	2 307	2 223
Nb	41	18 986	2 698	2 465	2 371
Mo	42	20 000	2 866	2 625	2 520
Tc	43	21 044	3 043	2 793	2 677
Ru	44	22 117	3 224	2 967	2 838
Rh	45	23 220	3 412	3 146	3 004
Pd	46	24 350	3 604	3 330	3 173
Ag	47	25 514	3 806	3 524	3 351
Cd	48	26 711	4 018	3 727	3 538

X-ray Absorption edge energies

Table 3. Electron binding energies, in eV, from [Elam 2002] (continued)

element	Z	K-edge	L₁-edge	L₂-edge	L₃-edge
In	49	27 940	4 238	3 938	3 730
Sn	50	29 200	4 465	4 156	3 929
Sb	51	30 491	4 698	4 380	4 132
Te	52	31 814	4 939	4 612	4 341
I	53	33 169	5 188	4 852	4 557
Xe	54	34 561	5 453	5 107	4 786
Cs	55	35 985	5 714	5 359	5 012
Ba	56	37 441	5 989	5 624	5 247
La	57	38 925	6 266	5 891	5 483
Ce	58	40 443	6 548	6 164	5 723
Pr	59	41 991	6 835	6 440	5 964
Nd	60	43 569	7 126	6 722	6 208
Pm	61	45 184	7 428	7 013	6 459
Sm	62	46 834	7 737	7 312	6 716
Eu	63	48 519	8 052	7 617	6 977
Gd	64	50 239	8 376	7 930	7 243
Tb	65	51 996	8 708	8 252	7 514
Dy	66	53 789	9 046	8 581	7 790
Ho	67	55 618	9 394	8 918	8 071
Er	68	57 486	9 751	9 264	8 358
Tm	69	59 390	10 116	9 617	8 648
Yb	70	61 332	10 486	9 978	8 944
Lu	71	63 314	10 870	10 349	9 244
Hf	72	65 351	11 271	10 739	9 561

X-ray Absorption edge energies

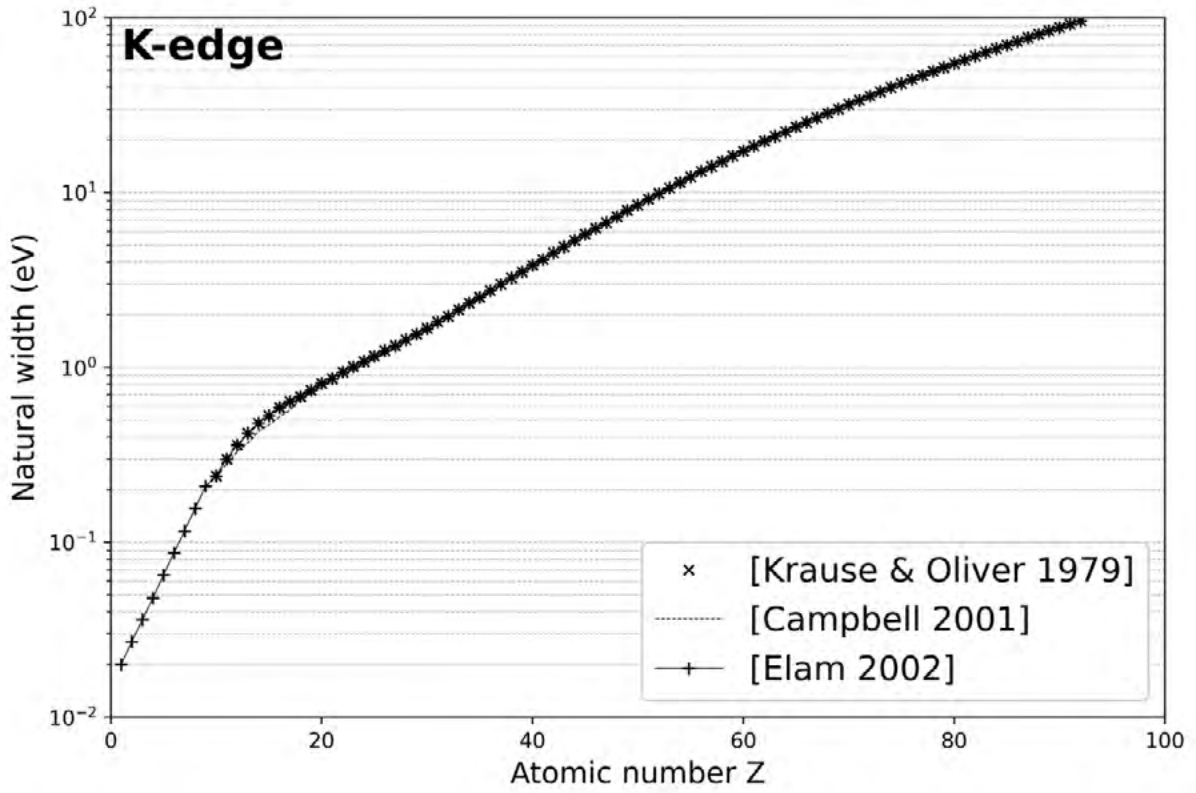
Table 3. Electron binding energies, in eV, from [Elam 2002] (continued)

element	Z	K-edge	L₁-edge	L₂-edge	L₃-edge
Ta	73	67 416	11 682	11 136	9 881
W	74	69 525	12 100	11 544	10 207
Re	75	71 676	12 527	11 959	10 535
Os	76	73 871	12 968	12 385	10 871
Ir	77	76 111	13 419	12 824	11 215
Pt	78	78 395	13 880	13 273	11 564
Au	79	80 725	14 353	13 734	11 919
Hg	80	83 102	14 839	14 209	12 284
Tl	81	85 530	15 347	14 698	12 658
Pb	82	88 005	15 861	15 200	13 035
Bi	83	90 526	16 388	15 711	13 419
Po	84	93 105	16 939	16 244	13 814
At	85	95 730	17 493	16 785	14 214
Rn	86	98 404	18 049	17 337	14 619
Fr	87	101 137	18 639	17 907	15 031
Ra	88	103 922	19 237	18 484	15 444
Ac	89	106 755	19 840	19 083	15 871
Th	90	109 651	20 472	19 693	16 300
Pa	91	112 601	21 105	20 314	16 733
U	92	115 606	21 757	20 948	17 166

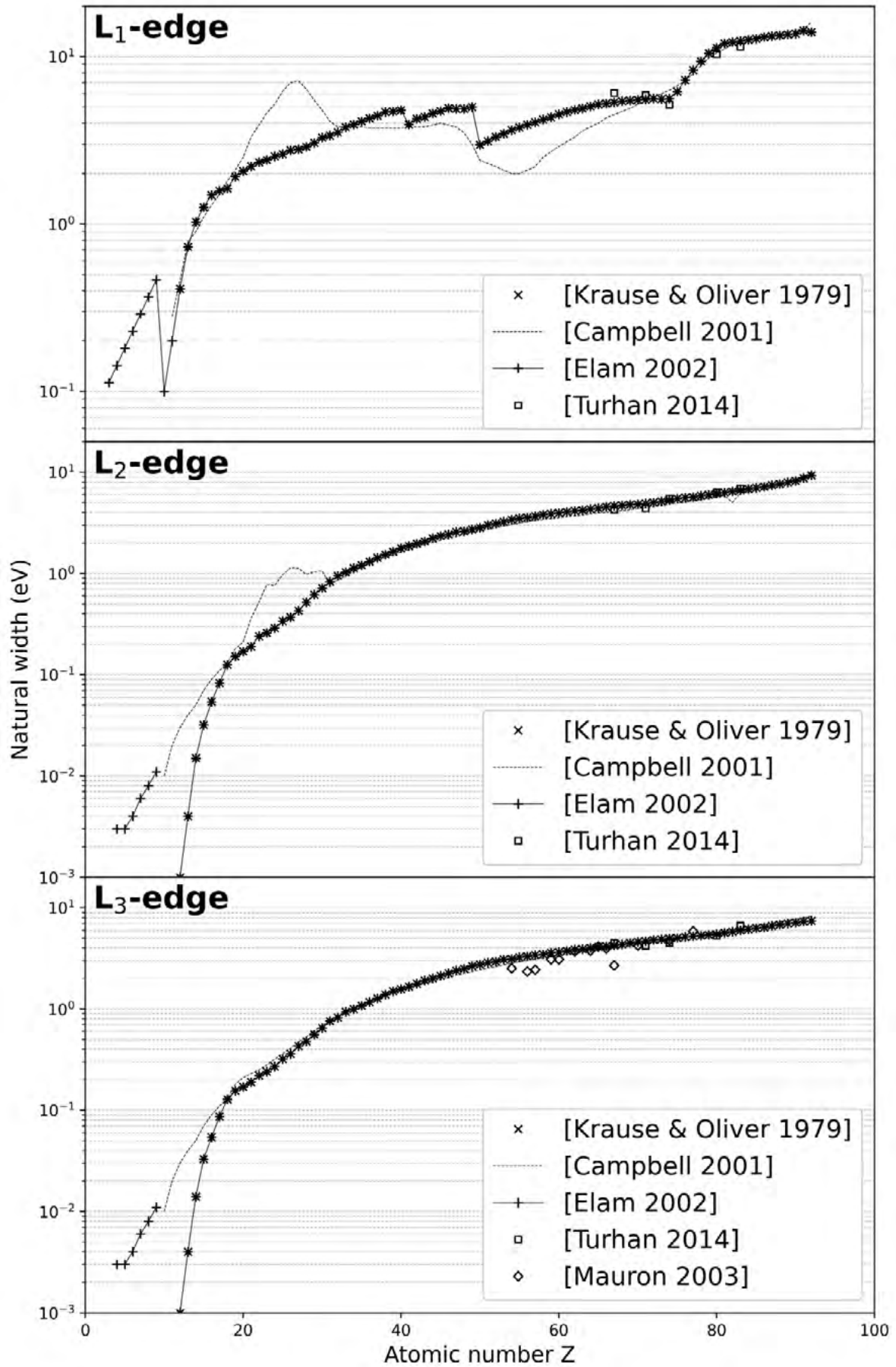
X-ray Absorption edge natural widths

X-ray Absorption edge natural widths

Comparison of different databases



X-ray Absorption edge natural widths



X-ray Absorption edge natural widths

Table 4. Natural width of atomic levels, in eV [Krause & Oliver 1979] except § [Elam 2002]

element	Z	K-edge	L ₁ -edge	L ₂ -edge	L ₃ -edge
H	1	0.02 [§]			
He	2	0.027 [§]			
Li	3	0.036 [§]			
Be	4	0.048 [§]			
B	5	0.065 [§]			
C	6	0.087 [§]			
N	7	0.116 [§]			
O	8	0.156 [§]			
F	9	0.209 [§]			
Ne	10	0.24			
Na	11	0.30			
Mg	12	0.36	0.41	0.001	0.001
Al	13	0.42	0.73	0.004	0.004
Si	14	0.48	1.03	0.015	0.014
P	15	0.53	1.26	0.032	0.033
S	16	0.59	1.49	0.054	0.054
Cl	17	0.64	1.58	0.083	0.087
Ar	18	0.68	1.63	0.126	0.128
K	19	0.74	1.92	0.152	0.156
Ca	20	0.81	2.07	0.17	0.17
Sc	21	0.86	2.21	0.19	0.19
Ti	22	0.94	2.34	0.24	0.22
V	23	1.01	2.41	0.26	0.24
Cr	24	1.08	2.54	0.29	0.27

X-ray Absorption edge natural widths

Table 4. Natural width of atomic levels, in eV [Krause & Oliver 1979] (cont.)

element	Z	K-edge	L₁-edge	L₂-edge	L₃-edge
Mn	25	1.16	2.62	0.34	0.32
Fe	26	1.25	2.76	0.37	0.36
Co	27	1.33	2.79	0.43	0.43
Ni	28	1.44	2.89	0.52	0.48
Cu	29	1.55	3.06	0.62	0.56
Zn	30	1.67	3.28	0.72	0.65
Ga	31	1.82	3.38	0.83	0.76
Ge	32	1.96	3.53	0.95	0.82
As	33	2.14	3.79	1.03	0.94
Se	34	2.33	3.94	1.13	1.00
Br	35	2.52	4.11	1.21	1.08
Kr	36	2.75	4.28	1.31	1.17
Rb	37	2.99	4.44	1.43	1.27
Sr	38	3.25	4.67	1.54	1.39
Y	39	3.52	4.71	1.65	1.50
Zr	40	3.84	4.78	1.78	1.57
Nb	41	4.14	3.94	1.87	1.66
Mo	42	4.52	4.25	1.97	1.78
Tc	43	4.91	4.36	2.08	1.91
Ru	44	5.33	4.58	2.23	2.00
Rh	45	5.77	4.73	2.35	2.13
Pd	46	6.24	4.93	2.43	2.25
Ag	47	6.75	4.88	2.57	2.4
Cd	48	7.28	4.87	2.62	2.5

X-ray Absorption edge natural widths

Table 4. Natural width of atomic levels, in eV [Krause & Oliver 1979] (cont.)

element	Z	K-edge	L₁-edge	L₂-edge	L₃-edge
In	49	7.91	5.00	2.72	2.65
Sn	50	8.49	2.97	2.84	2.75
Sb	51	9.16	3.13	3.00	2.87
Te	52	9.89	3.32	3.12	2.95
I	53	10.6	3.46	3.25	3.08
Xe	54	11.4	3.64	3.4	3.13
Cs	55	12.3	3.78	3.51	3.25
Ba	56	13.2	3.92	3.57	3.32
La	57	14.1	4.06	3.68	3.41
Ce	58	15.1	4.21	3.8	3.48
Pr	59	16.2	4.34	3.89	3.6
Nd	60	17.3	4.52	3.97	3.65
Pm	61	18.5	4.67	4.06	3.75
Sm	62	19.7	4.80	4.15	3.86
Eu	63	21.0	4.91	4.23	3.91
Gd	64	22.3	5.05	4.32	4.01
Tb	65	23.8	5.19	4.43	4.12
Dy	66	25.2	5.25	4.55	4.17
Ho	67	26.8	5.33	4.66	4.26
Er	68	28.4	5.43	4.73	4.35
Tm	69	30.1	5.47	4.79	4.48
Yb	70	31.9	5.53	4.82	4.60
Lu	71	33.7	5.54	4.92	4.68
Hf	72	35.7	5.63	5.02	4.80

X-ray Absorption edge natural widths

Table 4. Natural width of atomic levels, in eV [Krause & Oliver 1979] (cont.)

element	Z	K-edge	L₁-edge	L₂-edge	L₃-edge
Ta	<i>73</i>	37.7	5.58	5.15	4.88
W	<i>74</i>	39.9	5.61	5.33	4.98
Re	<i>75</i>	42.1	6.18	5.48	5.04
Os	<i>76</i>	44.4	7.25	5.59	5.16
Ir	<i>77</i>	46.8	8.30	5.69	5.25
Pt	<i>78</i>	49.3	9.39	5.86	5.31
Au	<i>79</i>	52.0	10.5	6.00	5.41
Hg	<i>80</i>	54.6	11.3	6.17	5.50
Tl	<i>81</i>	57.4	12.0	6.32	5.65
Pb	<i>82</i>	60.4	12.2	6.48	5.81
Bi	<i>83</i>	63.4	12.4	6.67	5.98
Po	<i>84</i>	66.6	12.6	6.83	6.13
At	<i>85</i>	69.8	12.8	7.01	6.29
Rn	<i>86</i>	73.3	13.1	7.20	6.41
Fr	<i>87</i>	76.8	13.3	7.47	6.65
Ra	<i>88</i>	80.4	13.4	7.68	6.82
Ac	<i>89</i>	84.1	13.6	7.95	6.98
Th	<i>90</i>	88.0	13.7	8.18	7.13
Pa	<i>91</i>	91.9	14.3	8.75	7.33
U	<i>92</i>	96.1	14.0	9.32	7.43

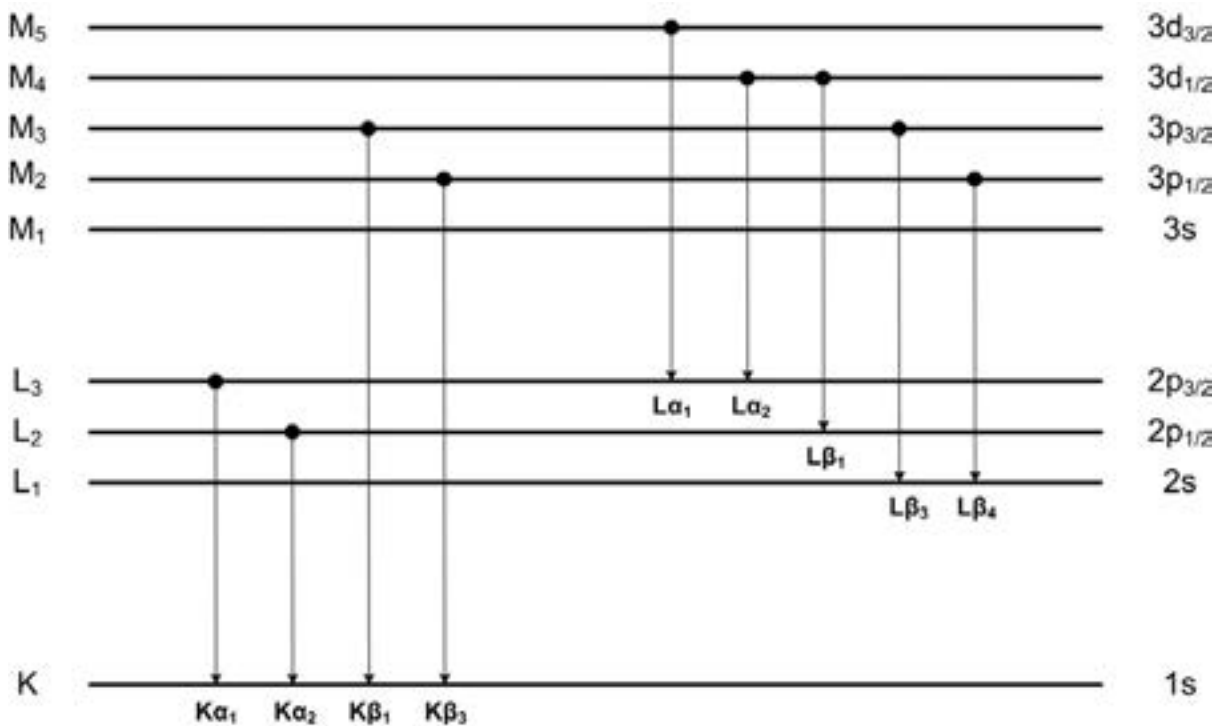
X-ray Fluorescence line energies

X-ray Fluorescence line energies

Table 5. Emission lines notation

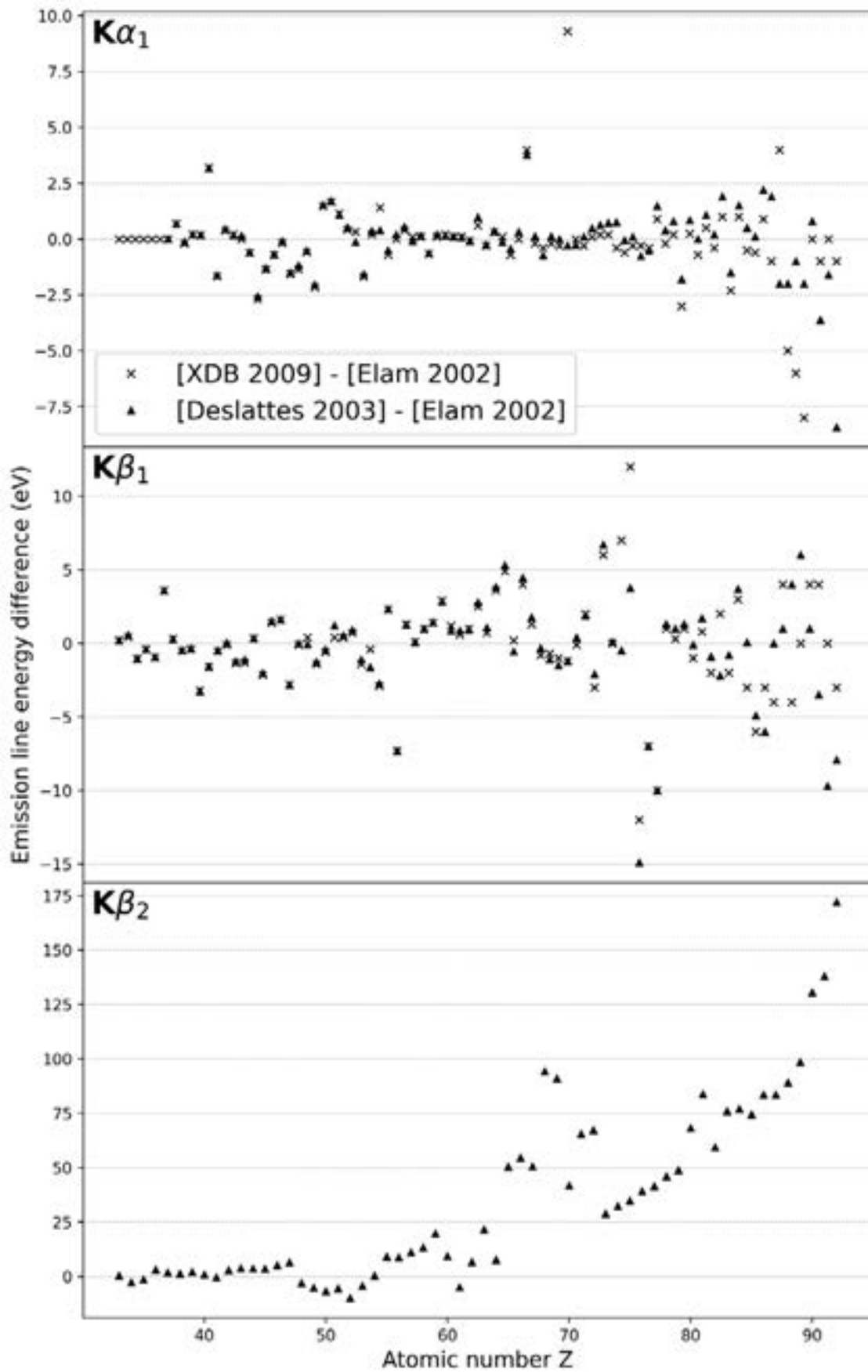
K-edge		L ₁ -edge		L ₂ -edge		L ₃ -edge	
Siegbahn	IUPAC	Siegbahn	IUPAC	Siegbahn	IUPAC	Siegbahn	IUPAC
Kα ₁	K-L ₃	Lβ ₃	L ₁ -M ₃	Lβ ₁	L ₂ -M ₄	Lα ₁	L ₃ -M ₅
Kα ₂	K-L ₂	Lβ ₄	L ₁ -M ₂	Lβ ₁₇	L ₂ -M ₃	Lα ₂	L ₃ -M ₄
Kβ ₁	K-M ₃	Lβ ₉	L ₁ -M ₅	Lγ ₁	L ₂ -N ₄	Lβ ₂	L ₃ -N ₅
Kβ ₂ ^I	K-N ₃	Lβ ₁₀	L ₁ -M ₄	Lγ ₅	L ₂ -N ₁	Lβ ₅	L ₃ -O _{4, 5}
Kβ ₂ ^{II}	K-N ₂	Lγ ₂	L ₁ -N ₂	Lγ ₆	L ₂ -O ₄	Lβ ₆	L ₃ -N ₁
Kβ ₃	K-M ₂	Lγ ₃	L ₁ -N ₃	Lγ ₈	L ₂ -O ₁	Lβ ₇	L ₃ -O ₁
Kβ ₄ ^I	K-N ₅	Lγ ₄	L ₁ -O ₃	Lγ ₈ [']	L ₂ -N ₆₍₇₎	Lβ ₇ [']	L ₃ -N _{6, 7}
Kβ ₄ ^{II}	K-N ₄	Lγ ₄ [']	L ₁ -O ₂	Lη	L ₂ -M ₁	Lβ ₁₅	L ₃ -N ₄
Kβ _{4x}	K-N ₄			L _v	L ₂ -N ₆₍₇₎	L _i	L ₃ -M ₁
Kβ ₅ ^I	K-M ₅					L _s	L ₃ -M ₃
Kβ ₅ ^{II}	K-M ₄					L _t	L ₃ -M ₂
						L _u	L ₃ -N _{6, 7}

Main emission lines based on the electron orbital diagram

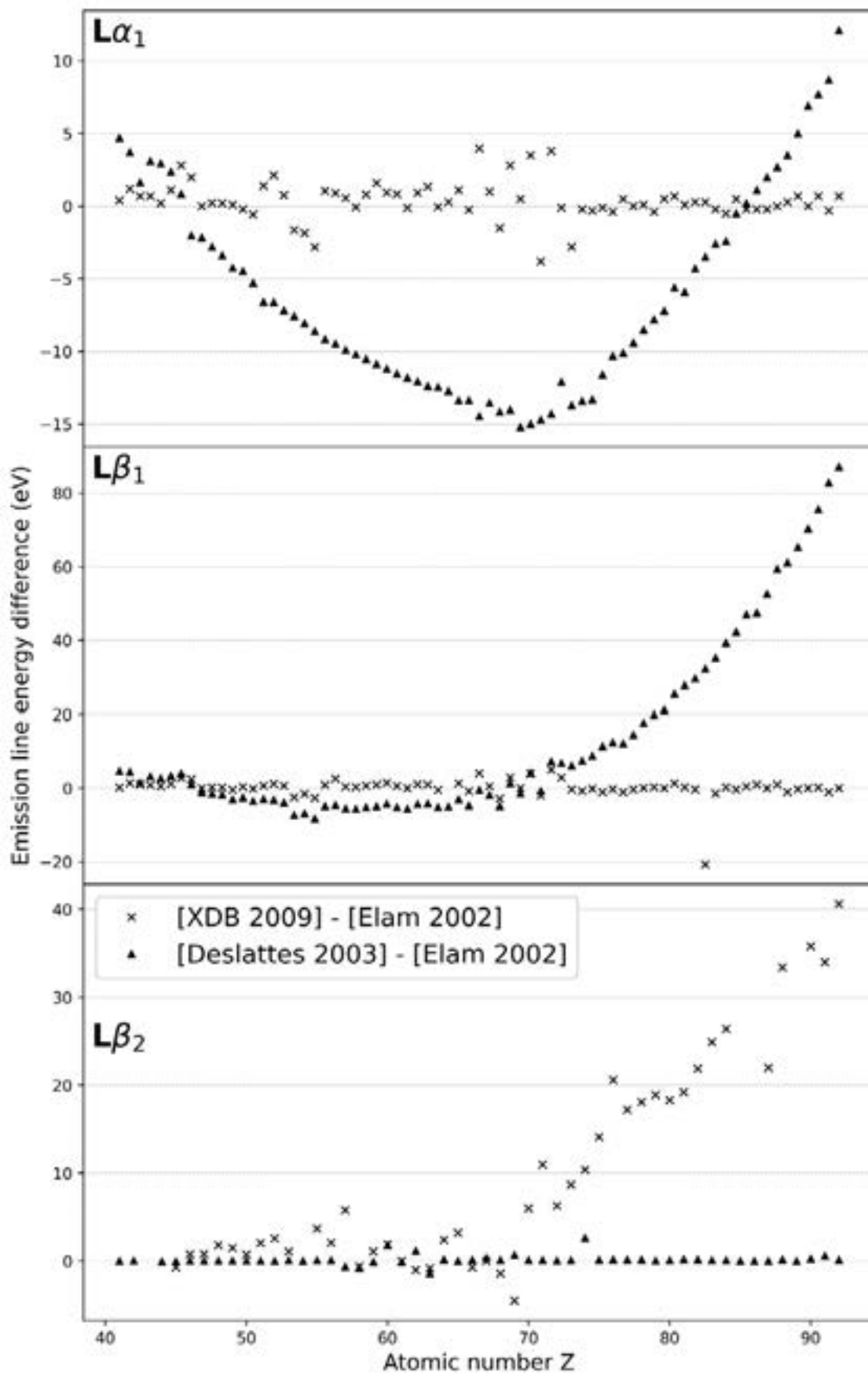


X-ray Fluorescence line energies

Comparison of different databases



X-ray Fluorescence line energies



X-ray Fluorescence line energies

Table 6. K emission line energies, in eV. Values from [Elam 2002] except when marked § [Bearden 1967] and # [XDB 2009]

element	Z	K_{α1}	K_{α2}	K_{β1}	K_{β2}
H	1				
He	2				
Li	3				
Be	4	108.5	108.5		
B	5	183.3	183.3		
C	6	277	277		
N	7	392.4	392.4		
O	8	524.9	524.9		
F	9	676.8	676.8		
Ne	10	848.6	848.5		
Na	11	1 040.3	1 040.4		
Mg	12	1 253.8	1 253.4	1 302	
Al	13	1 486.5	1 486.1	1 557	
Si	14	1 739.8	1 739.2	1 837	
P	15	2 010.5	2 009.5	2 139.5	
S	16	2 309.5	2 308.4	2 465	
Cl	17	2 622	2 620	2 812	
Ar	18	2 957.5	2 955.3	3 190.2	
K	19	3 313.8	3 311.1	3 590.1	
Ca	20	3 692.3	3 688.8	4 013.1	
Sc	21	4 093.3	4 088.4	4 463.7	
Ti	22	4 512.2	4 505.8	4 933.4	
V	23	4 952.9	4 945.2	5 427.8	
Cr	24	5 414.9	5 405.2	5 946.8	

X-ray Fluorescence line energies

Table 6. K emission line energies, in eV [Elam 2002] (continued)

element	Z	K α_1	K α_2	K β_1	K β_2
Mn	25	5 900.3	5 889.1	6 491.8	
Fe	26	6 405.2	6 392.1	7 059.3	
Co	27	6 930.9	6 915.8	7 649.1	
Ni	28	7 480.3	7 463	8 266.8	
Cu	29	8 046.3	8 026.7	8 903.9	
Zn	30	8 637.2	8 614.1	9 570.4	9 658 [§]
Ga	31	9 250.6	9 223.8	10 267	10 366.3 [§]
Ge	32	9 886	9 854.9	10 982	11 100.8 [§]
As	33	10 543.4	10 508	11 726	11 864
Se	34	11 224.1	11 184	12 497	12 655
Br	35	11 924	11 878	13 292	13 471
Kr	36	12 647.6	12 595	14 112	14 312
Rb	37	13 396	13 336	14961	15 184
Sr	38	14 165	14 098	15 835	16 083
Y	39	14 958	14 882	16 739	17 014
Zr	40	15 775	15 691	17 668	17 970
Nb	41	16 615	16 521	18 625	18 953
Mo	42	17 480	17 375	19 606	19 962
Tc	43	18 367	18 251	20 626	21 002
Ru	44	19 279	19 150	21 656	22 071
Rh	45	20 216	20 074	22 724	23 170
Pd	46	21 177	21 020	23 818	24 294
Ag	47	22 163	21 990	24 941	25 450
Cd	48	23 173	22 984	26 093	26 647

X-ray Fluorescence line energies

Table 6. K emission line energies, in eV [Elam 2002] (continued)

element	Z	K_{α1}	K_{α2}	K_{β1}	K_{β2}
In	49	24 210	24 002	27 274.7	27 866.5
Sn	50	25 271	25 044	28 485.4	29 116.4
Sb	51	26 359	26 111	29 724.6	30 395.4
Te	52	27 473	27 202	30 993.2	31 710.7
I	53	28 612	28 317	32 294	33 046
Xe	54	29 775	29 454	33 620.4	34 414.3
Cs	55	30 973	30 626	34 982	35 812.6
Ba	56	32 194	31 817	36 378	37 249
La	57	33 442	33 034	37 797	38 719.2
Ce	58	34 720	34 279	39 256	40 219.8
Pr	59	36 027	35 551	40 749	41 754.7
Nd	60	37 361	36 847	42 272	43 325.7
Pm	61	38 725	38 171	43 827	44 942
Sm	62	40 118	39 522	45 414.2	46 568.4
Eu	63	41 542	40 902	47 038	48 235
Gd	64	42 996	42 309	48 695	49 953
Tb	65	44 482	43 744	50 385	51 673.6
Dy	66	45 999	45 208	52 113	53 455.5
Ho	67	47 547	46 700	53 877	55 274.5
Er	68	49 128	48 222	55 674	57 119.8
Tm	69	50 742	49 773	57 505	59 004.1
Yb	70	52 388	51 354	59 382	60 943.3
Lu	71	54 070	52 965	61 290	62 901.6
Hf	72	55 790	54 612	63 244	64 912.8

X-ray Fluorescence line energies

Table 6. K emission line energies, in eV [Elam 2002] (continued)

element	Z	K_{α1}	K_{α2}	K_{β1}	K_{β2}
Ta	73	57 535	56 280	65 222	66 953
W	74	59 318	57 981	67 244	69 035
Re	75	61 141	59 717	69 309	71 157
Os	76	63 000	61 486	71 414	73 322
Ir	77	64 896	63 287	73 560	75 533
Pt	78	66 831	65 122	75 750	77 786
Au	79	68 806	66 991	77 982	80 082
Hg	80	70 818	68 893	80 255	82 422
Tl	81	72 872	70 832	82 573	84 810
Pb	82	74 970	72 805	84 939	87 243
Bi	83	77 107	74 815	87 349	89 721
Po	84	79 291	76 861	89 803	92 254
At	85	81 516	78 945	92 304	94 844
Rn	86	83 785	81 067	94 866	97 475
Fr	87	86 106	83 230	97 474	100 157
Ra	88	88 478	85 438	100 130	102 864
Ac	89	90 884	87 672	102 846	105 675
Th	90	93 351	89 958	105 605	108 483
Pa	91	95 868	92 287	108 427	111 377
U	92	98 440	94 658	111 303	114 335

X-ray Fluorescence line energies

Table 7. L emission line energies, in eV [Elam 2002]

element	Z	L_{α1}	L_{β1}	L_{β2}	L_{β3}	L_{β4}
H	1					
He	2					
Li	3					
Be	4					
B	5					
C	6					
N	7					
O	8					
F	9					
Ne	10					
Na	11					
Mg	12				87.6	87.6
Al	13				115.8	115.8
Si	14				147.7	147.7
P	15				183	182
S	16				223.9	222.9
Cl	17				260	260
Ar	18				310.6	310.4
K	19				360.3	360.3
Ca	20	341.3 [#]	344.9 [#]		413	413
Sc	21	395.4 [#]	399.6 [#]		469.7	469.7
Ti	22	451.8	458.2		528.3	528.3
V	23	510.1	517.8		589.5	589.5
Cr	24	572.1	581.8		653.8	653.8

X-ray Fluorescence line energies

Table 7. L emission line energies, in eV [Elam 2002] (continued)

element	Z	L_{α1}	L_{β1}	L_{β2}	L_{β3}	L_{β4}
Mn	25	636.7	647.9		721.9	721.9
Fe	26	704.8	717.9		791.9	791.9
Co	27	775.1	790.2		865.2	866.2
Ni	28	848.7	866		942.4	940.6
Cu	29	927.7	947.3		1 021.6	1 019.4
Zn	30	1 011.7	1 034.7		1 107.6	1 104.8
Ga	31	1 097.7	1 124.5		1 199	1 195.5
Ge	32	1 187.8	1 218.3		1 293.8	1 289.7
As	33	1 281.9	1 317.4		1 385.8	1 380.8
Se	34	1 379.3	1 418.8		1 491.3	1 485.5
Br	35	1 481	1 526		1 600	1 593
Kr	36	1 584.6	1 635.9		1 706.6	1 698.8
Rb	37	1 692	1 751		1 825.9	1 816.3
Sr	38	1 805.8	1 871		1 946	1 935.7
Y	39	1 924.2	1 998.3		2 074.2	2 062.4
Zr	40	2 044.2	2 125.9		2 202.2	2 188.5
Nb	41	2 168.7	2 260		2 337.4	2 321.9
Mo	42	2 292.1	2 393.9		2 472	2 454.4
Tc	43	2 423.1	2 535.4		2 625.3	2 595.4
Ru	44	2 558	2 682.8		2 762.5	2 740.7
Rh	45	2 696.8	2 834.1	3 002	2 915.5	2 890.7
Pd	46	2 837.8	2 989.5	3 171	3 071.7	3 044.1
Ag	47	2 982.7	3 150	3 347	3 233	3 202.2
Cd	48	3 132.8	3 315.1	3 526.3	3 399.6	3 365.4

X-ray Fluorescence line energies

Table 7. K emission line energies, in eV [Elam 2002] (continued)

element	Z	L_{α1}	L_{β1}	L_{β2}	L_{β3}	L_{β4}
In	49	3 286.1	3 486.6	3 712.3	3 572.7	3 534.8
Sn	50	3 444.1	3 662.8	3 904.1	3 750.4	3 708.5
Sb	51	3 603.8	3 842.5	4 098.7	3 931.6	3 885.3
Te	52	3 768	4 028.6	4 299.1	4 118.2	4 068.2
I	53	3 937.7	4 221.2	4 506.4	4 313	4 257
Xe	54	4 109.6	4 418	4 716.5	4 512.4	4 450.9
Cs	55	4 285.4	4 618.5	4 932.2	4 711	4 643
Ba	56	4 466.5	4 828.3	5 154.4	4 926	4 852
La	57	4 647	5 038	5 377.7	5 138	5 057
Ce	58	4 839.2	5 261.6	5 614	5 361	5 274
Pr	59	5 035.2	5 491.7	5 848.9	5 593	5 498
Nd	60	5 227.6	5 718.7	6 087.5	5 829	5 723
Pm	61	5 432	5 961	6 339	6 071	5 956.6
Sm	62	5 632.6	6 201.1	6 587	6 317.2	6 196
Eu	63	5 849.5	6 458.4	6 844	6 571	6 438
Gd	64	6 053.4	6 708.1	7 100.4	6 832	6 688
Tb	65	6 272.9	6 975.1	7 363.5	7 097	6 940
Dy	66	6 498	7 248	7 636.4	7 370	7 204
Ho	67	6 720	7 526	7 911	7 653	7 471
Er	68	6 949	7 811	8 190.4	7 939	7 745
Tm	69	7 180	8 102	8 472.5	8 231	8 026
Yb	70	7 416	8 402	8 752.8	8 536	8 313
Lu	71	7 655	8 710	9 037.9	8 846	8 606
Hf	72	7 899	9 023	9 341	9 164	8 906

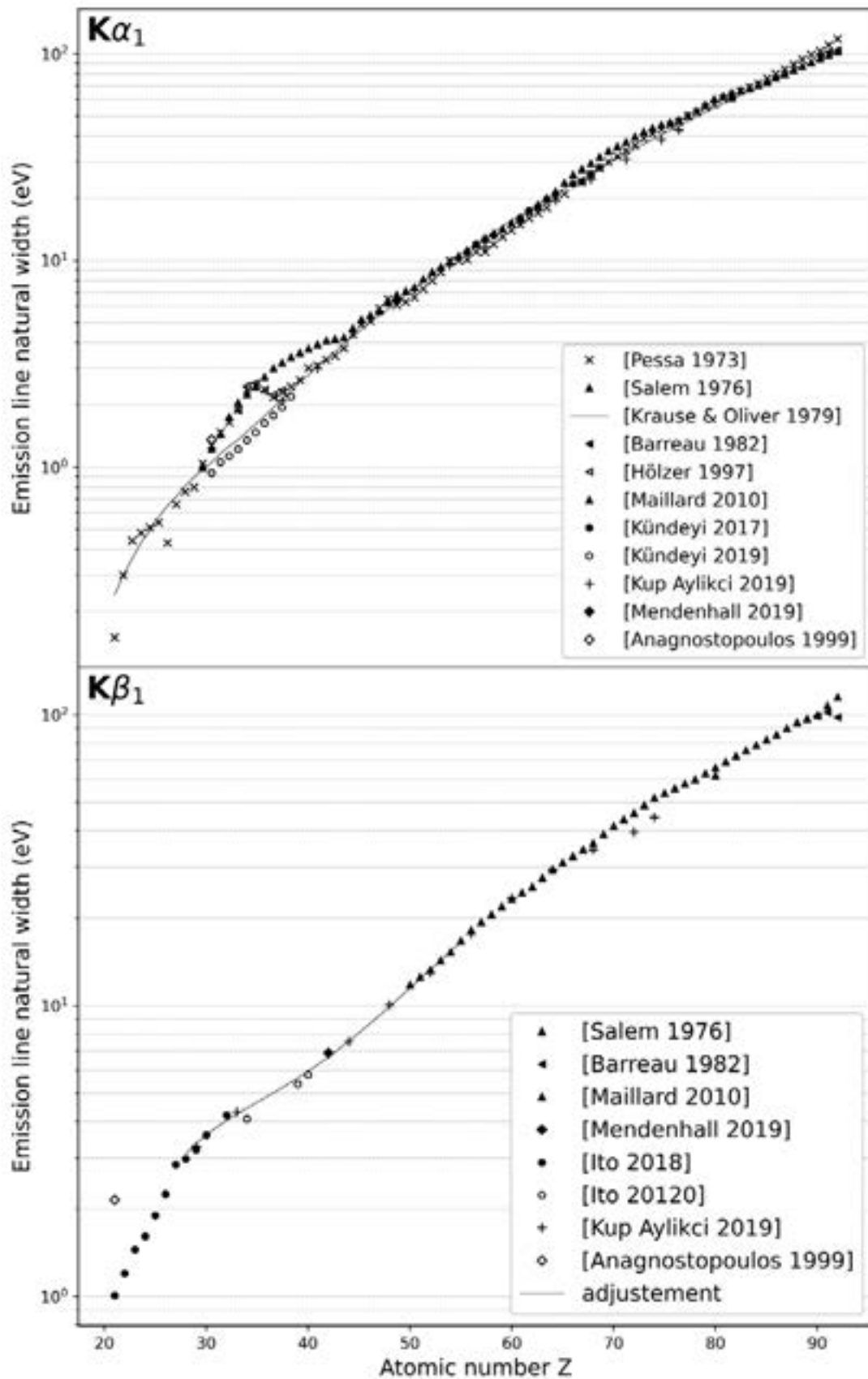
X-ray Fluorescence line energies

Table 7. K emission line energies, in eV [Elam 2002] (continued)

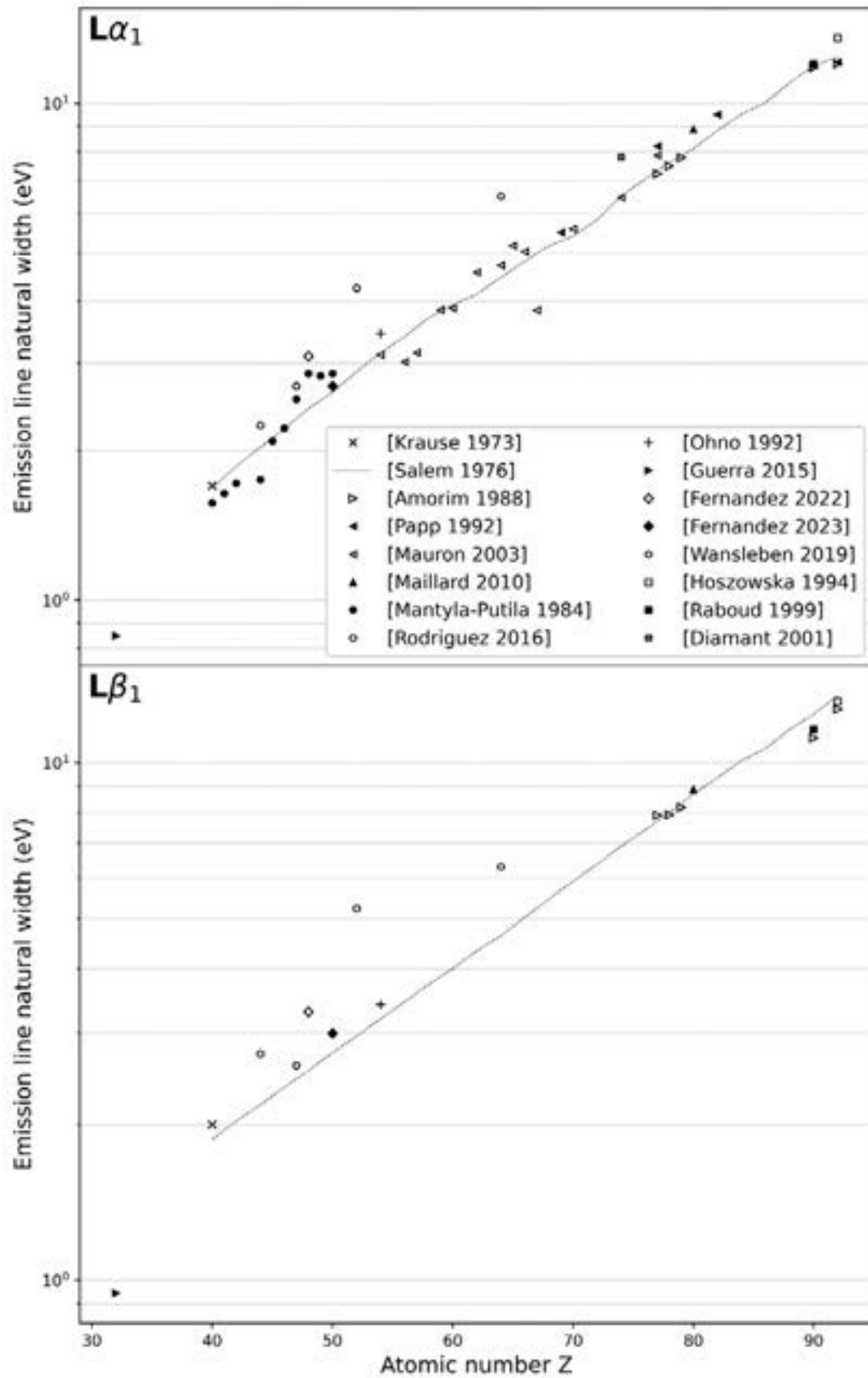
element	Z	L_{α1}	L_{β1}	L_{β2}	L_{β3}	L_{β4}
Ta	73	8 146	9 343	9 643.1	9 488	9 213
W	74	8 398	9 672	9 951.1	9 819	9 525
Re	75	8 652	10 010	10 261	10 160	9 845
Os	76	8 911	10 354	10 578	10 511	10 176
Ir	77	9 175	10 708	10 903	10 868	10 510
Pt	78	9 442	11 071	11 232	11 235	10 853
Au	79	9 713	11 443	11 566	11 610	11 205
Hg	80	9 989	11 824	11 906	11 992	11 560
Tl	81	10 269	12 213	12 252	12 390	11 931
Pb	82	10 551	12 614	12 601	12 795	12 307
Bi	83	10 839	13 023	12 955	13 211	12 692
Po	84	11 131	13 446	13 314	13 637	13 085
At	85	11 427	13 876	13 681	14 067	13 485
Rn	86	11 727	14 315	14 052	14 511	13 890
Fr	87	12 031	14 771	14 428	14 976	14 312
Ra	88	12 339	15 236	14 808	15 445	14 747
Ac	89	12 652	15 713	15 196	15 931	15 184
Th	90	12 968	16 202	15 588	16 426	15 642
Pa	91	13 291	16 703	15 990	16 931	16 104
U	92	13 614	17 220	16 388	17 454	16 575

X-ray Fluorescence line natural widths

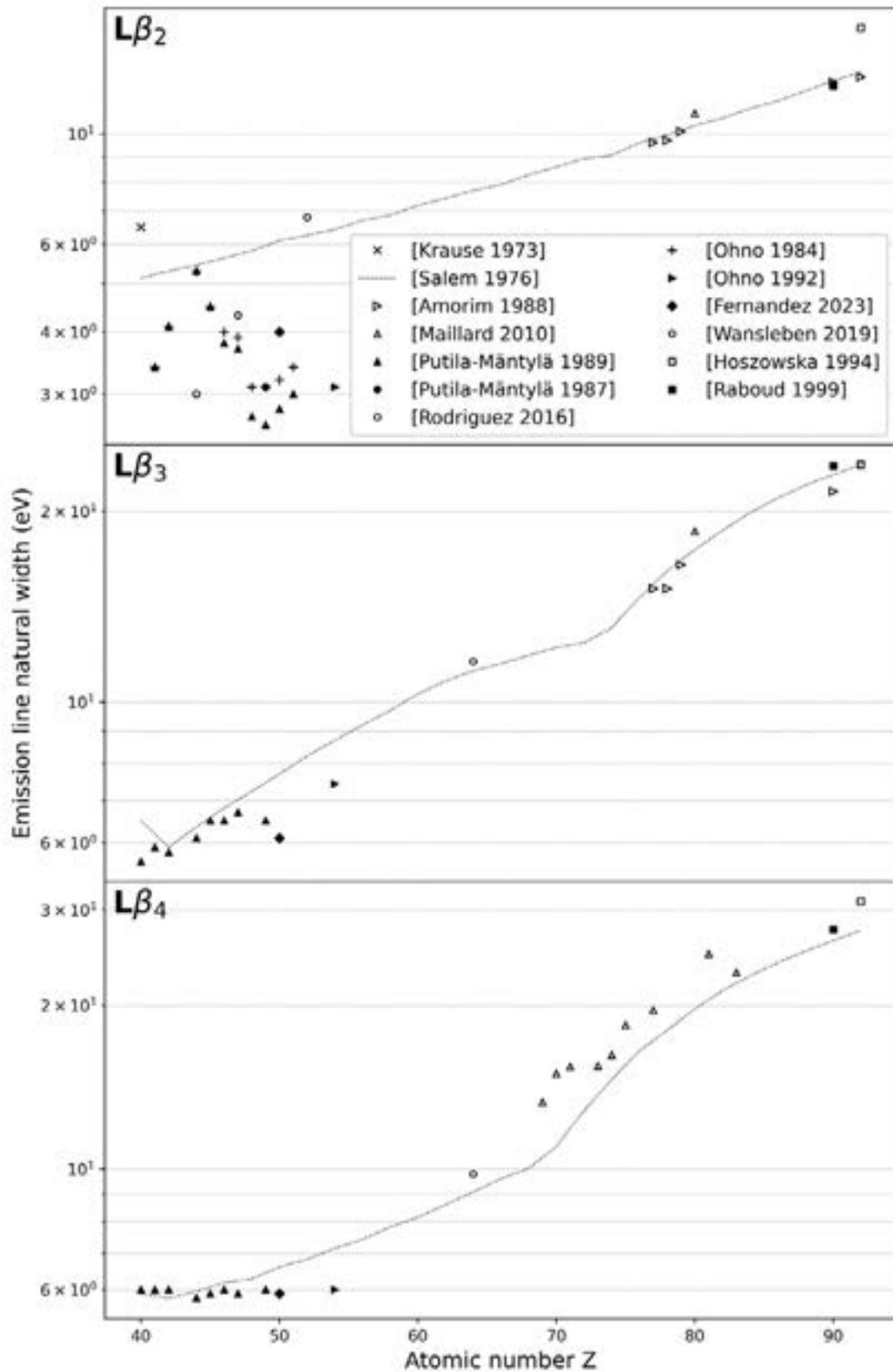
Comparison of different databases



X-ray Fluorescence line natural widths



X-ray Fluorescence line natural widths



X-ray Fluorescence line natural widths

Table 8. K emission line natural width, in eV.

Values from Krause & Oliver [Krause & Oliver 1979] except when marked. 1 [Ito 2018]. 2 (and values in italic), extrapolation of experimental data. 3 [Kup Aylikci 2019]. 4 [Ito 2020]. 5 [Mendenhall 2019]. 6 [Maillard 2010]. 7 [Barreau 1982]

element	Z	Kα₁	Kβ₁	Kβ₁ (other)
Ne	<i>10</i>	0.24		
Na	<i>11</i>	0.3		
Mg	<i>12</i>	0.36		
Al	<i>13</i>	0.43		
Si	<i>14</i>	0.49		
P	<i>15</i>	0.57		
S	<i>16</i>	0.65		
Cl	<i>17</i>	0.72		
Ar	<i>18</i>	0.81		
K	<i>19</i>	0.89		
Ca	<i>20</i>	0.98		
Sc	<i>21</i>	1.05		1.007 ¹
Ti	<i>22</i>	1.16		1.200 ¹
V	<i>23</i>	1.26		1.448 ¹
Cr	<i>24</i>	1.35		1.611 ¹
Mn	<i>25</i>	1.48		1.899 ¹
Fe	<i>26</i>	1.61		2.251 ¹
Co	<i>27</i>	1.76		2.838 ¹
Ni	<i>28</i>	1.94		2.97 ¹
Cu	<i>29</i>	2.11		3.20 ¹
Zn	<i>30</i>	2.32		3.59 ¹

X-ray Fluorescence line natural widths

Table 8. K emission line natural width, in eV (continued)

element	Z	K_{α1}	K_{β1}	K_{β1}(other)
Ga	31	2.59		3.81 ²
Ge	32	2.78		4.2 ¹
As	33	3.08		4.32 ³
Se	34	3.33		4.085 ⁴
Br	35	3.6		4.66 ²
Kr	36	3.92		4.86 ²
Rb	37	4.26		5.11 ²
Sr	38	4.63		5.36 ²
Y	39	5.02		5.38 ⁴
Zr	40	5.4		5.791 ⁴
Nb	41	5.8		6.28 ²
Mo	42	6.31		6.88 ⁵
Tc	43	6.82		7.08 ²
Ru	44	7.33		7.53 ³
Rh	45	7.9		8.06 ²
Pd	46	8.49		8.62 ²
Ag	47	9.16		9.25 ²
Cd	48	9.79		10.06 ³
In	49	10.56		10.67 ²
Sn	50	11.2	11.8	11.47 ²
Sb	51	12	12.55	12.35 ²
Te	52	12.8	13.3	13 ³
I	53	13.7	14.3	14.29 ²
Xe	54	14.6	15.3	15.36 ²

X-ray Fluorescence line natural widths

Table 8. K emission line natural width, in eV (continued)

element	Z	K_{α1}	K_{β1}	K_{β1}(other)
Cs	55	15.6	16.725	16.50 ²
Ba	56	16.5	18.15	17.66 ³
La	57	17.6	19.375	
Ce	58	18.6	20.6	
Pr	59	19.8	21.93	
Nd	60	20.9	23.25	23.48 ³
Pm	61	22.2	24.45	
Sm	62	23.6	25.65	
Eu	63	24.9	27.51	
Gd	64	26.4	29.37	29.33 ³
Tb	65	27.9	31.05	
Dy	66	29.4	32.73	
Ho	67	31.1	34.47	
Er	68	32.7	36.2	34.34 ³
Tm	69	34.6	38.815	
Yb	70	36.5	41.43	
Lu	71	38.4	43.715	
Hf	72	40.5	46	39.5
Ta	73	42.6	48.915	
W	74	44.9	51.83	44.45 ³
Re	75	47.2	53.865	
Os	76	49.6	55.9	
Ir	77	52.1	57.94	
Pt	78	54.6	59.98	

X-ray Fluorescence line natural widths

Table 8. K emission line natural width, in eV (continued)

element	Z	K_{α1}	K_{β1}	K_{β1}(other)
Au	79	57.4	62.865	
Hg	80	60.1	65.75	61.9 ⁶
Tl	81	63.1	68.975	
Pb	82	66.2	72.2	
Bi	83	69.4	75.4	
Po	84	72.7	78.6	
At	85	76.1	82.05	
Rn	86	79.7	85.5	
Fr	87	83.4	89.85	
Ra	88	87.2	94.2	
Ac	89	91.1	96.95	
Th	90	95.2	99.7	99 ⁷
Pa	91	99.3	107.35	102 ⁷
U	92	103.5	115	98 ⁷

X-ray Fluorescence line natural widths

Table 9. L emission line natural width, in eV. Values from [Salem 1976]

element	Z	L_{α1}	L_{β1}	L_{β2}	L_{β3}	L_{β4}
Zr	40	1.68	1.87	5.13	6.5	5.9
Nb	41	1.77	1.95	5.215	6.2	5.84
Mo	42	1.86	2.03	5.3	5.9	5.78
Tc	43	1.95	2.11	5.38	6.13	5.87
Ru	44	2.03	2.18	5.45	6.35	5.96
Rh	45	2.12	2.27	5.54	6.58	6.07
Pd	46	2.21	2.36	5.63	6.8	6.18
Ag	47	2.32	2.45	5.73	7.02	6.23
Cd	48	2.43	2.54	5.82	7.23	6.28
In	49	2.53	2.65	5.96	7.47	6.44
Sn	50	2.62	2.75	6.1	7.7	6.6
Sb	51	2.75	2.86	6.18	7.96	6.71
Te	52	2.88	2.96	6.25	8.22	6.82
I	53	3.02	3.08	6.34	8.46	6.99
Xe	54	3.15	3.20	6.43	8.7	7.15
Cs	55	3.27	3.33	6.57	8.95	7.29
Ba	56	3.39	3.45	6.7	9.2	7.42
La	57	3.55	3.59	6.78	9.45	7.62
Ce	58	3.7	3.73	6.86	9.7	7.82
Pr	59	3.82	3.87	7.02	10	7.99
Nd	60	3.93	4.00	7.18	10.3	8.15
Pm	61	4.03	4.17	7.3	10.55	8.38
Sm	62	4.13	4.33	7.42	10.8	8.6
Eu	63	4.30	4.48	7.56	11	8.84

X-ray Fluorescence line natural widths

Table 9. L emission line natural width, in eV (continued)

element	Z	L _{α1}	L _{β1}	L _{β2}	L _{β3}	L _{β4}
Gd	64	4.46	4.63	7.7	11.2	9.08
Tb	65	4.64	4.83	7.8	11.35	9.34
Dy	66	4.81	5.03	7.9	11.5	9.6
Ho	67	4.99	5.24	8.09	11.67	9.82
Er	68	5.17	5.45	8.28	11.85	10.03
Tm	69	5.29	5.675	8.43	12.02	10.52
Yb	70	5.4	5.9	8.58	12.2	11
Lu	71	5.62	6.13	8.75	12.3	11.9
Hf	72	5.83	6.36	8.92	12.4	12.8
Ta	73	6.17	6.63	8.99	12.75	13.7
W	74	6.5	6.9	9.06	13.1	14.6
Re	75	6.77	7.16	9.33	13.85	15.55
Os	76	7.04	7.42	9.6	14.6	16.5
Ir	77	7.32	7.71	9.78	15.35	17.25
Pt	78	7.6	8	9.95	16.1	18
Au	79	7.85	8.35	10.18	16.75	18.85
Hg	80	8.1	8.7	10.4	17.4	19.7
Tl	81	8.46	9.03	10.58	18.02	20.5
Pb	82	8.82	9.35	10.75	18.65	21.3
Bi	83	9.16	9.73	11	19.28	22
Po	84	9.5	10.1	11.25	19.9	22.7
At	85	9.77	10.38	11.45	20.45	23.35
Rn	86	10.03	10.65	11.65	21	24
Fr	87	10.52	11.125	11.925	21.5	24.6

X-ray Fluorescence line natural widths

Table 9. L emission line natural width, in eV (continued)

element	Z	L_{α1}	L_{β1}	L_{β2}	L_{β3}	L_{β4}
Ra	88	11	11.6	12.2	22	25.2
Ac	89	11.45	12	12.5	22.43	25.78
Th	90	11.9	12.4	12.8	22.85	26.35
Pa	91	12.15	12.95	13.05	23.28	26.93
U	92	12.4	13.5	13.3	23.7	27.5

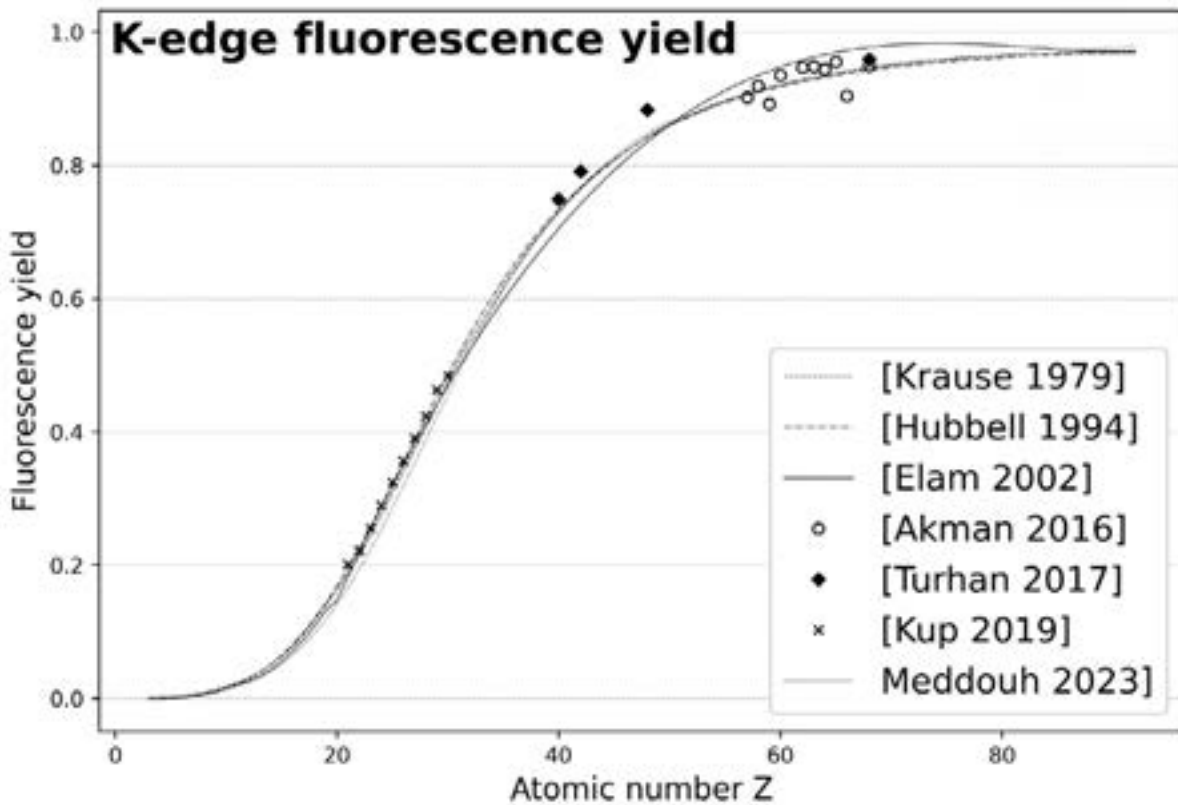
Fluorescence yields

Fluorescence yields

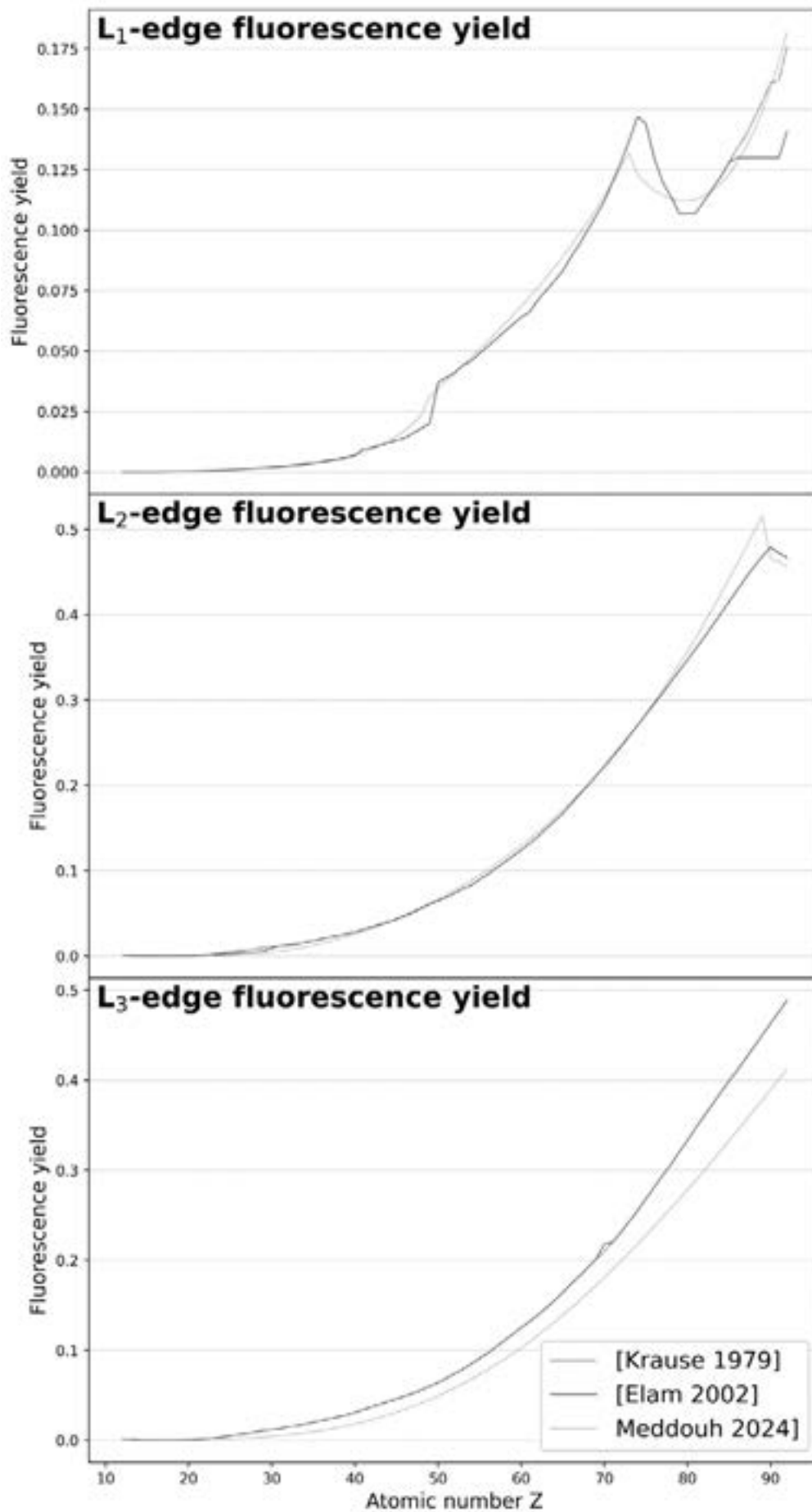
The fluorescence yield is the probability that an electronic vacancy occurring during the absorption process will be filled and will give a radiation (fluorescence) transition. The complementary non-radiative yield is the Auger yield.

$$1 = \omega_{fluorescence} + \omega_{Auger}$$

Comparison of different databases



Fluorescence yields



X-ray Emission Spectroscopy

X-ray Emission Spectroscopy

Energy shifts and chemical bonding

Literature on the subject is quite large, beginning in the 30' (e.g. [Tanaka 1935], [Okuno 1936]), with review articles (e.g. [Parrat 1959]), and books ([Agarwal 1991])... The electronic mechanisms involved in such chemical XES sensitivity may schematically arise from two effects (e.g. [Glatzel 2013]):

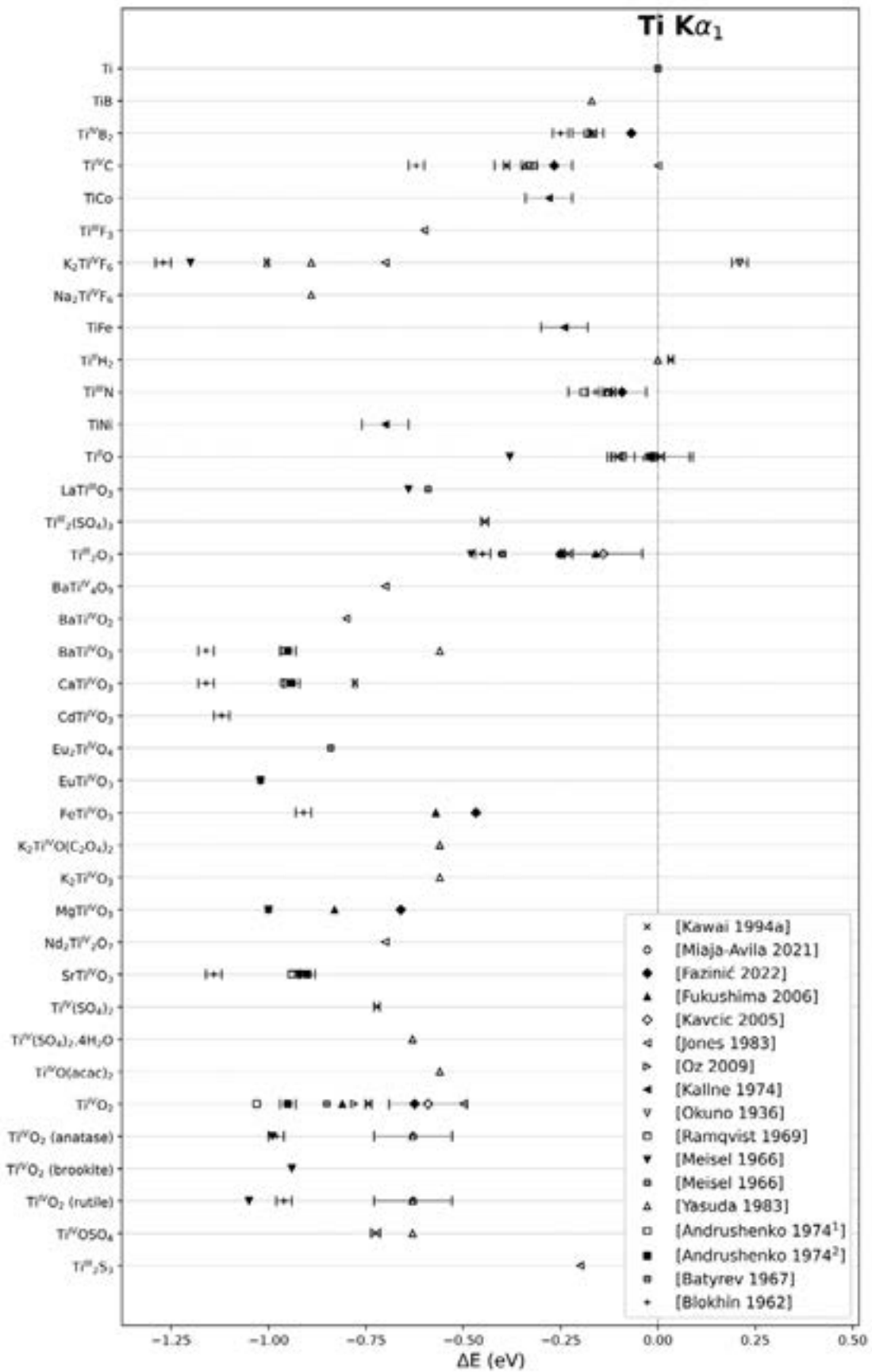
- Screening effects. When the valence configuration changes, all the core levels of an atom shift, to adjust the modifications of the electron density in the valence orbitals.
- Multiplet effects. The spin and orbital angular momentum of the core hole and valence electrons strongly couple inducing energy shifts and a multiplet structure.

These electron level shifts are around few eV, positive if electrons are gained, negative if electrons are lost. In first approximation the energy shifts are the same for all the level, but, in reality, small differences occur. Consequently, emission lines energies are slightly shifted.

In the following pages we present the energy shifts of the transition metals $K\alpha_1$ and $K\beta_1$ emission lines, the reference being taken for the metallic state. The aim of the figures is not to give an absolute value of the shift for a given material and a given emission line (dispersion of the experimental values is sometimes too large) but to give the main trends of the phenomena.

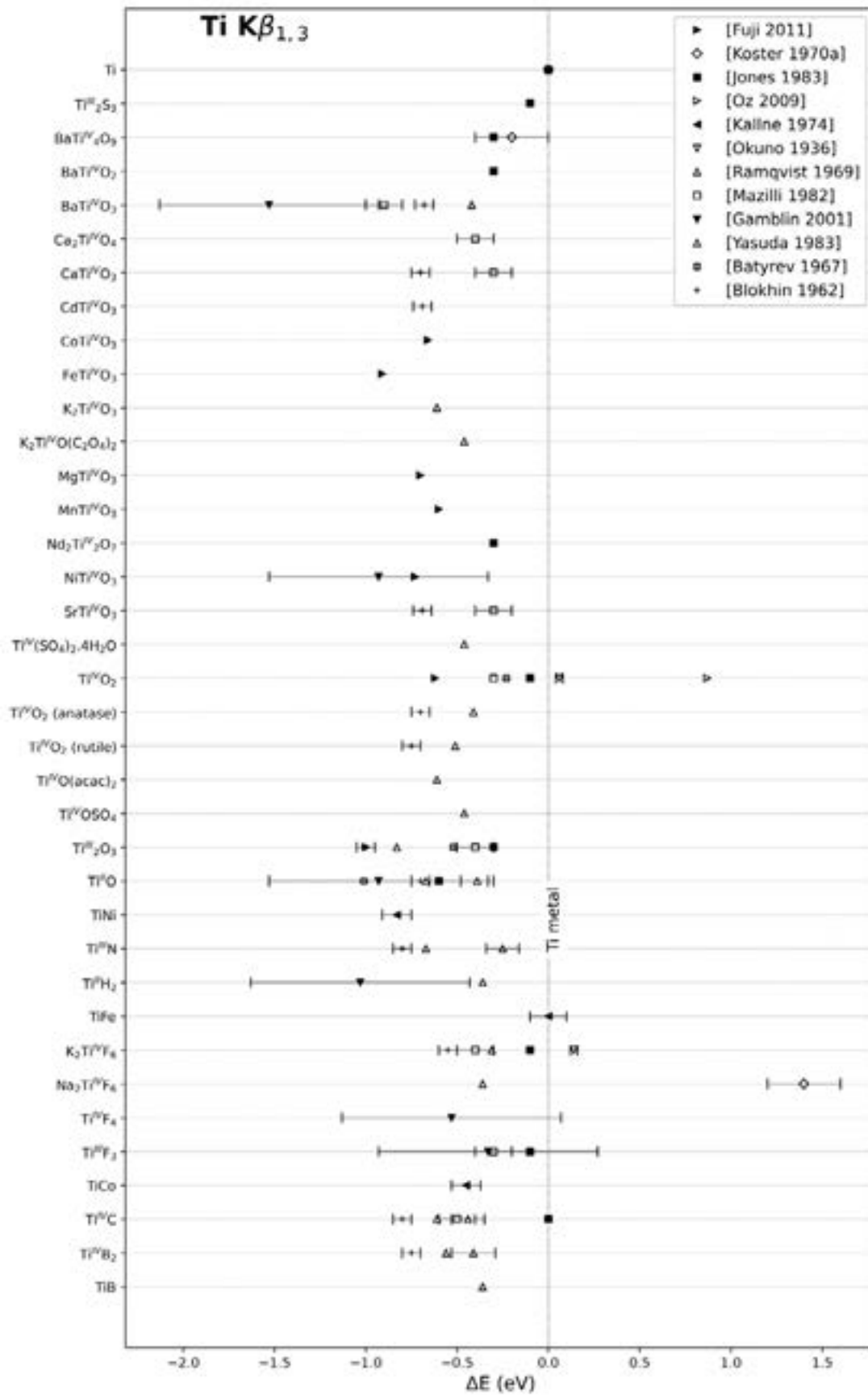
X-ray Emission Spectroscopy

Z=22 Ti $K\alpha_1$ energy shift



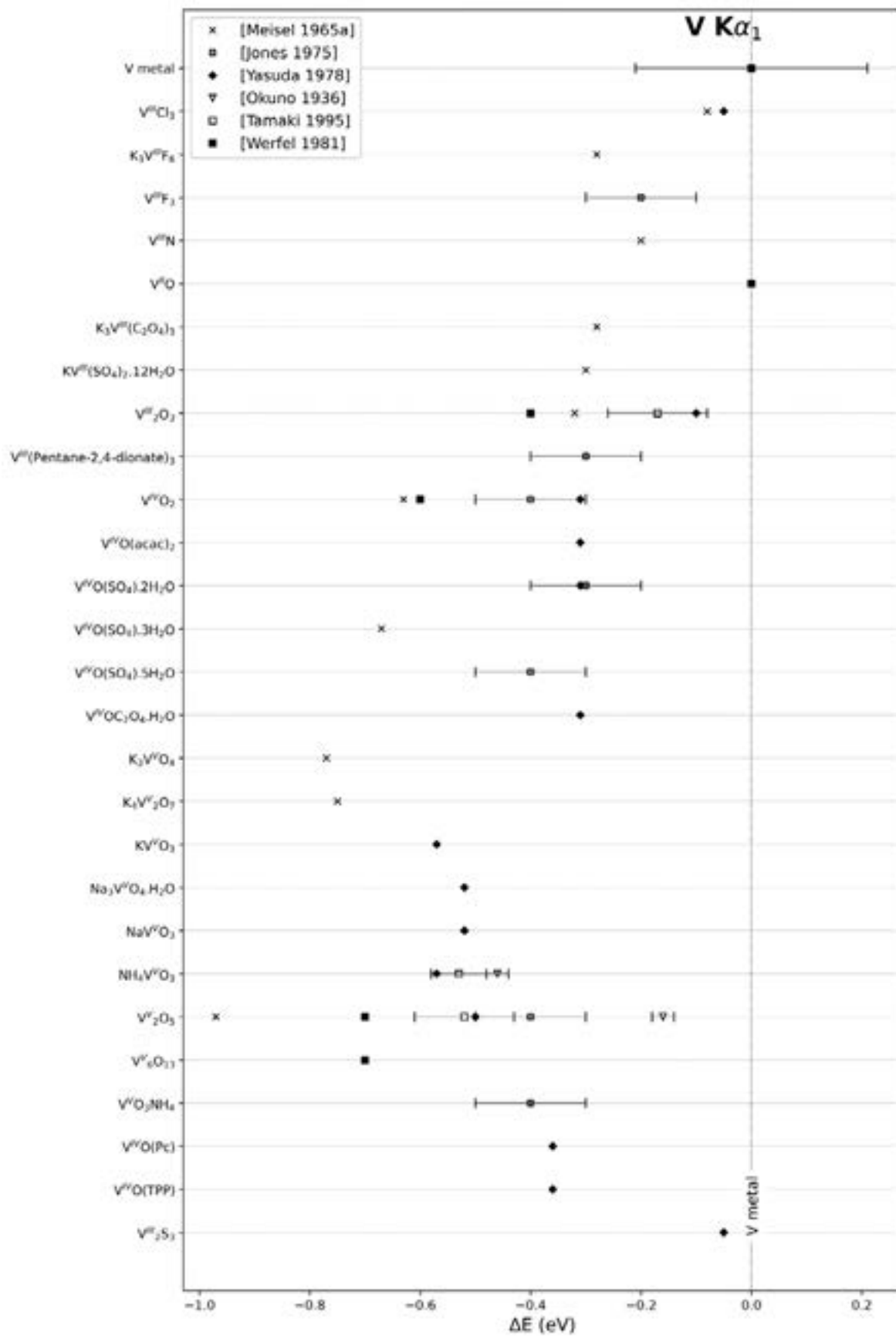
X-ray Emission Spectroscopy

Z=22 Ti $K\beta_{1,3}$ energy shift



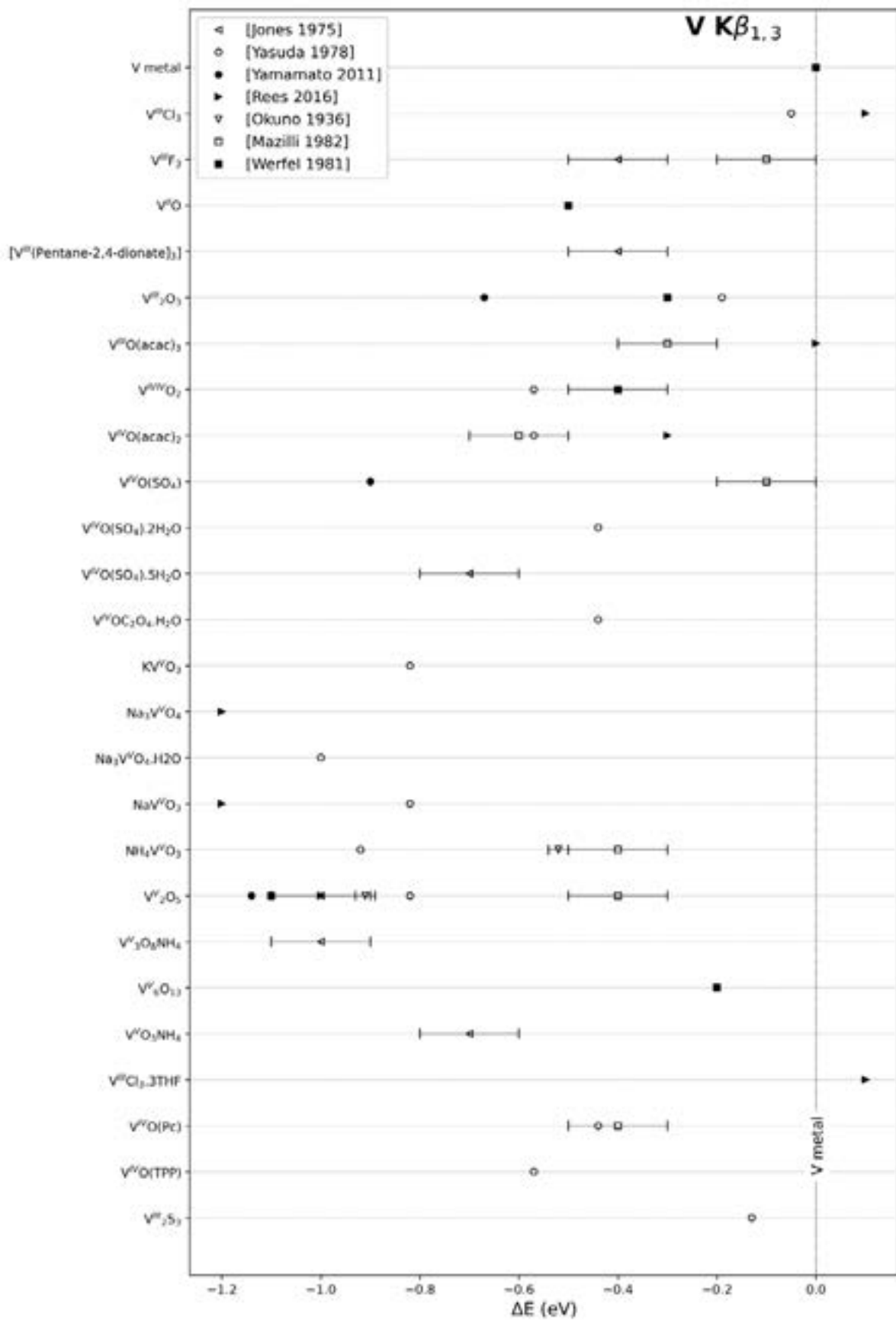
X-ray Emission Spectroscopy

Z=23 V $K\alpha_1$ energy shift



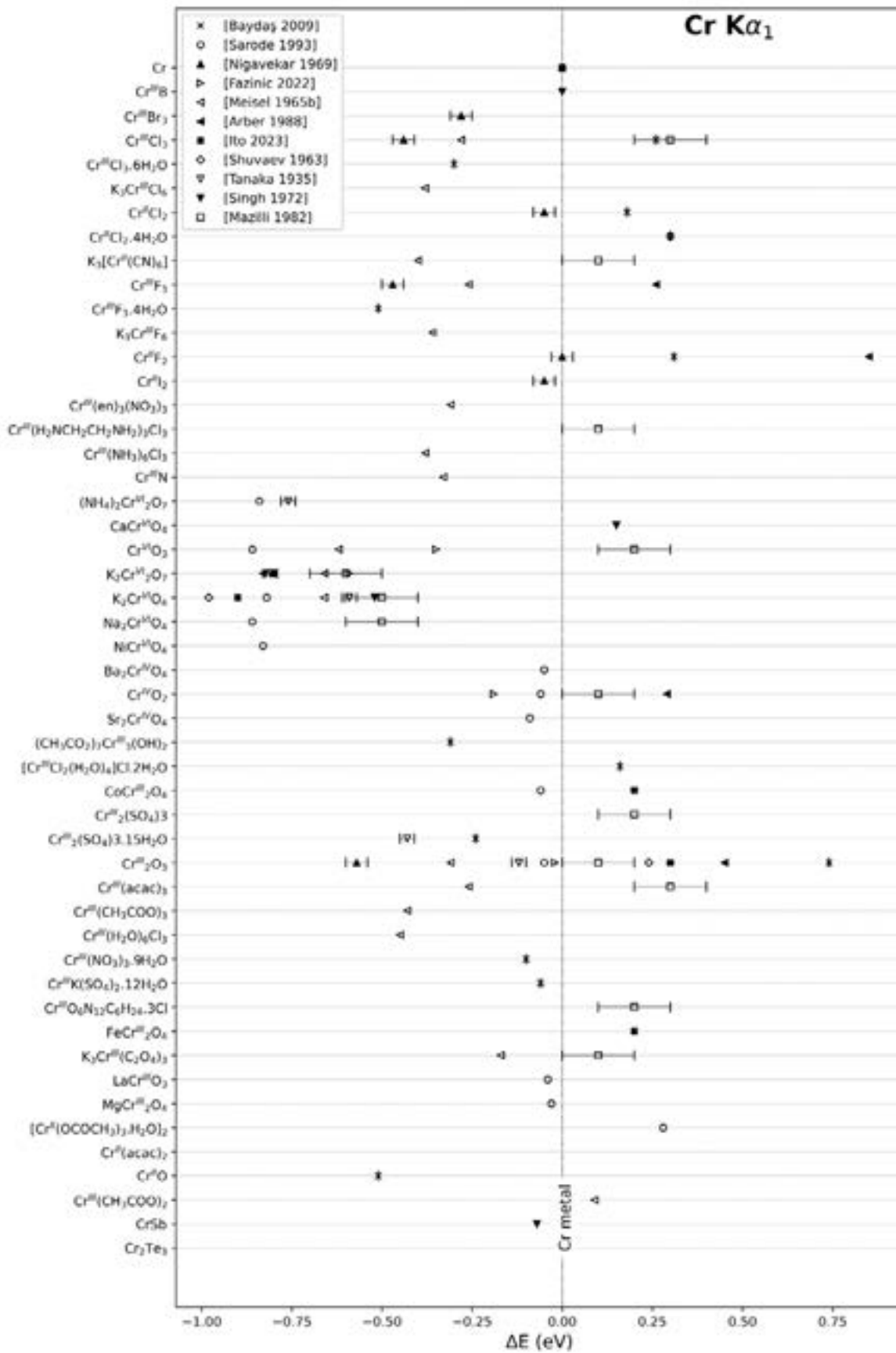
X-ray Emission Spectroscopy

Z=23 V $K\beta_{1,3}$ energy shift



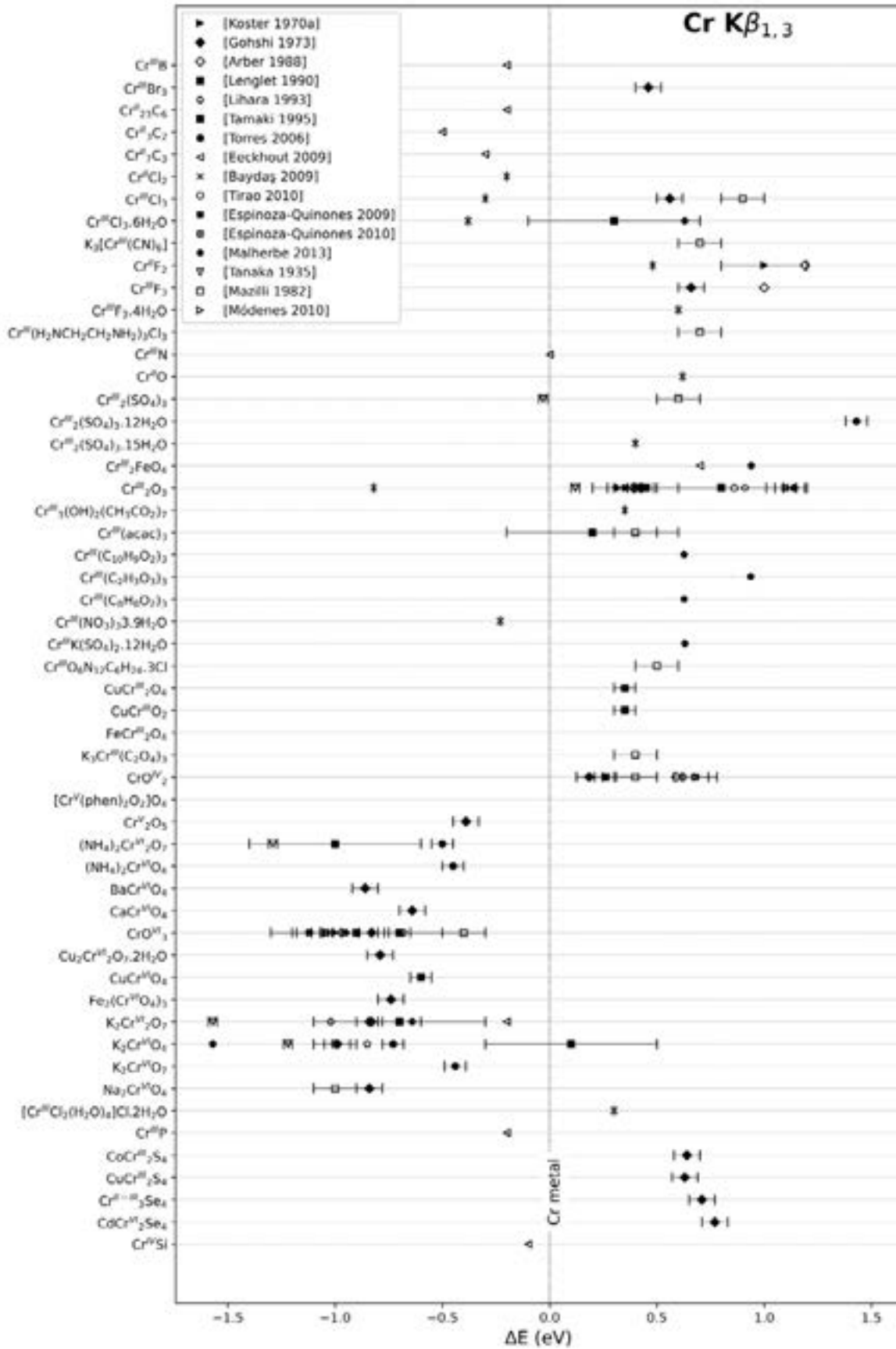
X-ray Emission Spectroscopy

Z=24 Cr $K\alpha_1$ energy shift



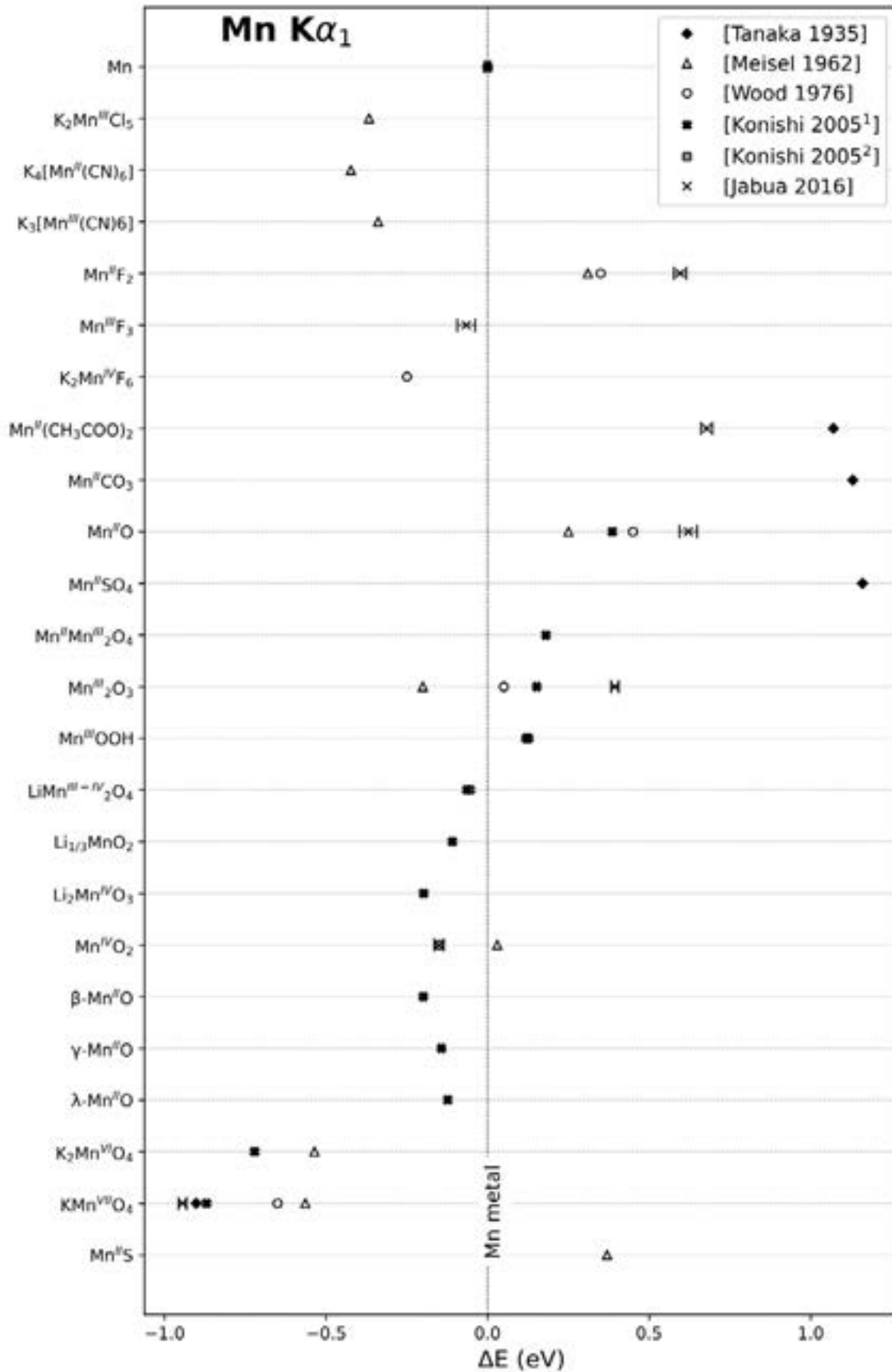
X-ray Emission Spectroscopy

Z=24 Cr $K\beta_{1,3}$ energy shift



X-ray Emission Spectroscopy

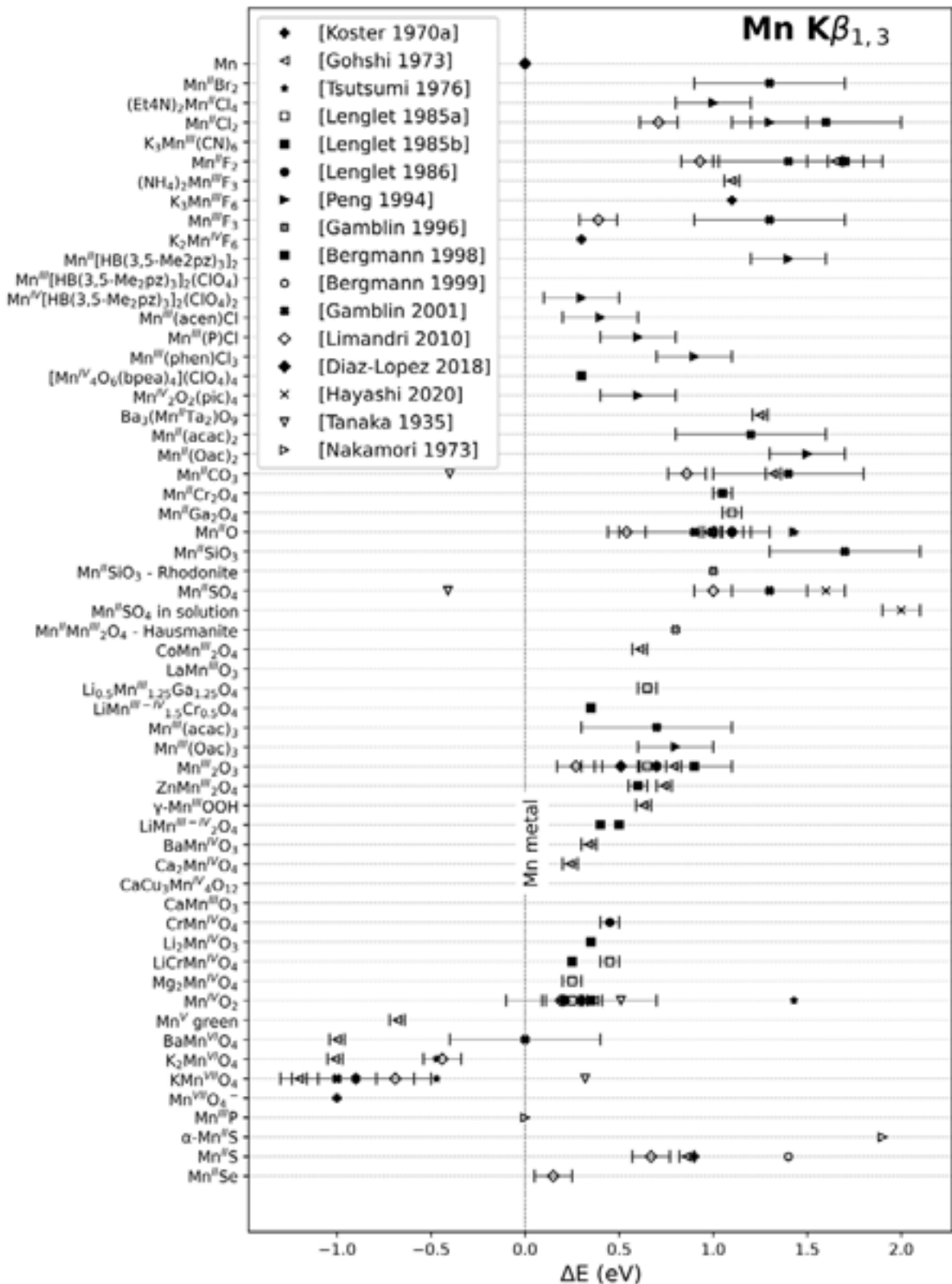
Z=25 Mn $K\alpha_1$ energy shift



X-ray Emission Spectroscopy

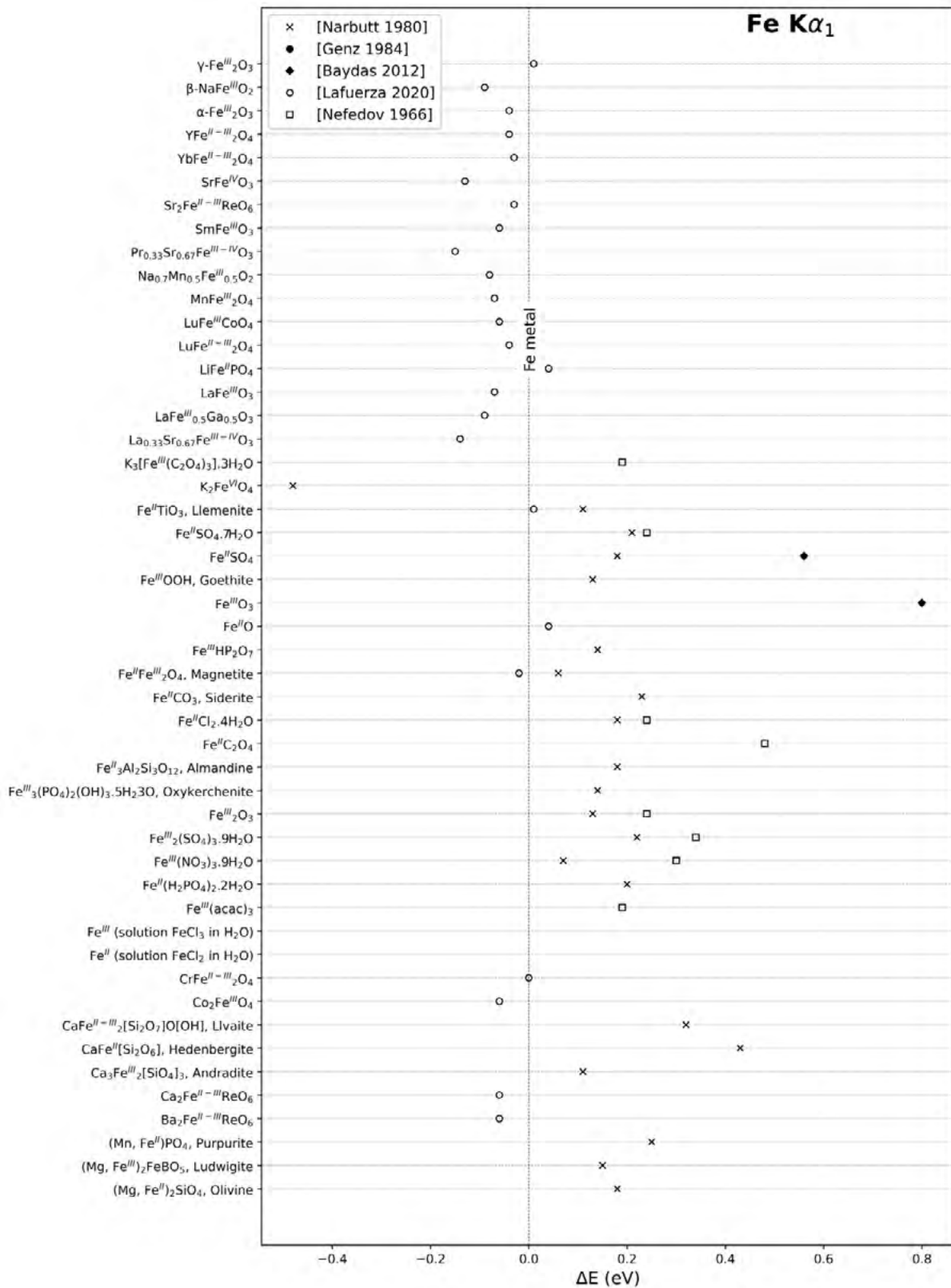
Z=25 Mn

K $\beta_{1,3}$ energy shift

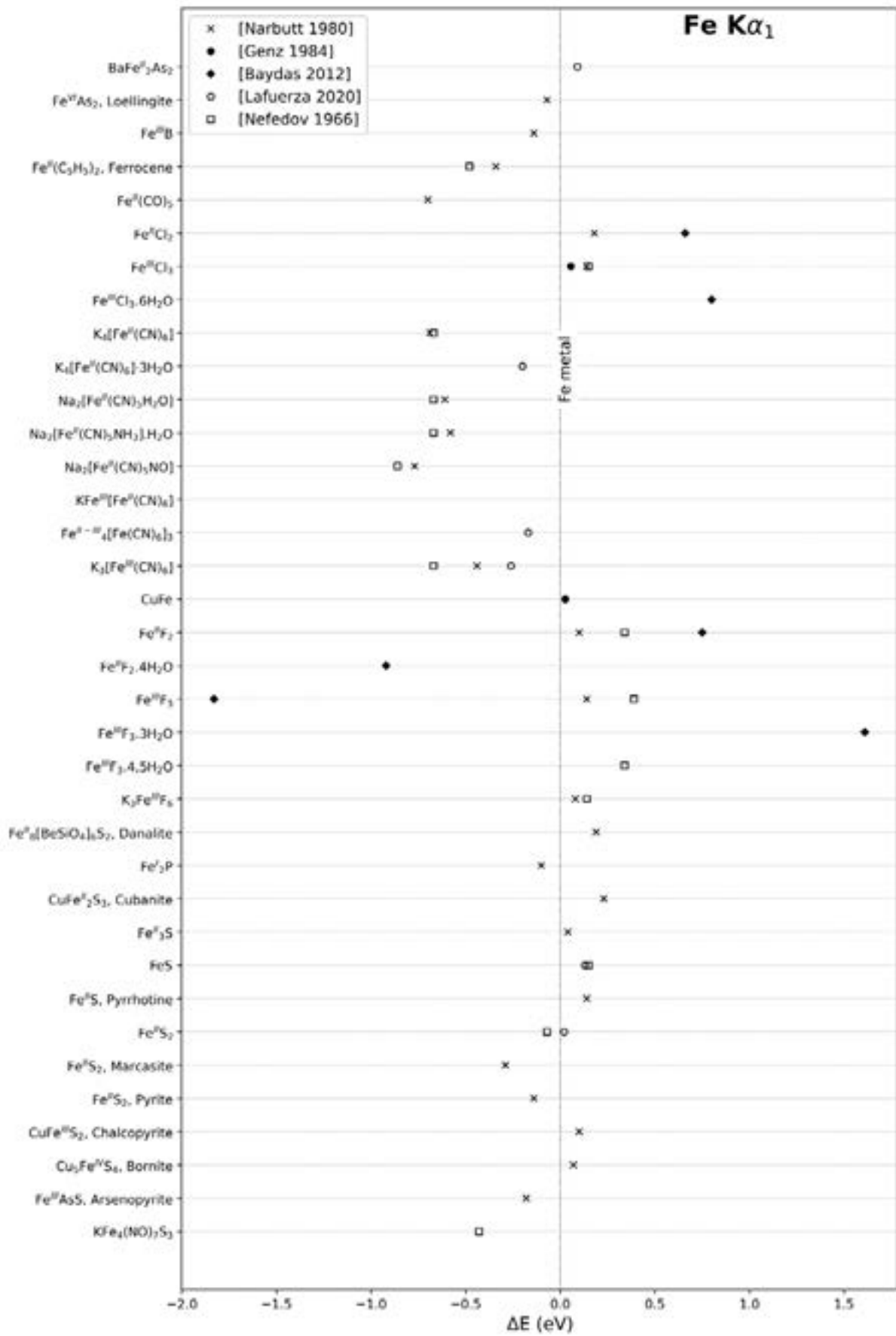


X-ray Emission Spectroscopy

Z=26 Fe $K\alpha_{1,3}$ energy shift

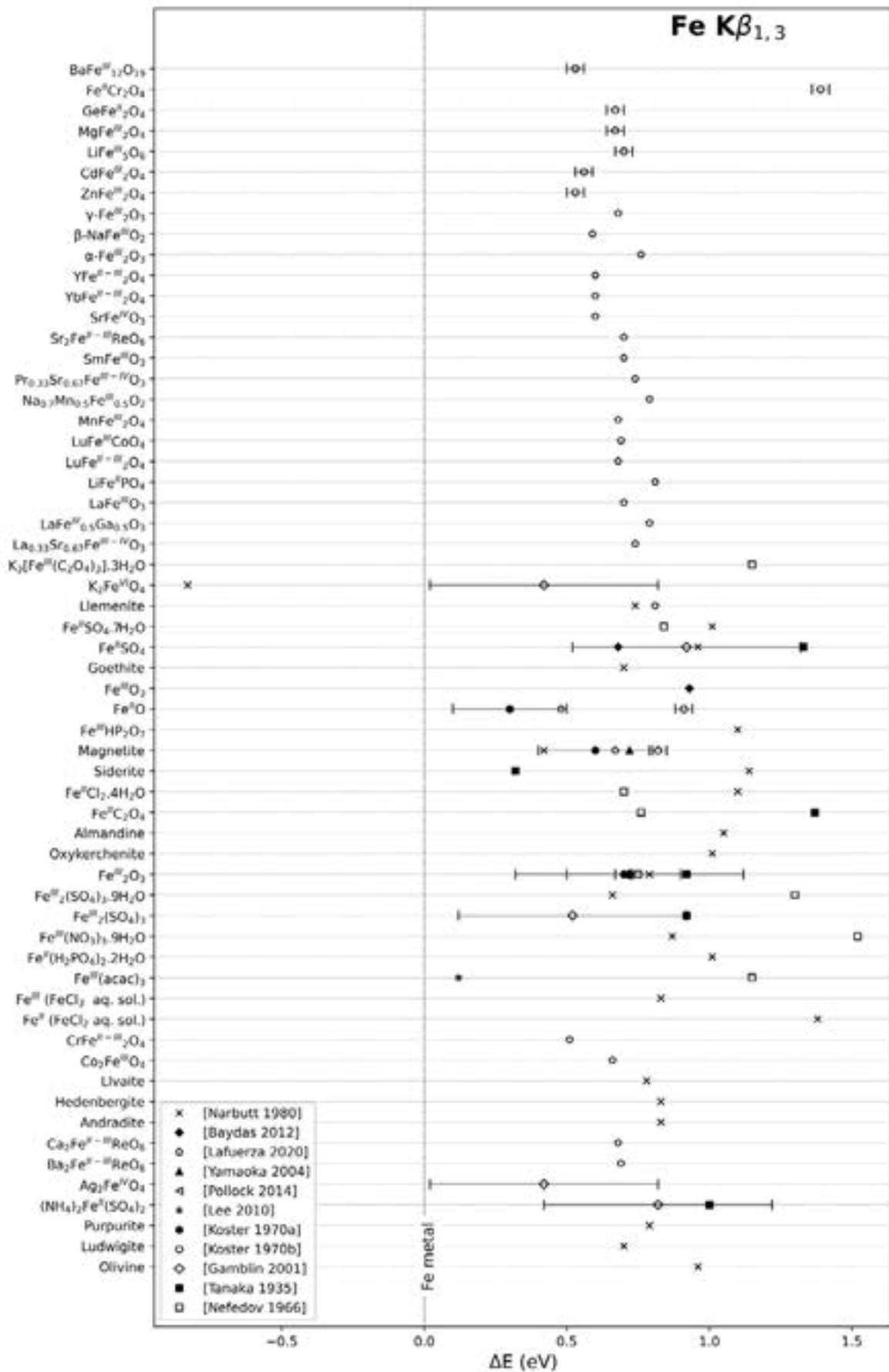


X-ray Emission Spectroscopy

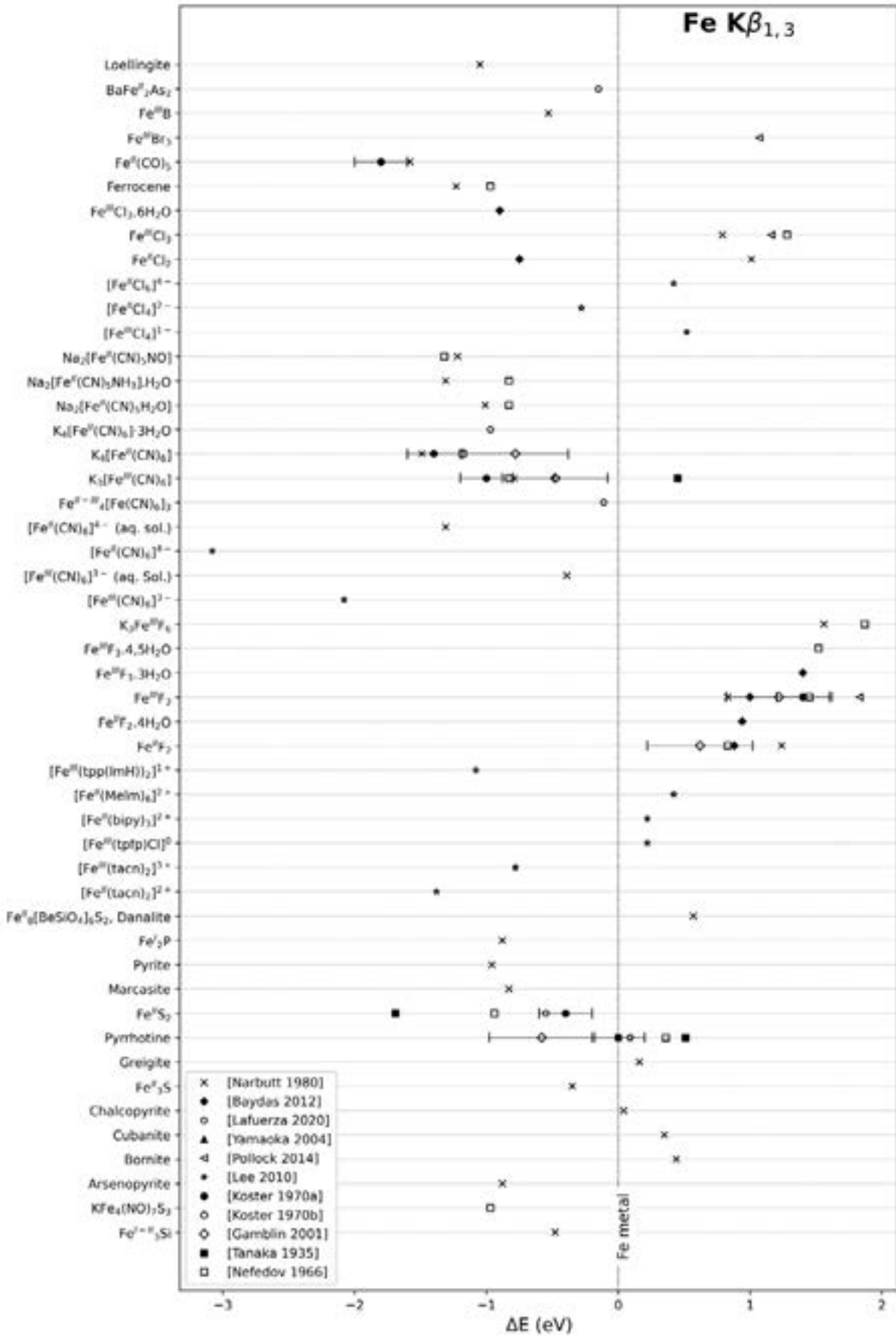


X-ray Emission Spectroscopy

Z=26 Fe $K\beta_{1,3}$ energy shift

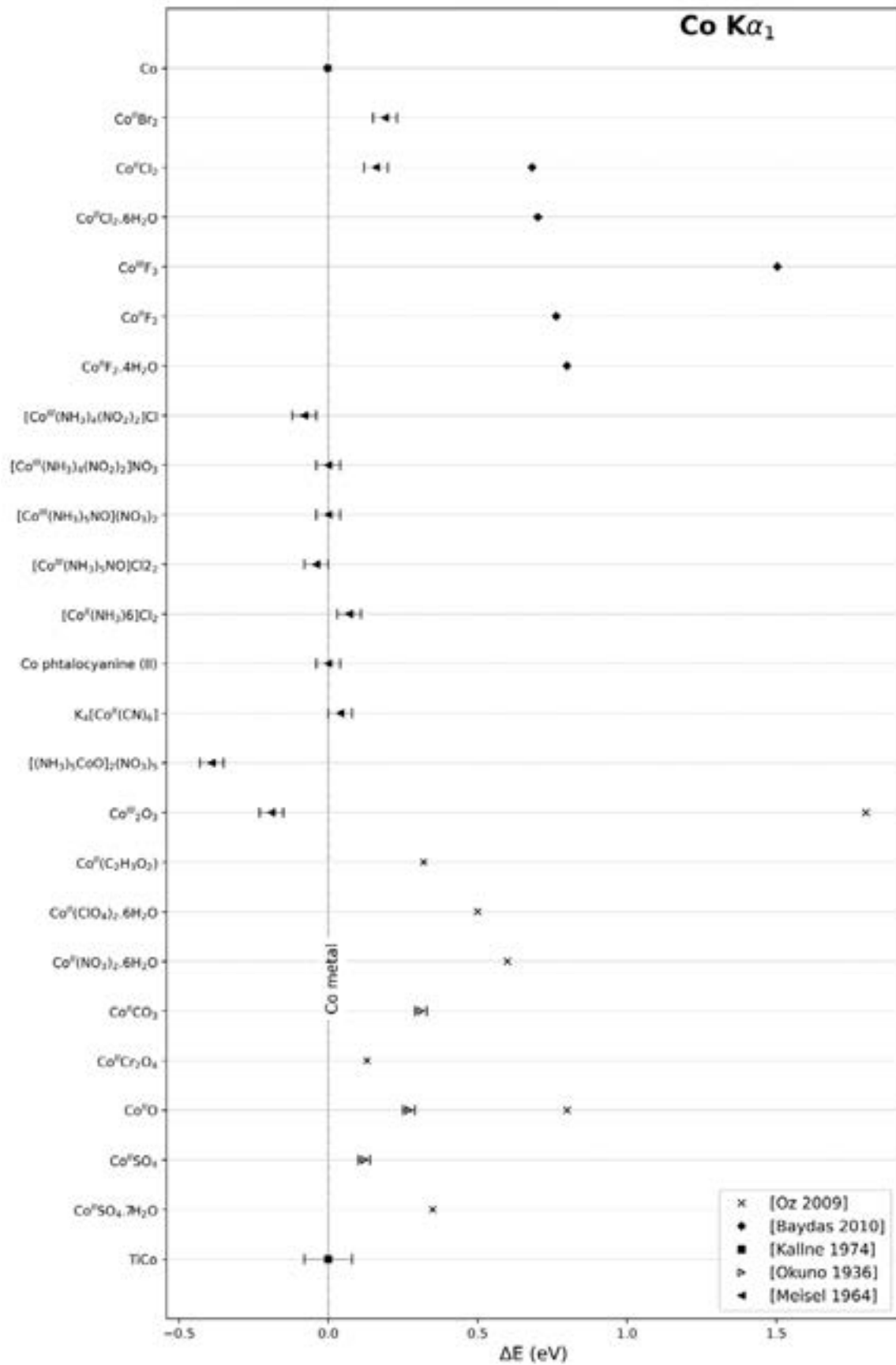


X-ray Emission Spectroscopy



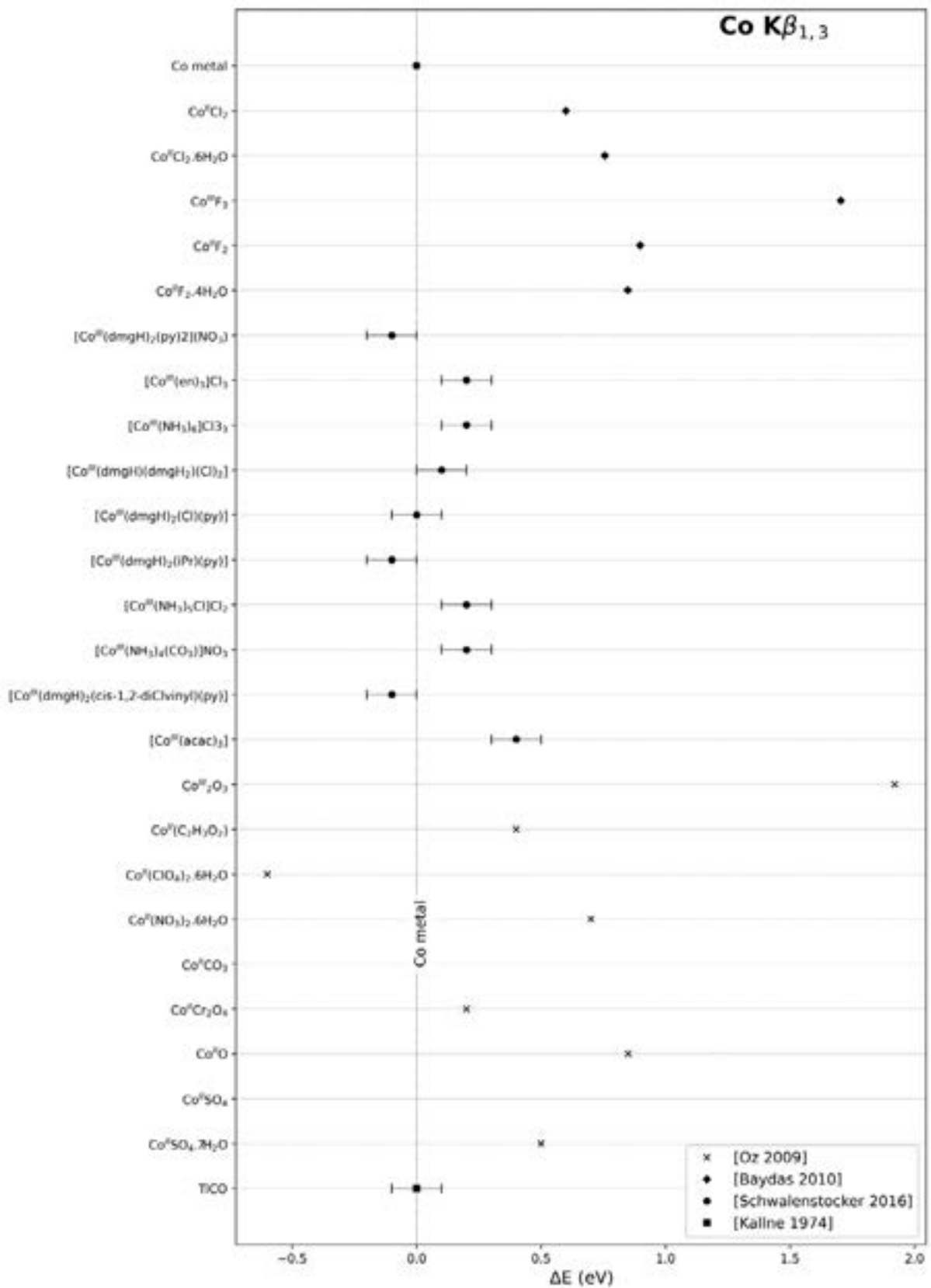
X-ray Emission Spectroscopy

Z=27 Co $K\alpha_{1,3}$ energy shift



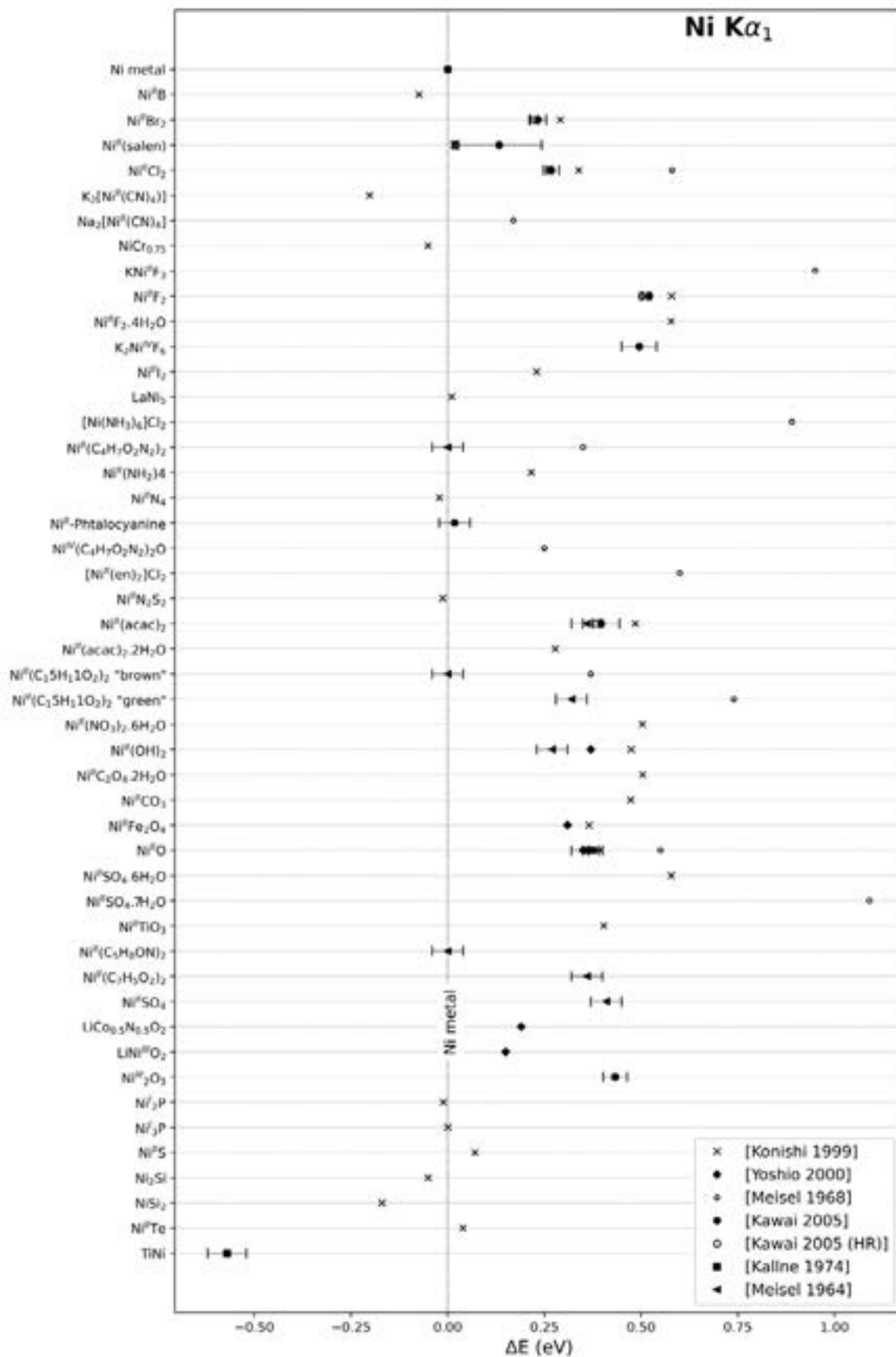
X-ray Emission Spectroscopy

Z=27 Co $K\beta_{1,3}$ energy shift



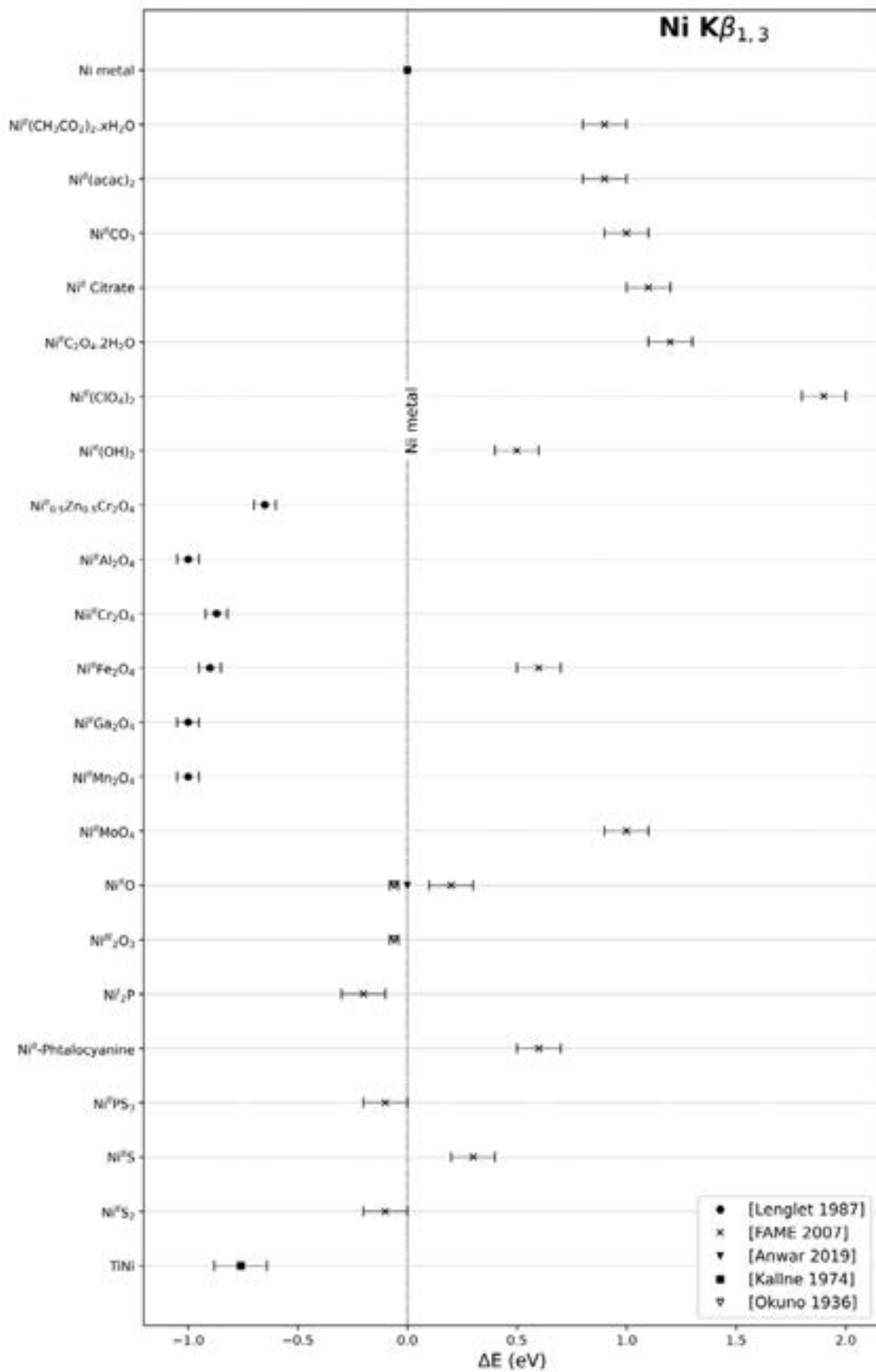
X-ray Emission Spectroscopy

Z=28 Ni $K\alpha_{1,3}$ energy shift



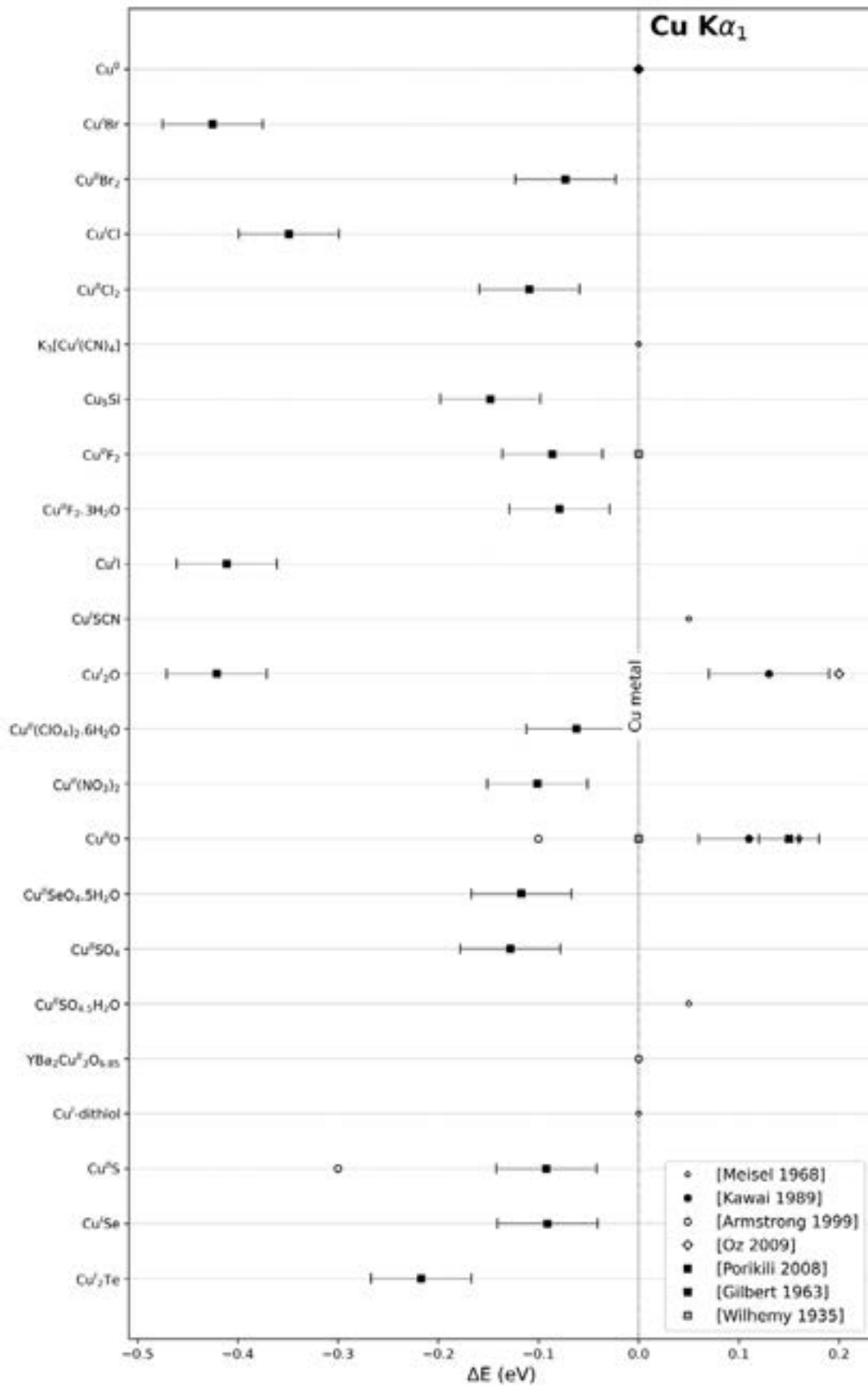
X-ray Emission Spectroscopy

Z=28 Ni $K\beta_{1,3}$ energy shift



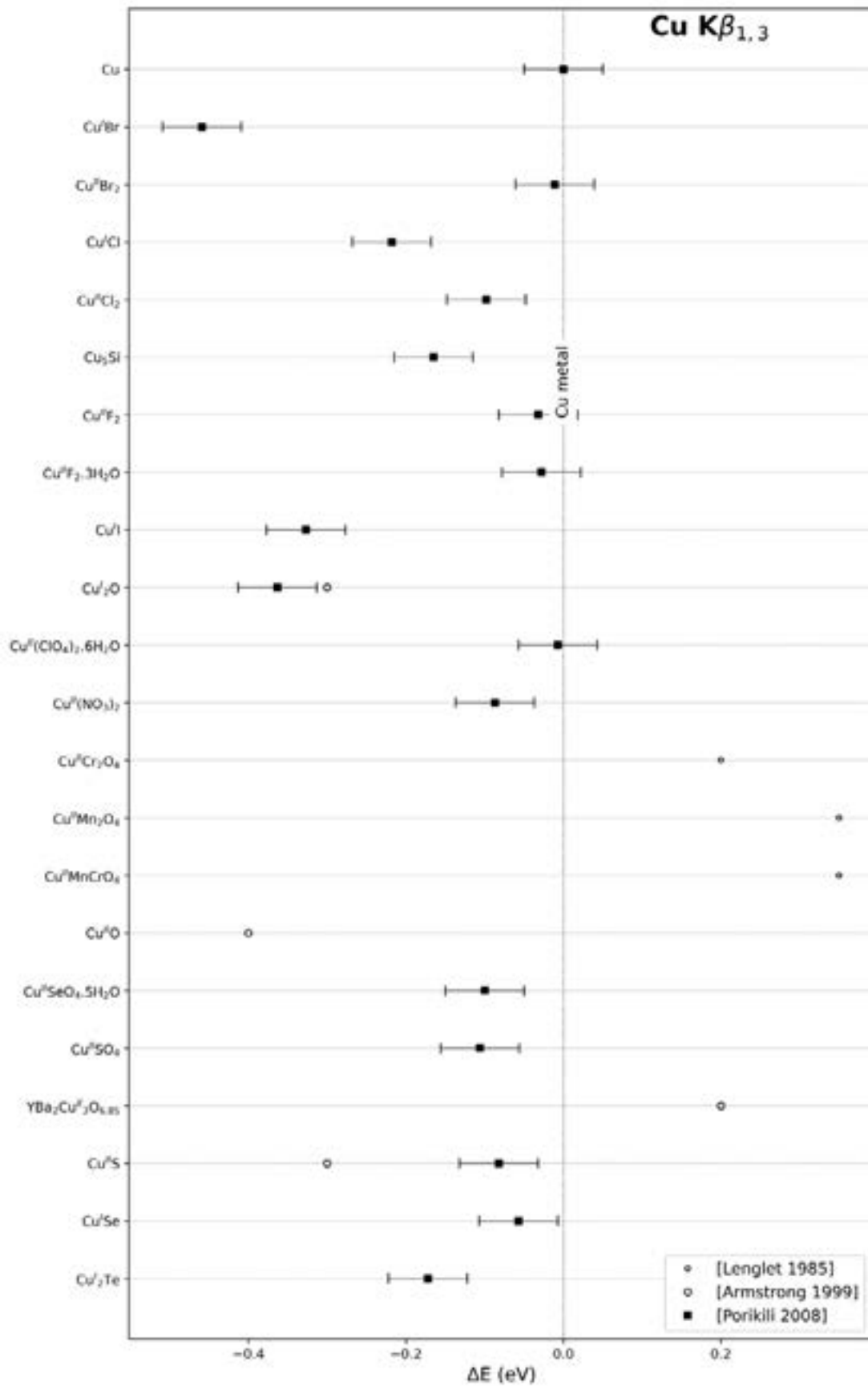
X-ray Emission Spectroscopy

Z=29 Cu $K\alpha_{1,3}$ energy shift



X-ray Emission Spectroscopy

Z=29 Cu $K\beta_{1,3}$ energy shift



X-ray Absorption Spectroscopy spectra

XAS database

Most of the spectra presented in the following pages have been measured on FAME or FAME-UHD beamlines with a Si220 monochromator, and either in transmission or in TFY. They can be found on the SSHADE database [Kieffer 2016]:

<https://www.sshade.eu/db/fame>



Do not hesitate to contact us to include your spectra obtained on FAME, soon FAME-PIX, or FAME-UHD on SSHADE, both model compounds reference spectra and your own samples ones.

Other databases exist and where sometimes also used here (a reference is then added on the figures, with the nature of the monochromator crystals when different from Si220), among:

- the database of the Canadian Light Source, <https://xasdb.lightsource.ca/>
- the XASLIB database, X-ray Absorption Data Library, of the International X-ray Absorption Society, <https://xaslib.xrayabsorption.org/>
- the MDR (Materials Data Repository) operated by the National Institute for Materials Science (Japan), <https://mdr.nims.go.jp/>
- AcReDaS (Actinide Reference Database for Spectroscopy), <https://www.hzdr.de/acredas>
- RefXAS, <http://xafsdb.ddns.net/>
- the database of Italian CRG beamline LISA, <https://lisa.iom.cnr.it/xasdb/>
- the Lytle database, http://ixs.iit.edu/database/data/Farrel_Lytle_data/
- International XAFS DB Portal gathers on a same site several databases (including SSHADE, MDR...s): <https://ixdb.ixafs.org/>

Z=22**Ti****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	4 966	4 512.2	4 933.4
Natural width	0.94	1.16	1.20

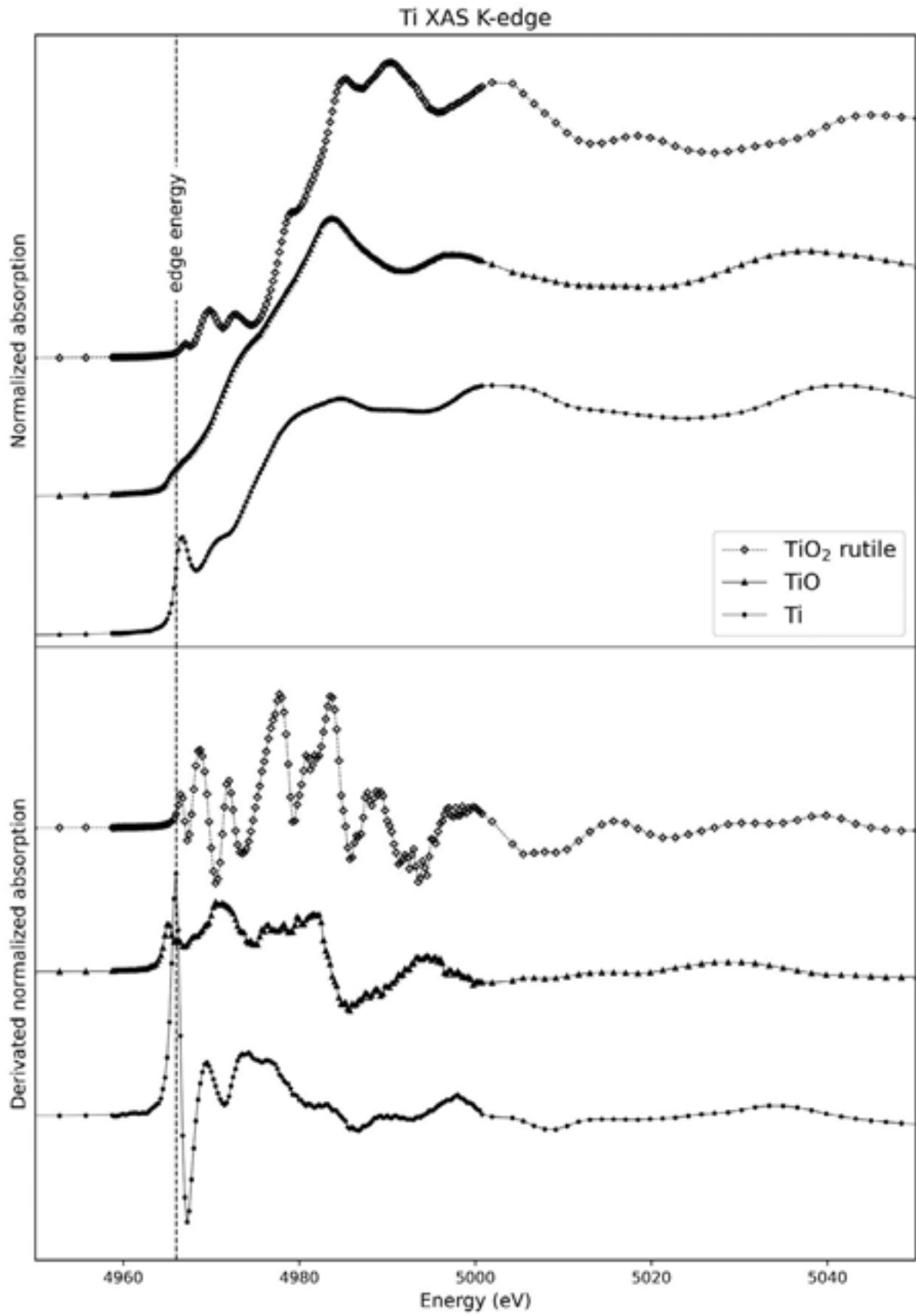
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	23.46	0.68
Si220	40.55	0.30

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge400	76.3
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge331	75.5

XAS Reference spectra



Z=23**V****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	5 465	4 952.9	5 427.8
Natural width	1.01	1.26	1.448

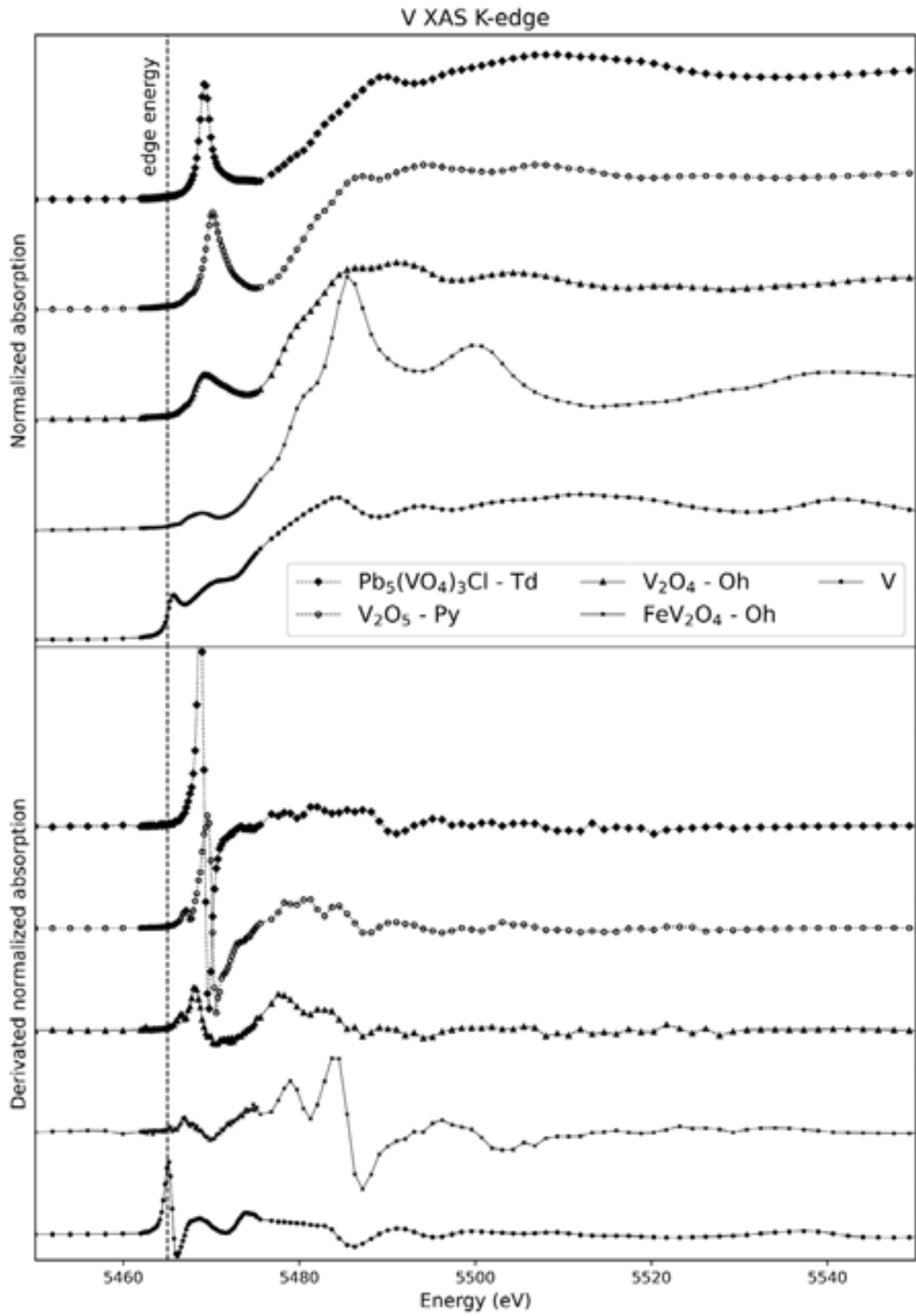
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	21.21	0.74
Si220	36.21	0.33

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge331	74.6
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge422	81.5

XAS Reference spectra



Z=24**Cr****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	5 989	5 414.9	5 946.8
Natural width	1.08	1.35	1.611

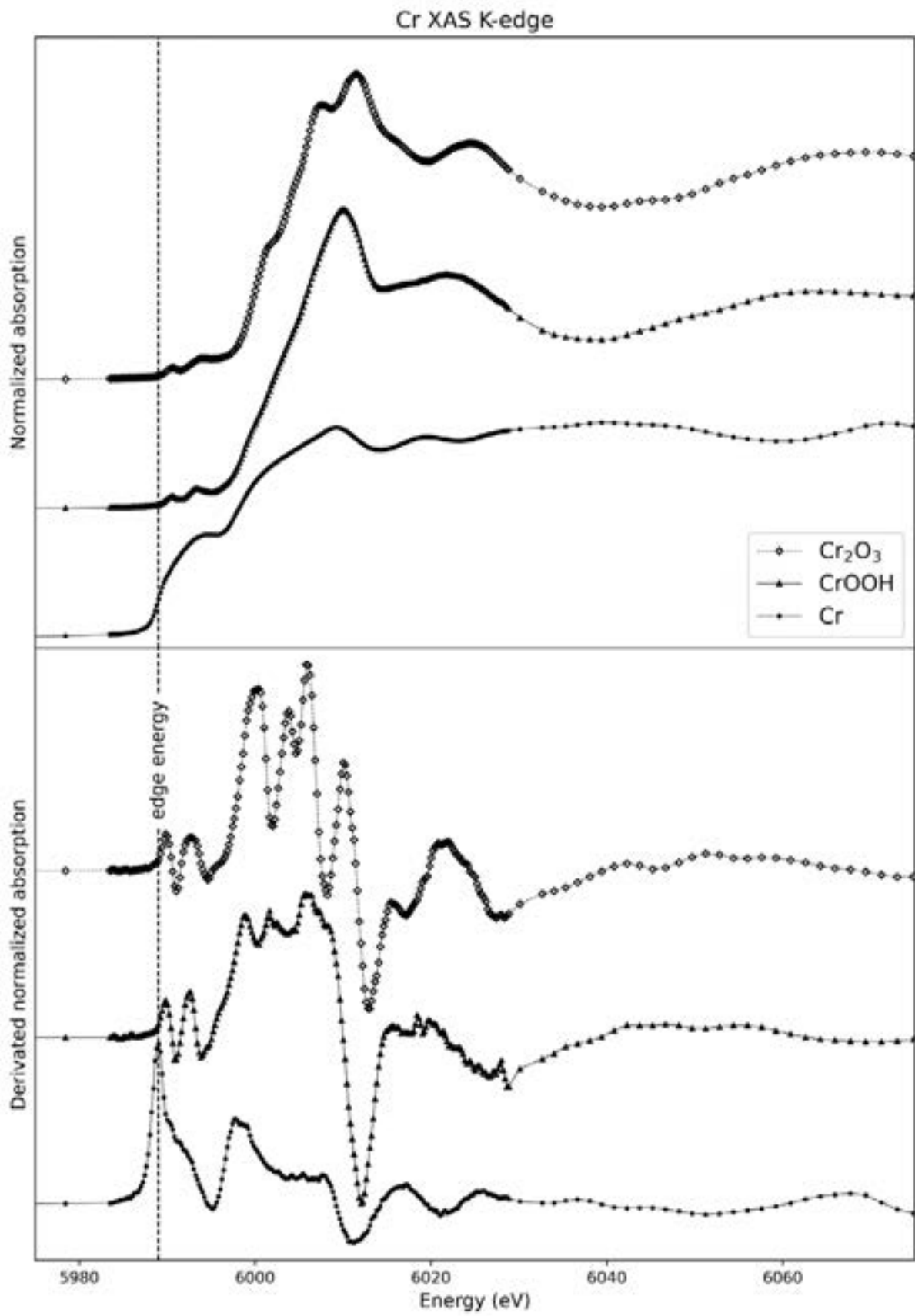
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	19.27	0.81
Si220	32.62	0.36

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge422	82.4
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si333	85.8

XAS Reference spectra



Z=25**Mn****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	6 539	5 900.3	6 491.8
Natural width	1.16	1.48	1.899

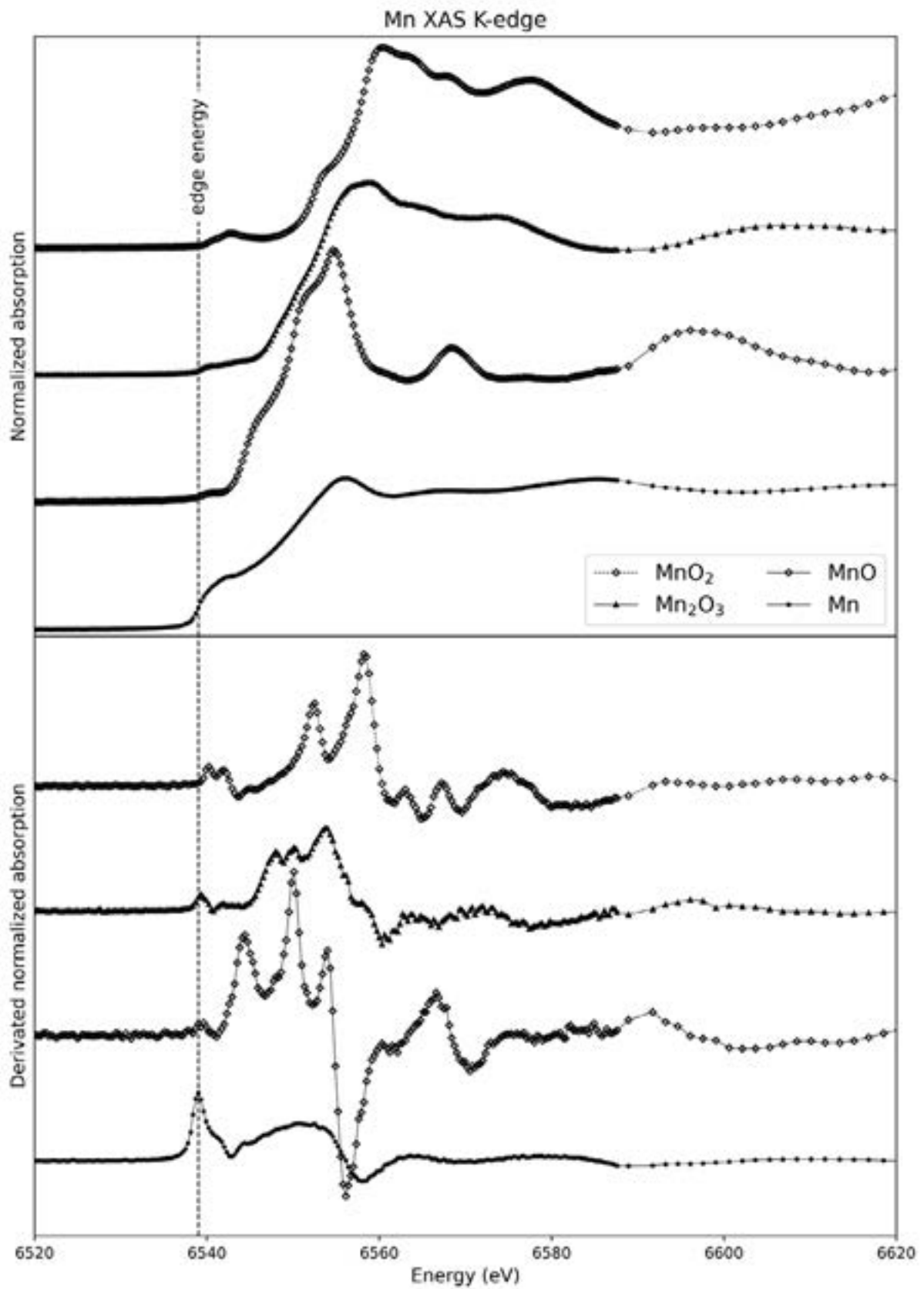
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	17.60	0.88
Si220	29.59	0.39

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge333	74.9
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si440	84.1

XAS Reference spectra



Z=26**Fe****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	7112	6405.2	7059.3
Natural width	1.25	1.61	2.25

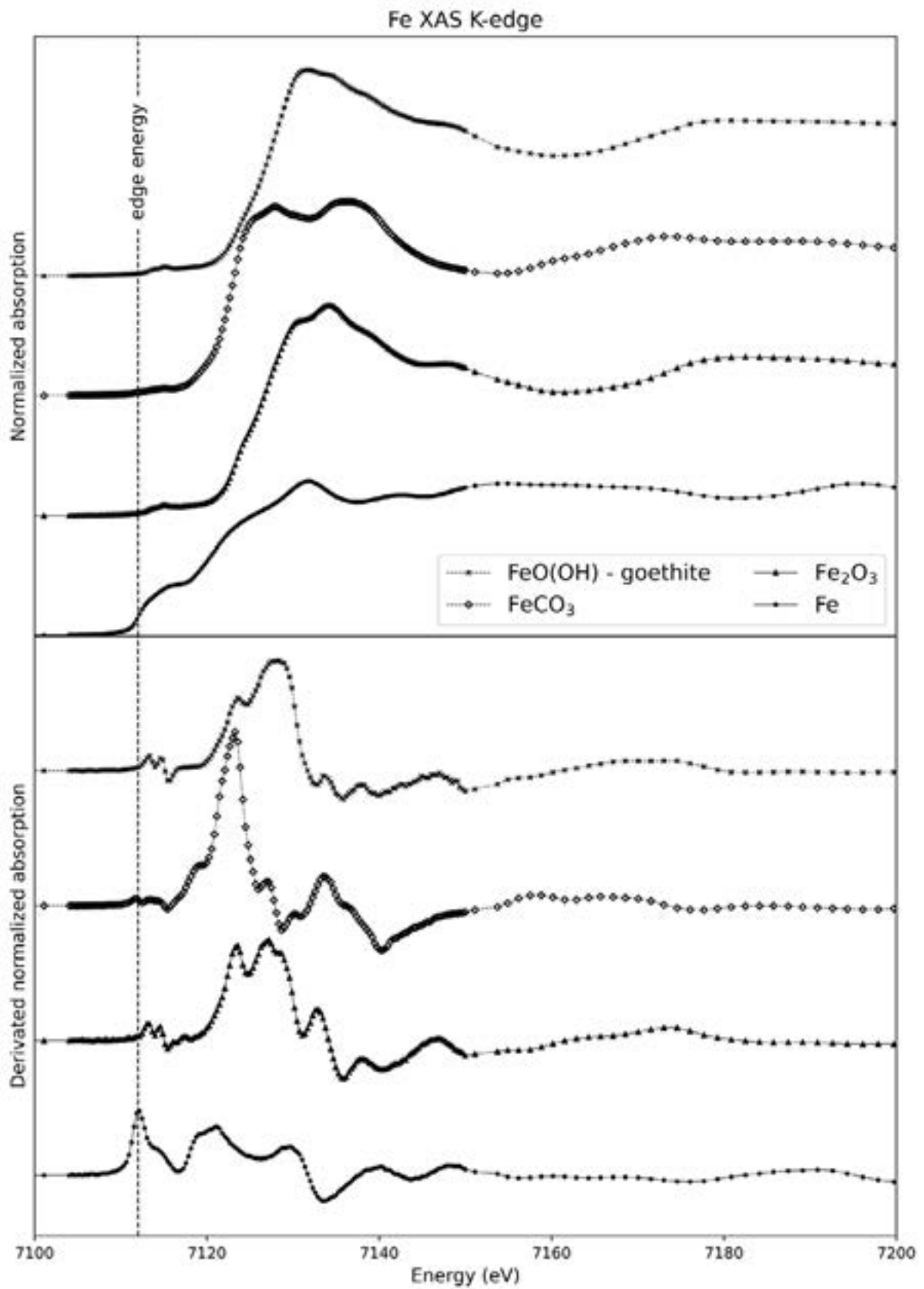
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	16.14	0.96
Si220	27.00	0.42

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge440	75.4
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge620	79.0
Si531	73.1

XAS Reference spectra



Z=27**Co****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	7 709	6 930.9	7 649.1
Natural width	1.33	1.76	2.84

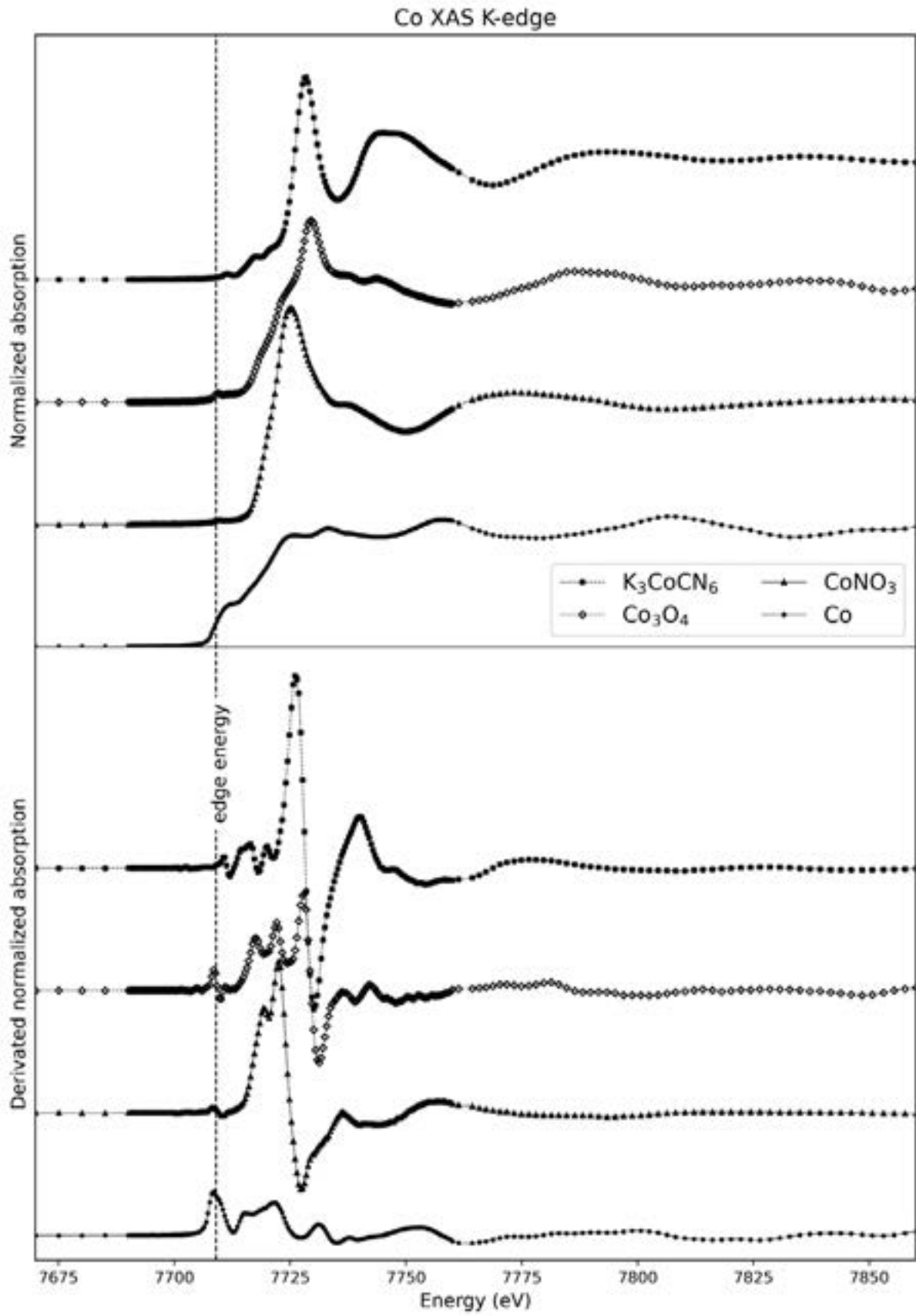
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	14.86	1.04
Si220	24.76	0.46

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge620	88.9
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge444	83.0

XAS Reference spectra



Z=28**Ni****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	8 333	7 480.3	8 266.8
Natural width	1.44	1.94	2.97

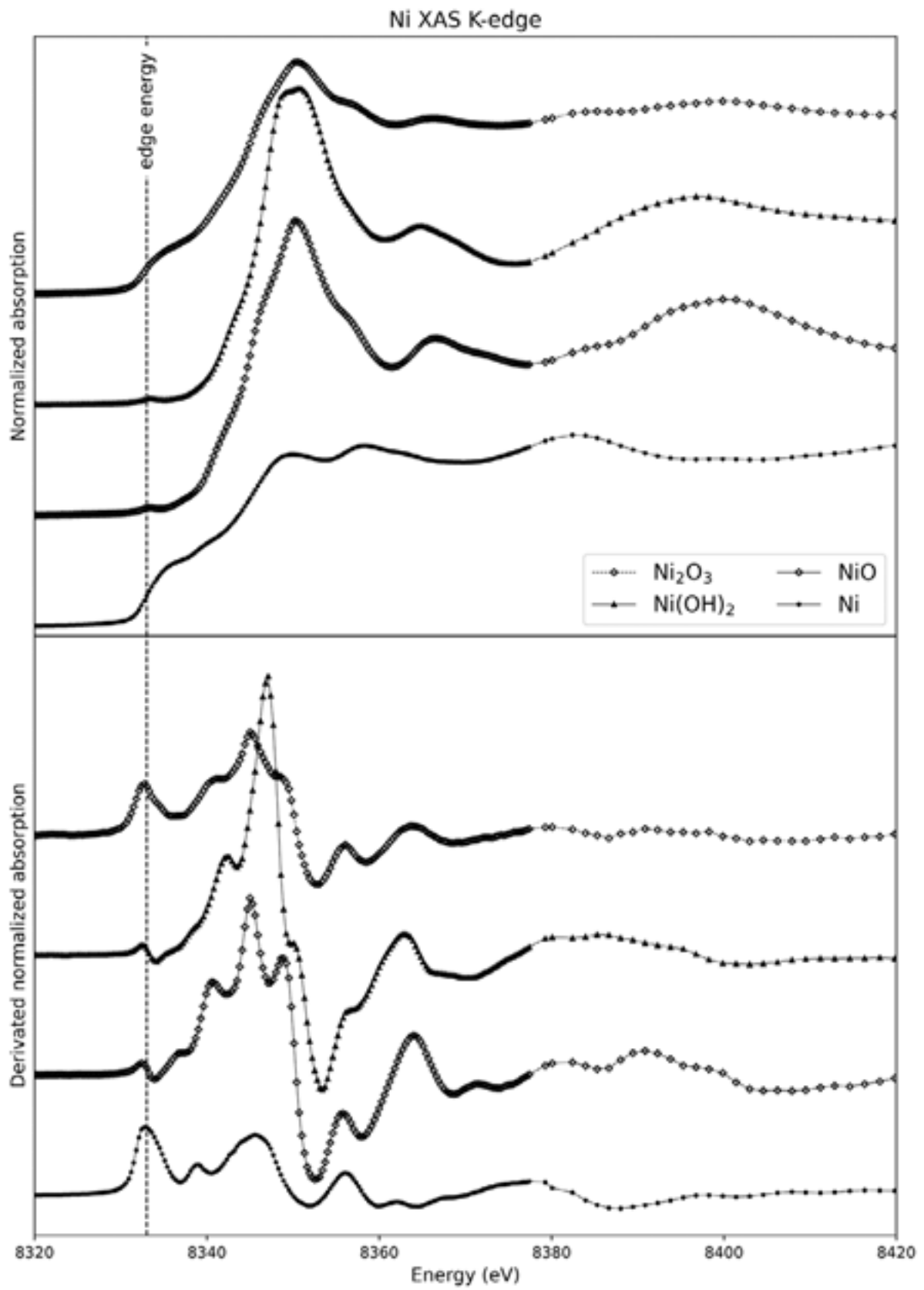
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	13.72	1.12
Si220	22.80	0.49

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si620	74.8
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si551	80.4

XAS Reference spectra



Z=29**Cu****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	8 979	8 046.3	8 903.9
Natural width	1.55	2.11	3.20

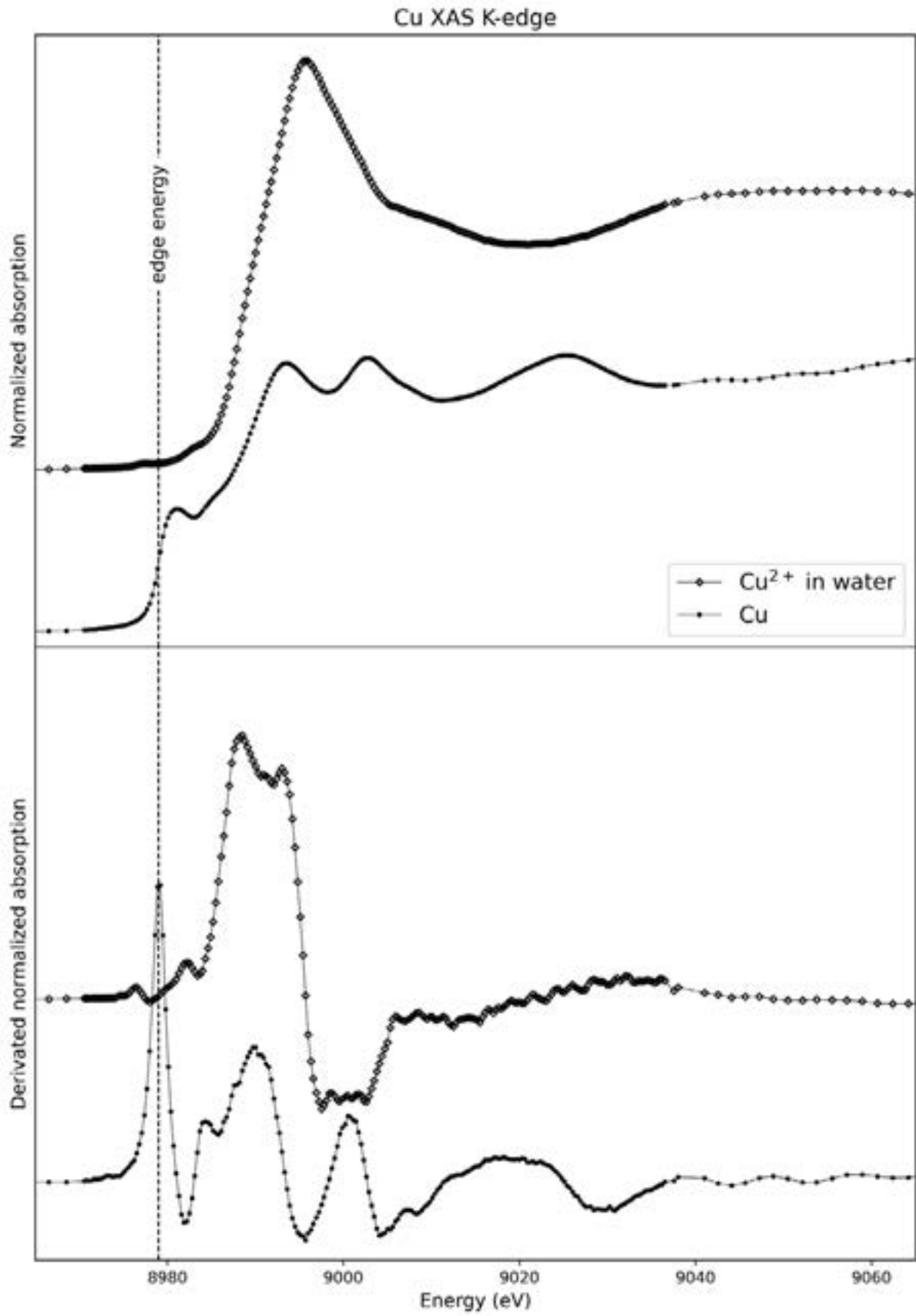
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	12.72	1.20
Si220	21.07	0.53

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si444	79.4
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge800	79.9

XAS Reference spectra



Z=30**Zn****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	9 659	8 637.2	9 570.4
Natural width	1.67	2.32	3.59

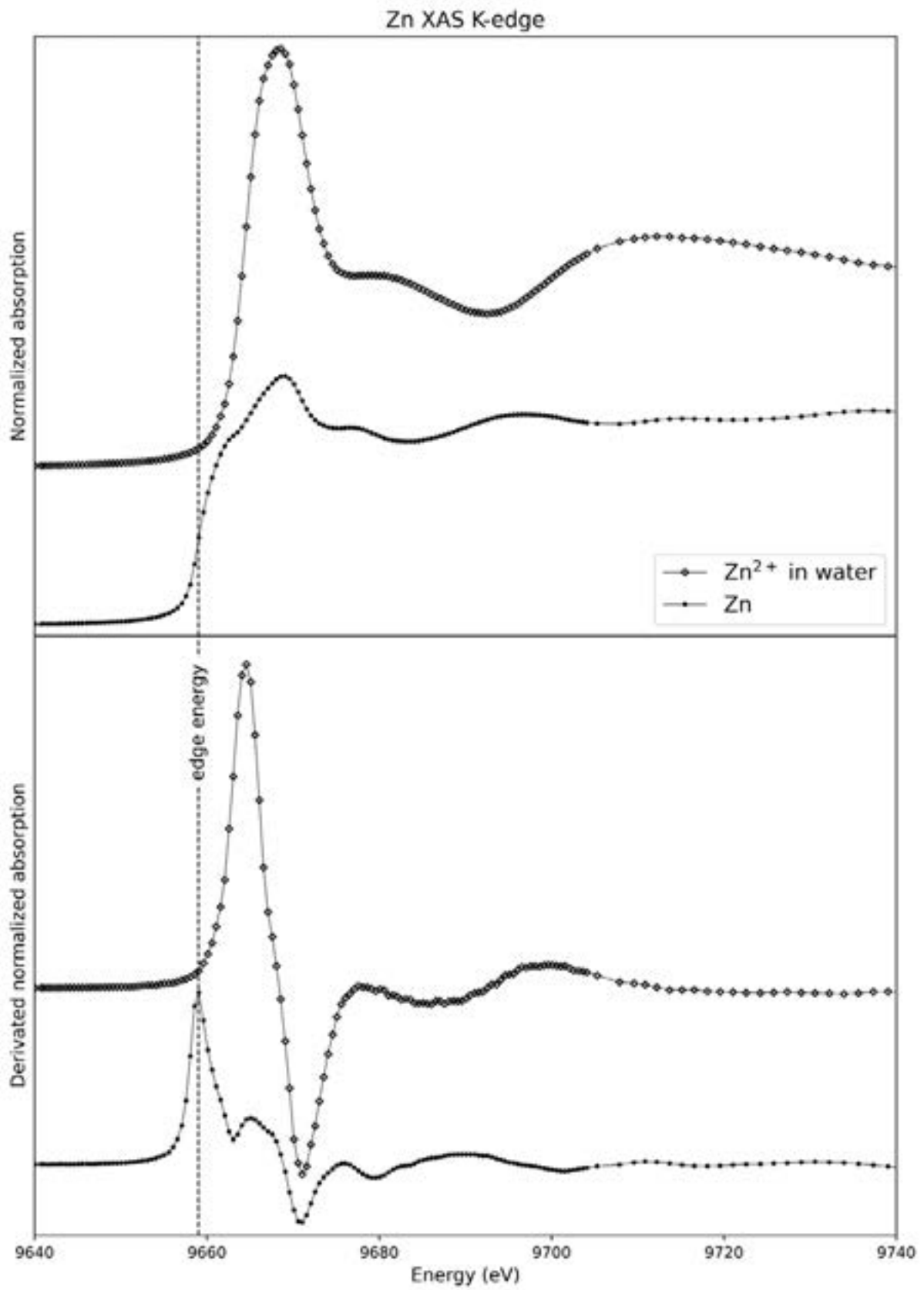
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	11.81	1.29
Si220	19.53	0.57

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si642	81.5
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge555	82.5

XAS Reference spectra



Z=31**Ga****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	10 367	9 250.6	10 267
Natural width	1.82	2.59	3.81

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	11.00	1.38
Si220	18.14	0.61

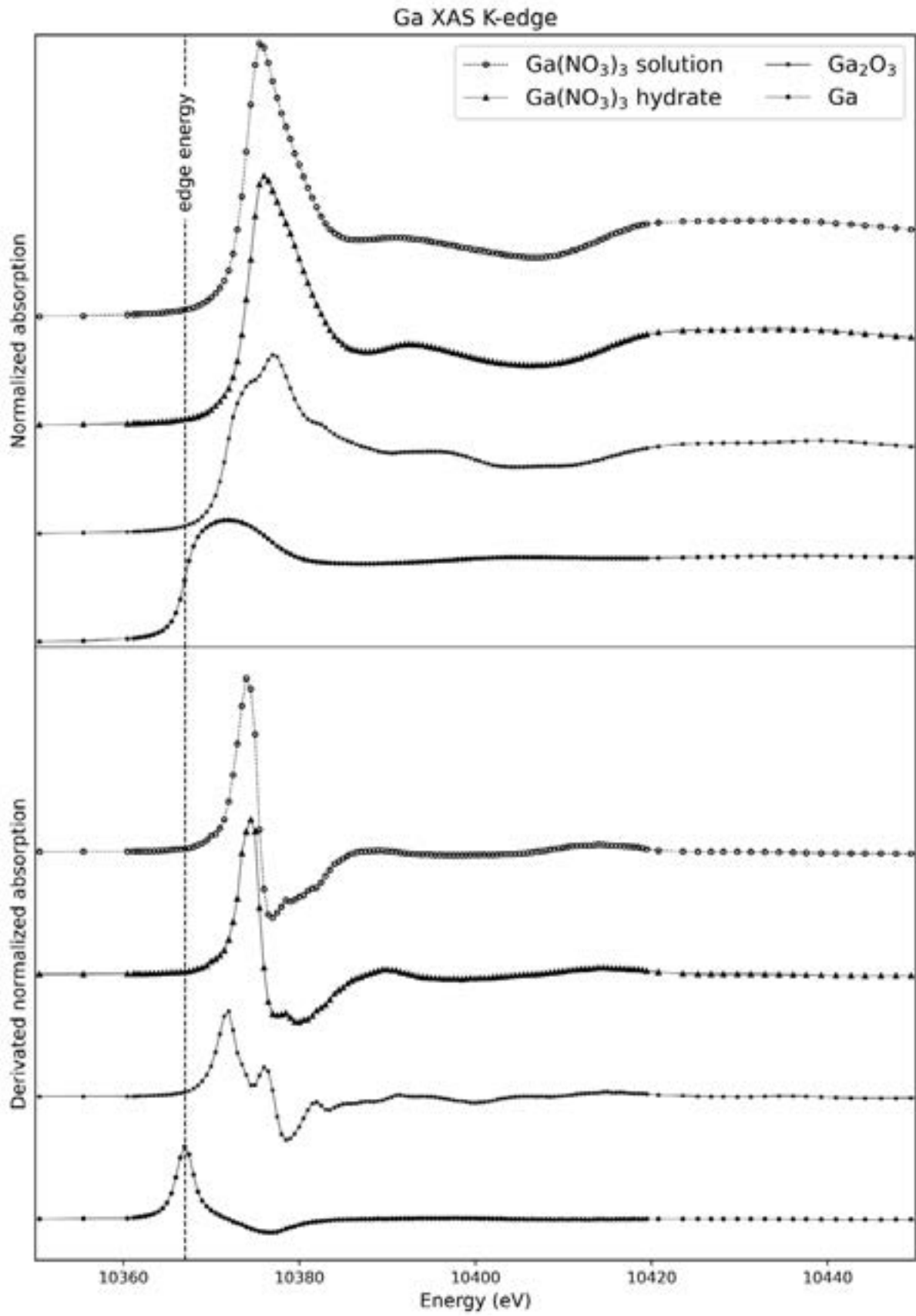
Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si800	80.8
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si555	74.3

Edges positions

Calibration (eV)	$Ga^{(0)}$ (eV)	$Ga^{(III)}$ solution (eV)
$W^{(0)}$ L _{III} -edge - 10 207		10 379.0
$Zn^{(0)}$ K-edge - 9 659	10 366.7	10 373.8
$Ga^{(0)}$ K-edge - 10 367	10 367.0	10 374.1

XAS Reference spectra



Z=32**Ge****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	11 103	9 886	10 982
Natural width	1.96	2.78	4.2

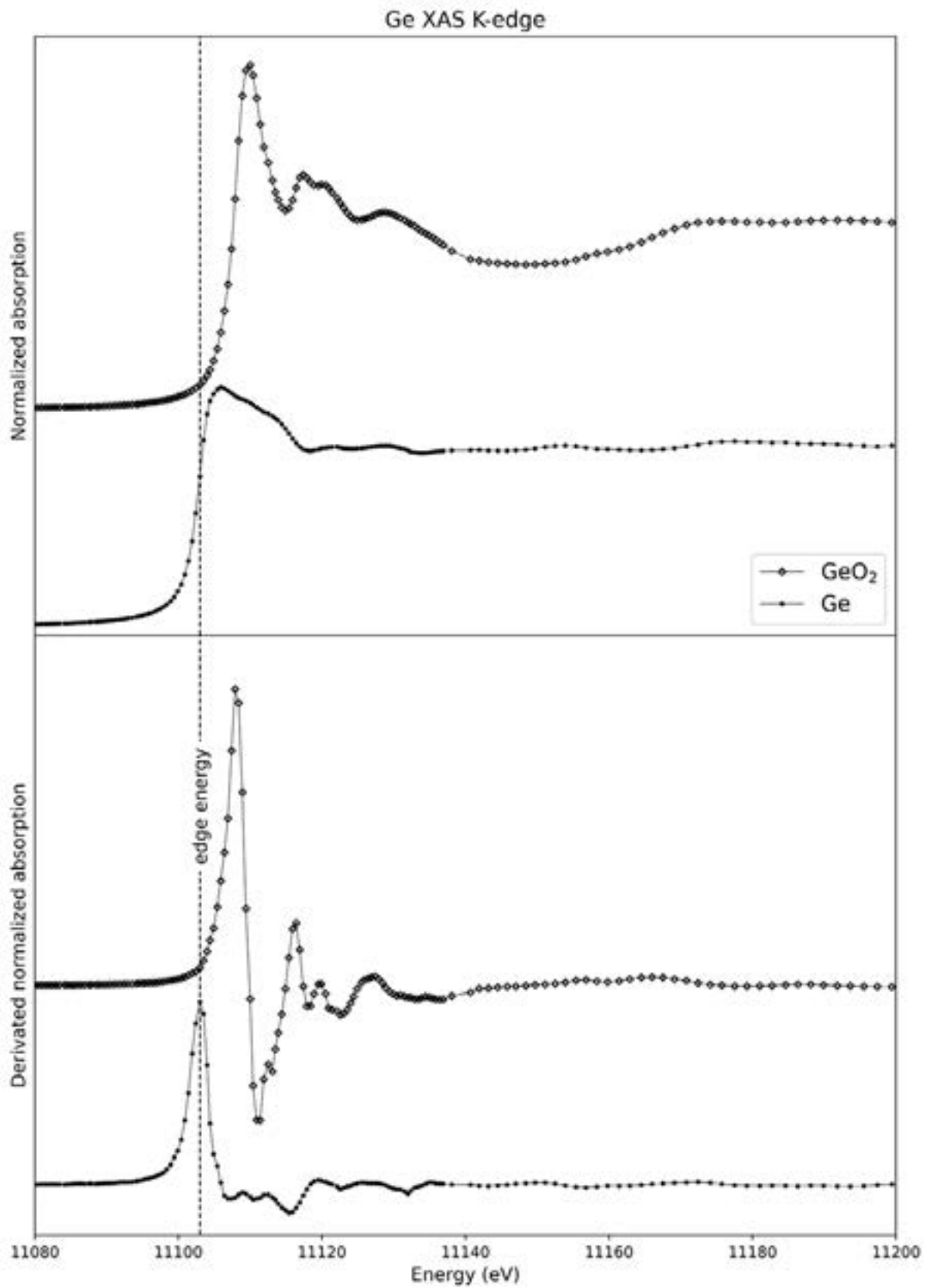
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	10.26	1.48
Si220	16.90	0.65

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si660	78.4
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge844	77.8

XAS Reference spectra



Z=33**As****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	11 867	10 543.4	11 726
Natural width	2.14	3.08	4.32

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	9.59	1.58
Si220	15.80	0.70

Crystal Analyzer Spectrometer parameters

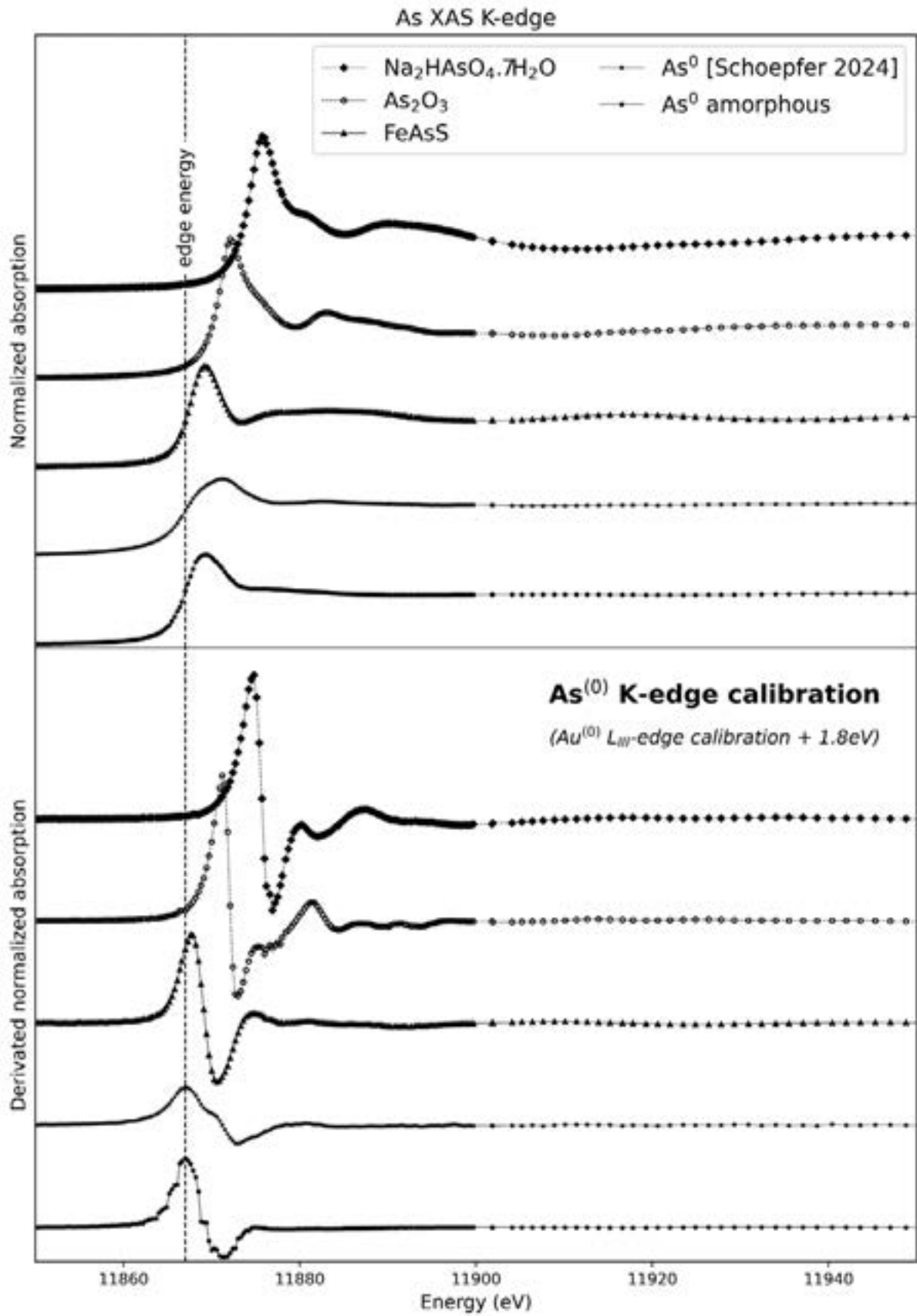
$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si555	69.7
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge844	72.5

Edges positions

Calibration (eV)	As ⁽⁰⁾ (eV)	As ₂ O ₃ (eV)
Au ⁽⁰⁾ L _{III} -edge - 11 919	11 865.2 ^(b)	11 869.5 ^(a)
As ⁽⁰⁾ K-edge - 11 867	11 867	11 871

(a) [Borisova 2010] and SSHADE data – (b) [Schoepfer 2024]

XAS Reference spectra



Z=34**Se****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	12 658	11 224.1	12 497
Natural width	2.33	3.33	4.085

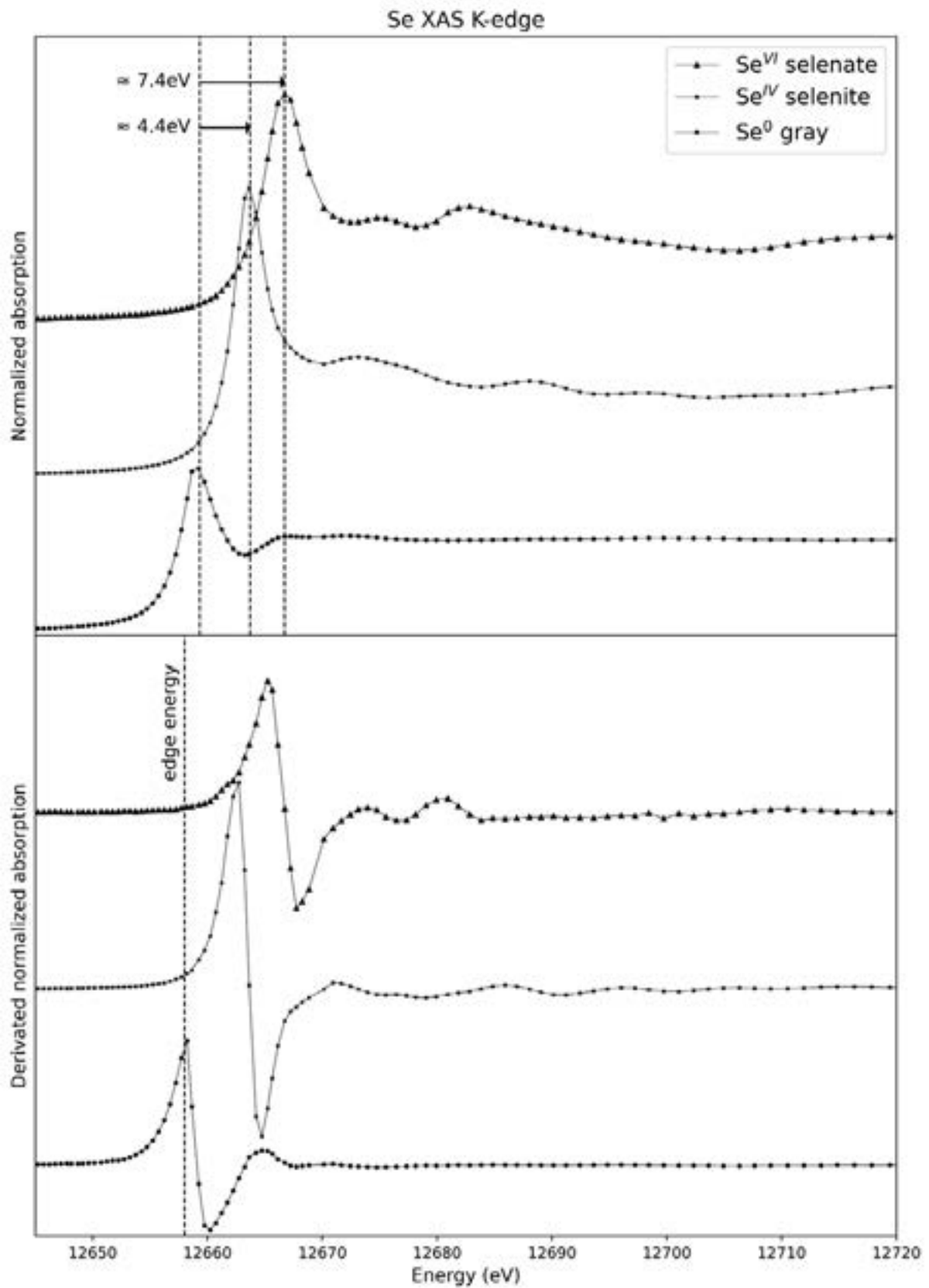
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	8.99	1.68
Si220	14.75	0.74

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si844	85.2
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge880	82.7

XAS Reference spectra



Z=35**Br****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	13 474	11 924	13 292
Natural width	2.52	3.60	4.66

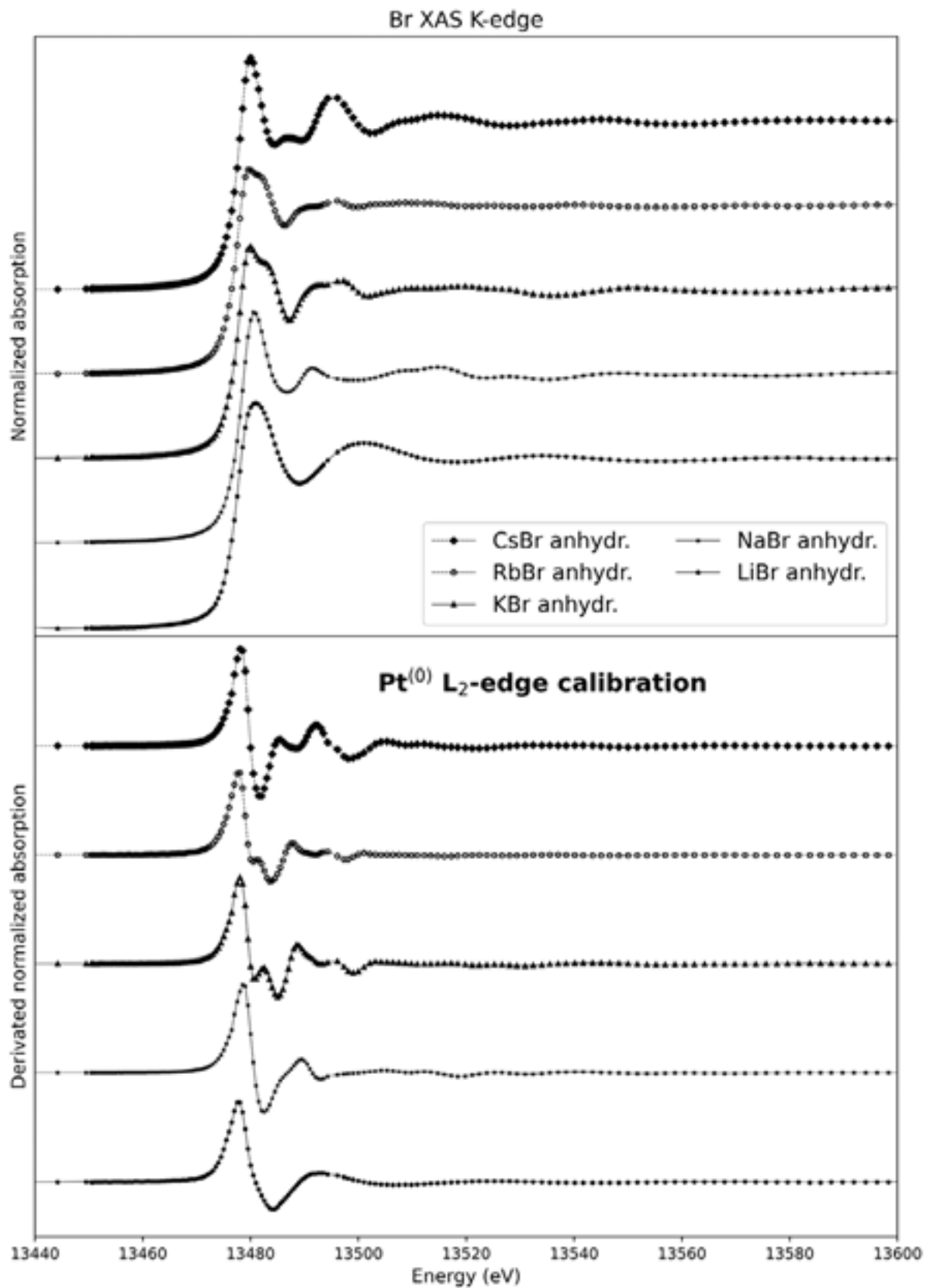
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	8.44	1.79
Si220	13.86	0.79

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si951	82.0
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si880	76.3

XAS Reference spectra



Z=36**Kr****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	14 326	12 647	14 112
Natural width	2.52	3.92	4.86

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	7.94	1.90
Si220	13.02	0.84

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge880	78.6
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si777	78.7

XAS Reference spectra

Z=37**Rb****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	15 200	13 396	14 961
Natural width	2.99	4.26	5.11

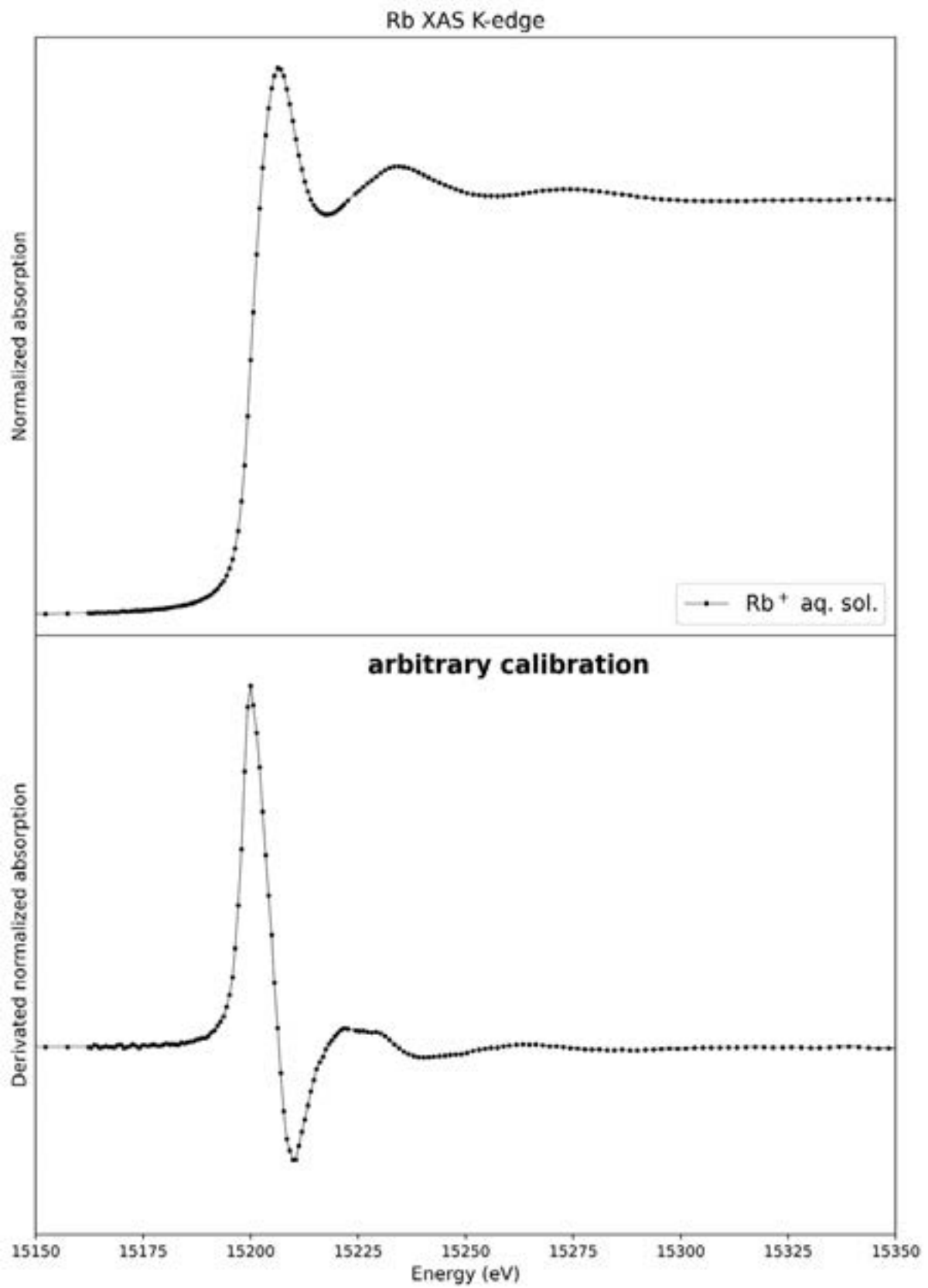
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	7.47	2.01
Si220	12.26	0.89

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge777	82.7
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si993	86.1

XAS Reference spectra



Z=38**Sr****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	16 105	14 165	15 835
Natural width	3.25	4.63	5.36

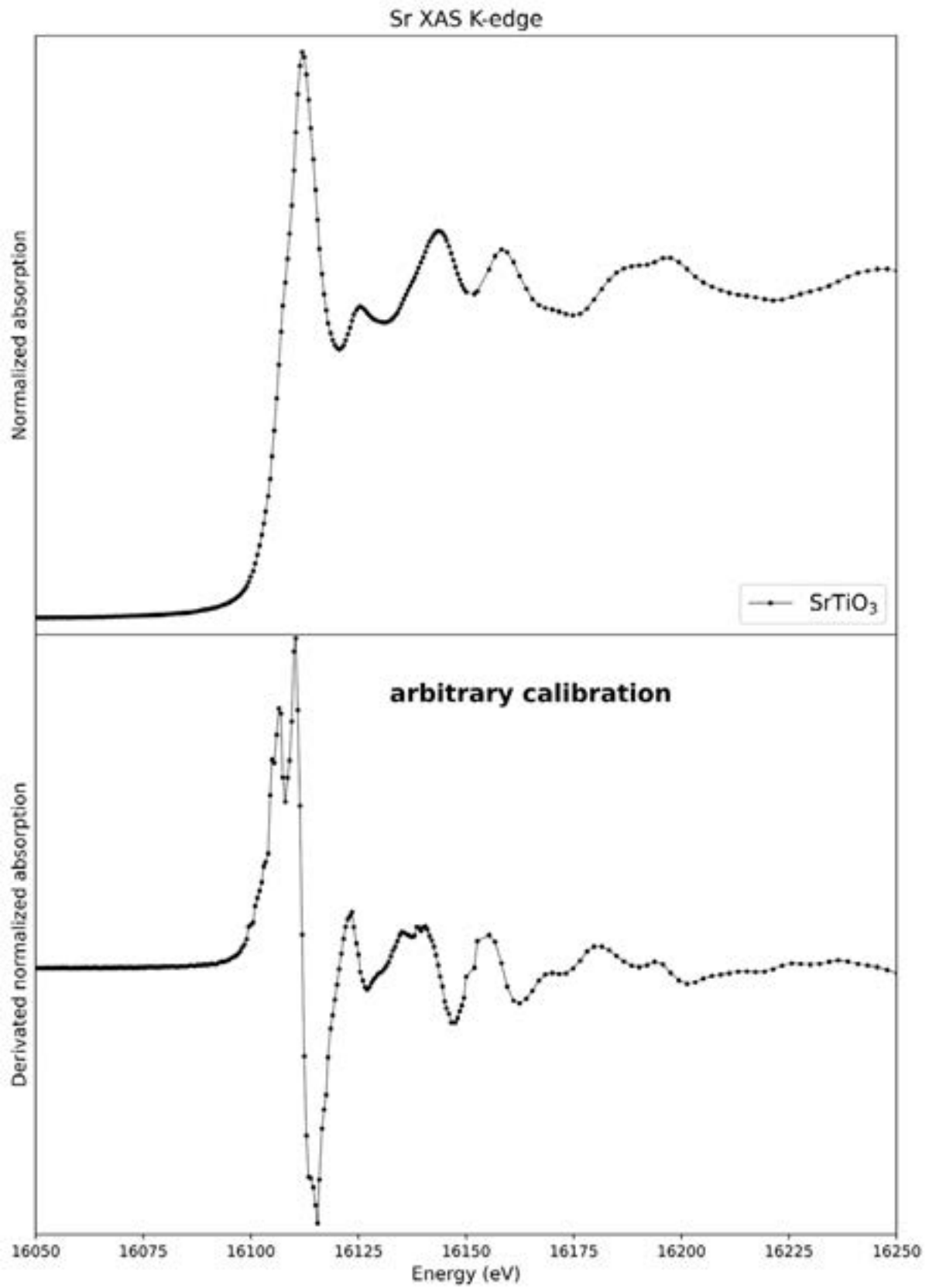
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	7.05	2.13
Si220	11.56	0.94

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si777	77.7
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si888	87.2

XAS Reference spectra



Z=39**Y****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	17 038	14 958	16 739.2
Natural width	3.52	5.02	5.38

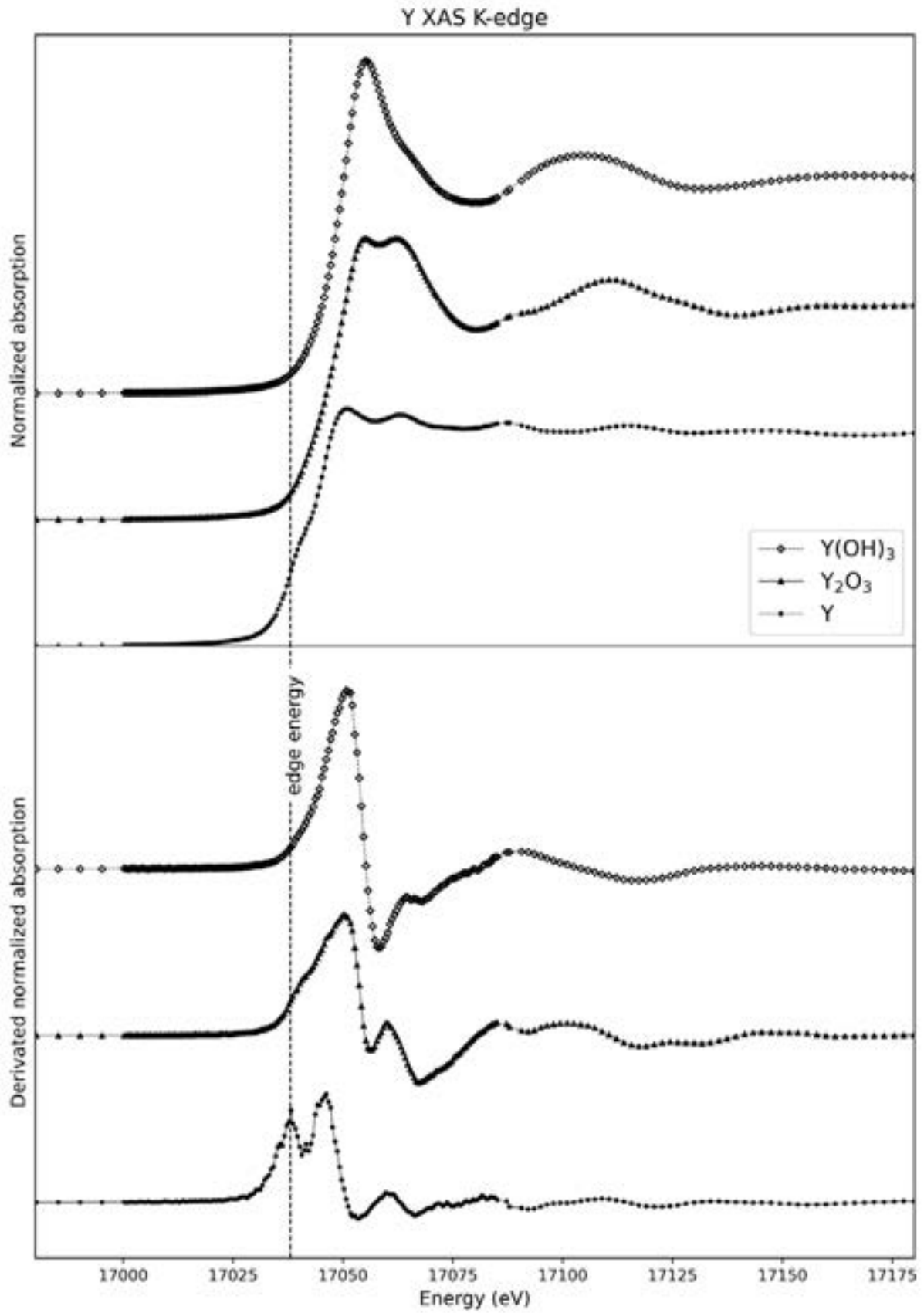
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	6.66	2.25
Si220	10.92	0.99

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si993	86.3
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si 10 10 0	74.7

XAS Reference spectra



Z=40**Zr****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	17 998	15 775	17 668
Natural width	3.84	5.4	5.791

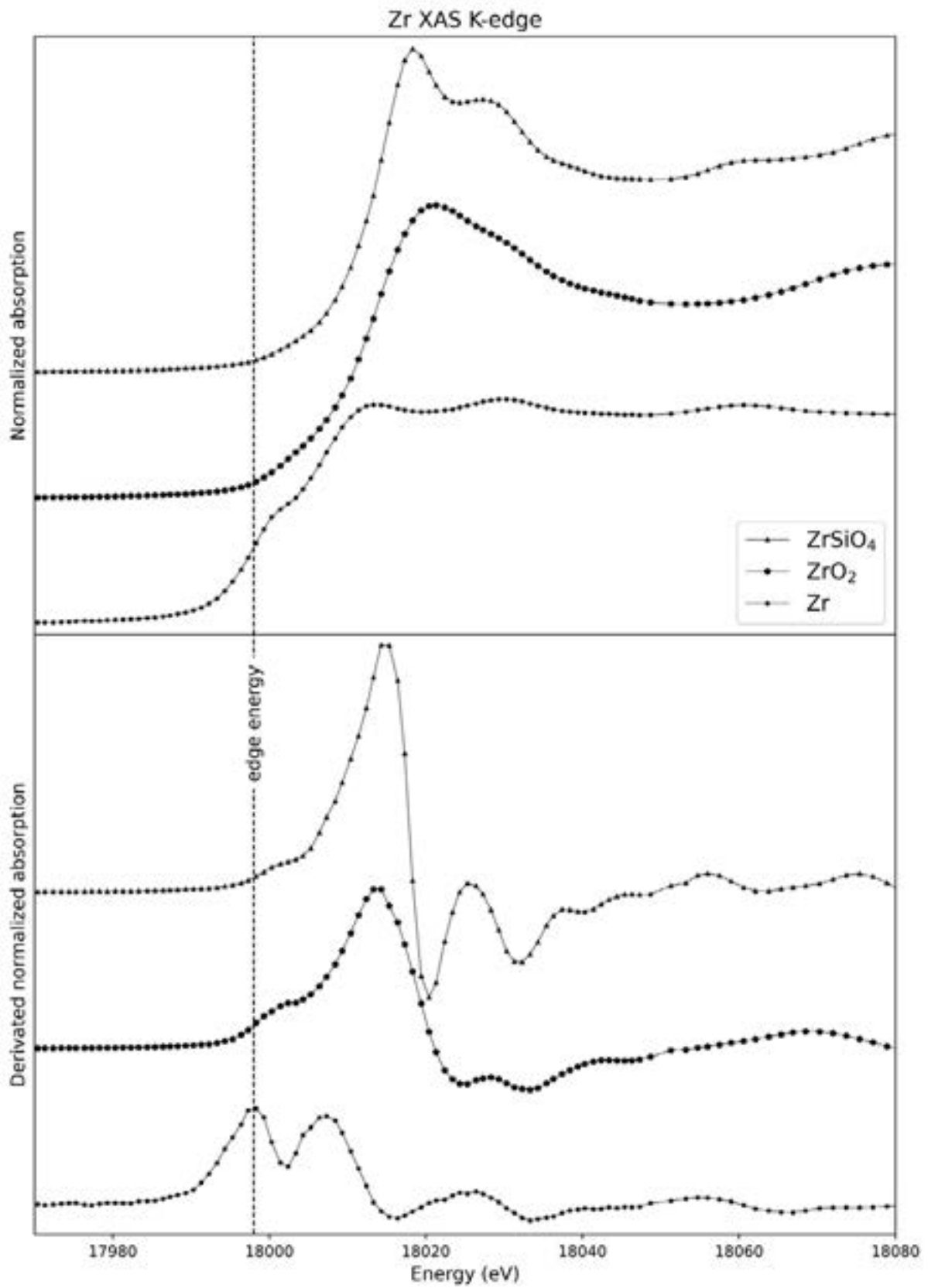
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	6.31	2.38
Si220	10.33	1.04

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge 10 10 0	79.2
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge999	75.2

XAS Reference spectra



Z=41**Nb****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	18 986	16 615	18 625
Natural width	4.14	5.8	6.28

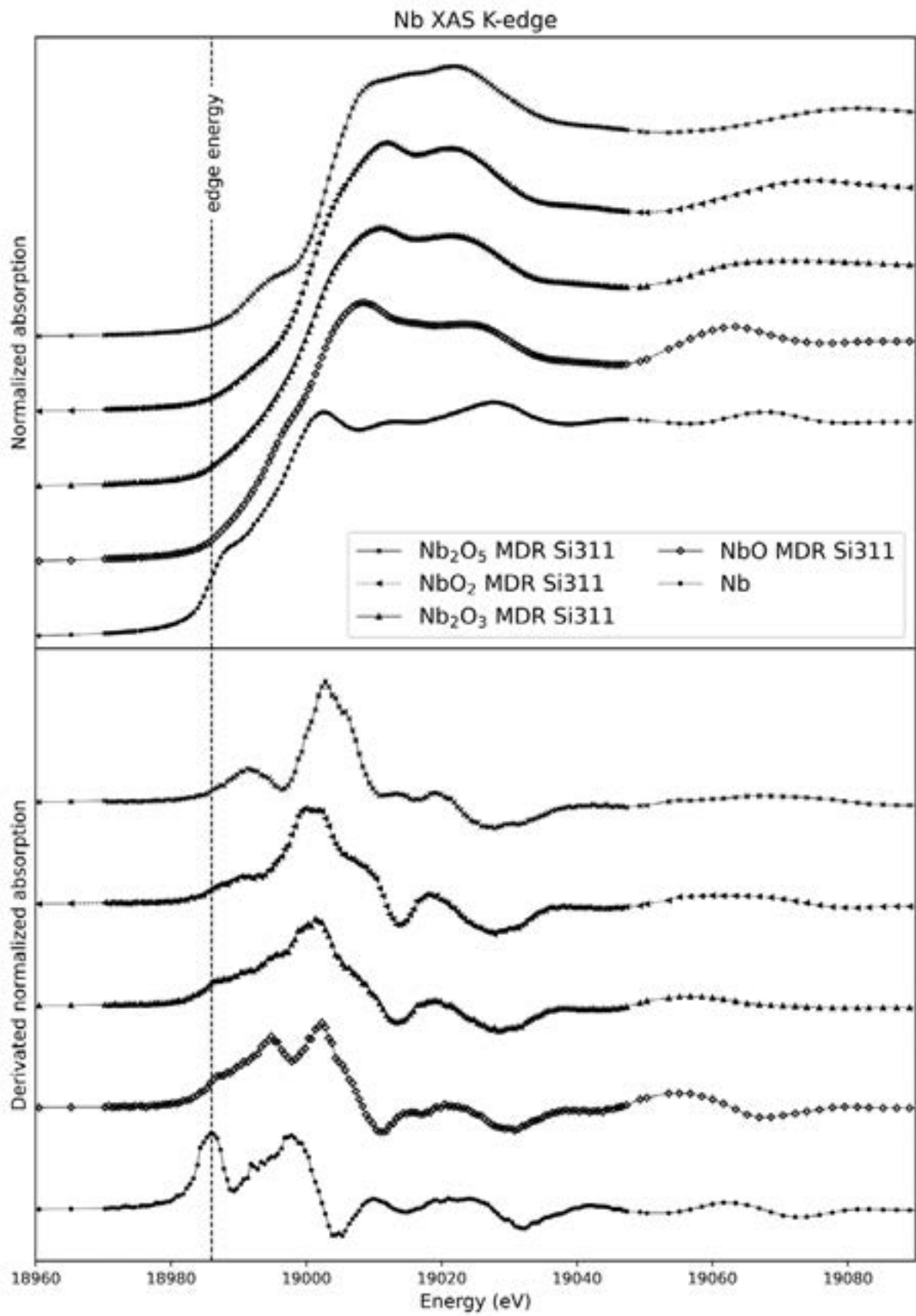
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	5.98	2.51
Si220	9.79	1.10

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Si 10 10 0	76.3
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Si 11 11 11	87

XAS Reference spectra



Z=42**Mo****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	20 000	17 480	19 606
Natural width	4.52	6.31	6.88

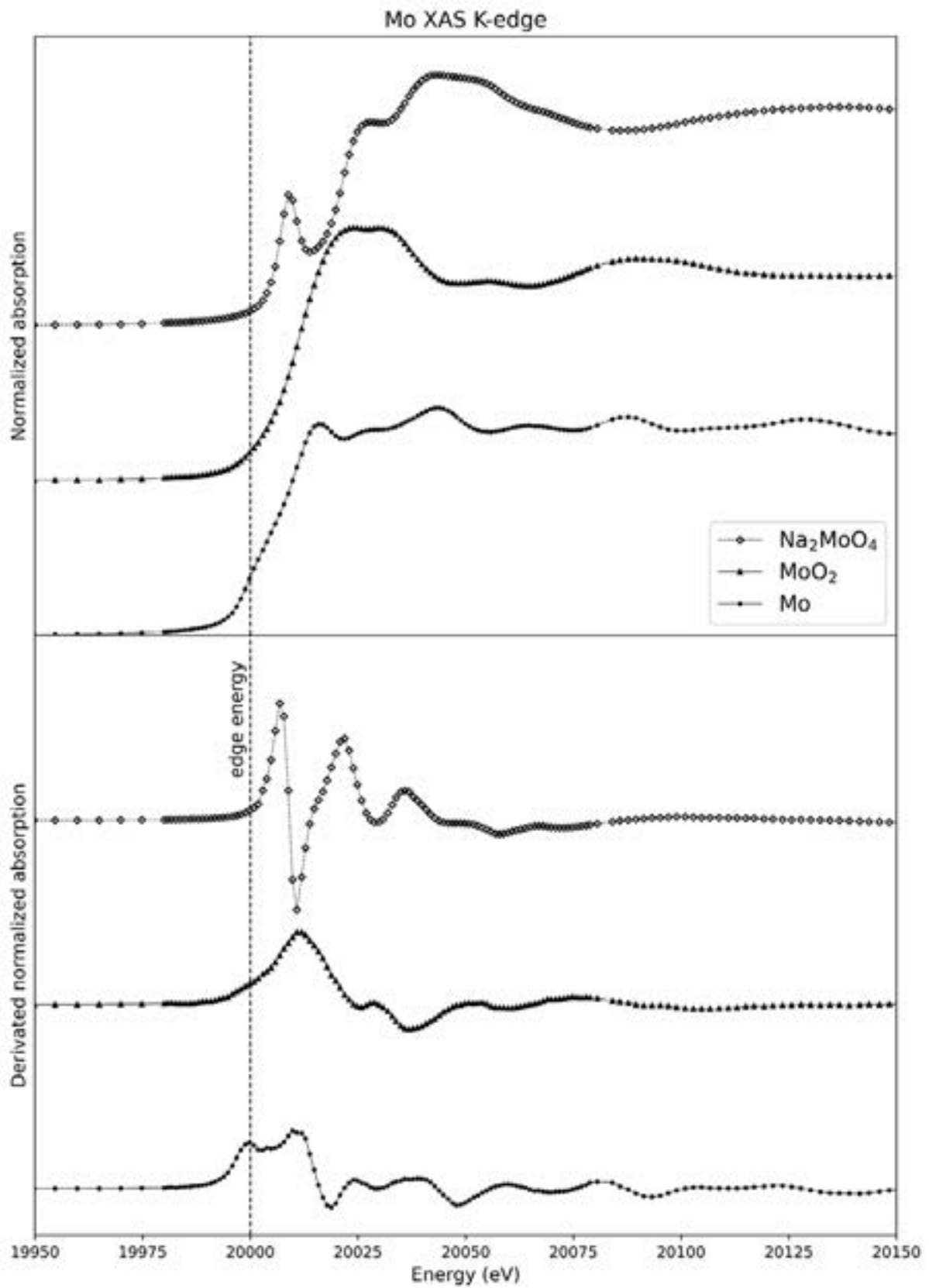
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	5.67	2.64
Si220	9.29	1.16

Crystal Analyzer Spectrometer parameters

$K_{\alpha 1}$ emission line	
Crystals	Bragg Angle (°)
Ge999	77.8
$K_{\beta 1}$ emission line	
Crystals	Bragg Angle (°)
Ge 12 12 0	71.5

XAS Reference spectra



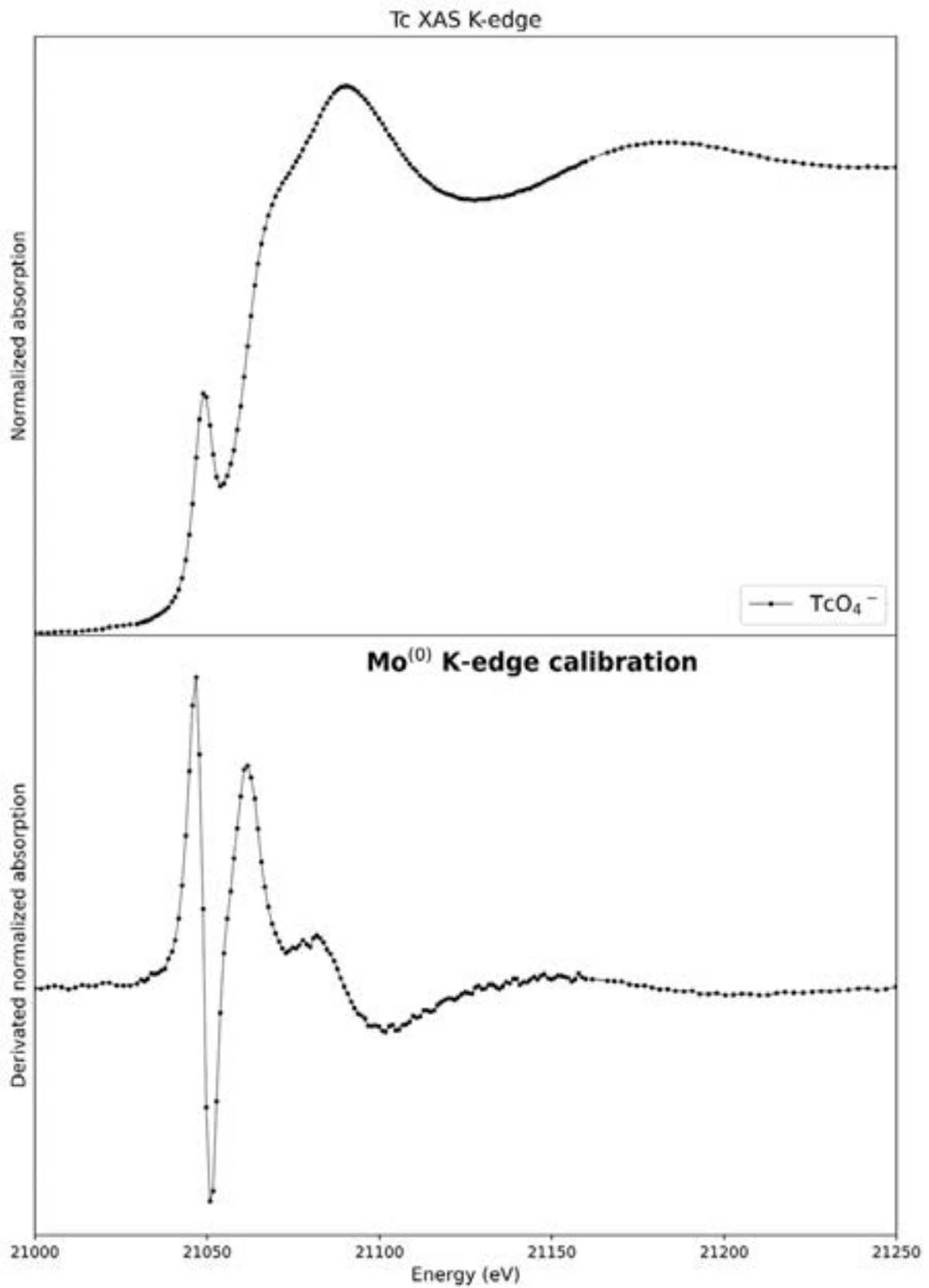
Z=43**Tc****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	21 044	18 367	20 626
Natural width	4.91	6.82	7.08

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	5.39	2.78
Si220	8.82	1.22

XAS Reference spectra



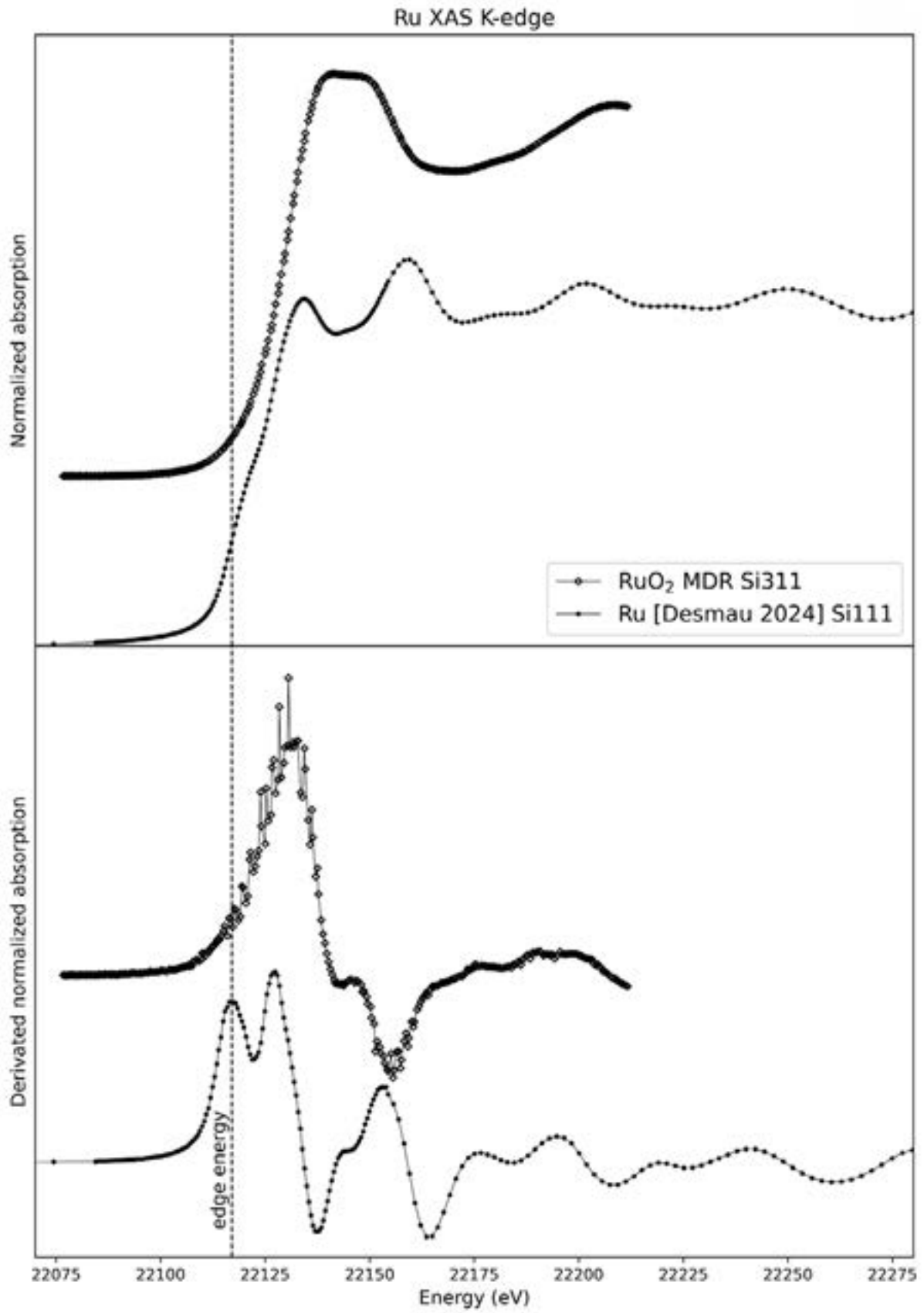
Z=44**Ru****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	22 117	19 279	21 656
Natural width	5.33	7.33	7.53

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	2.13	2.92
Si220	8.39	1.28

XAS Reference spectra



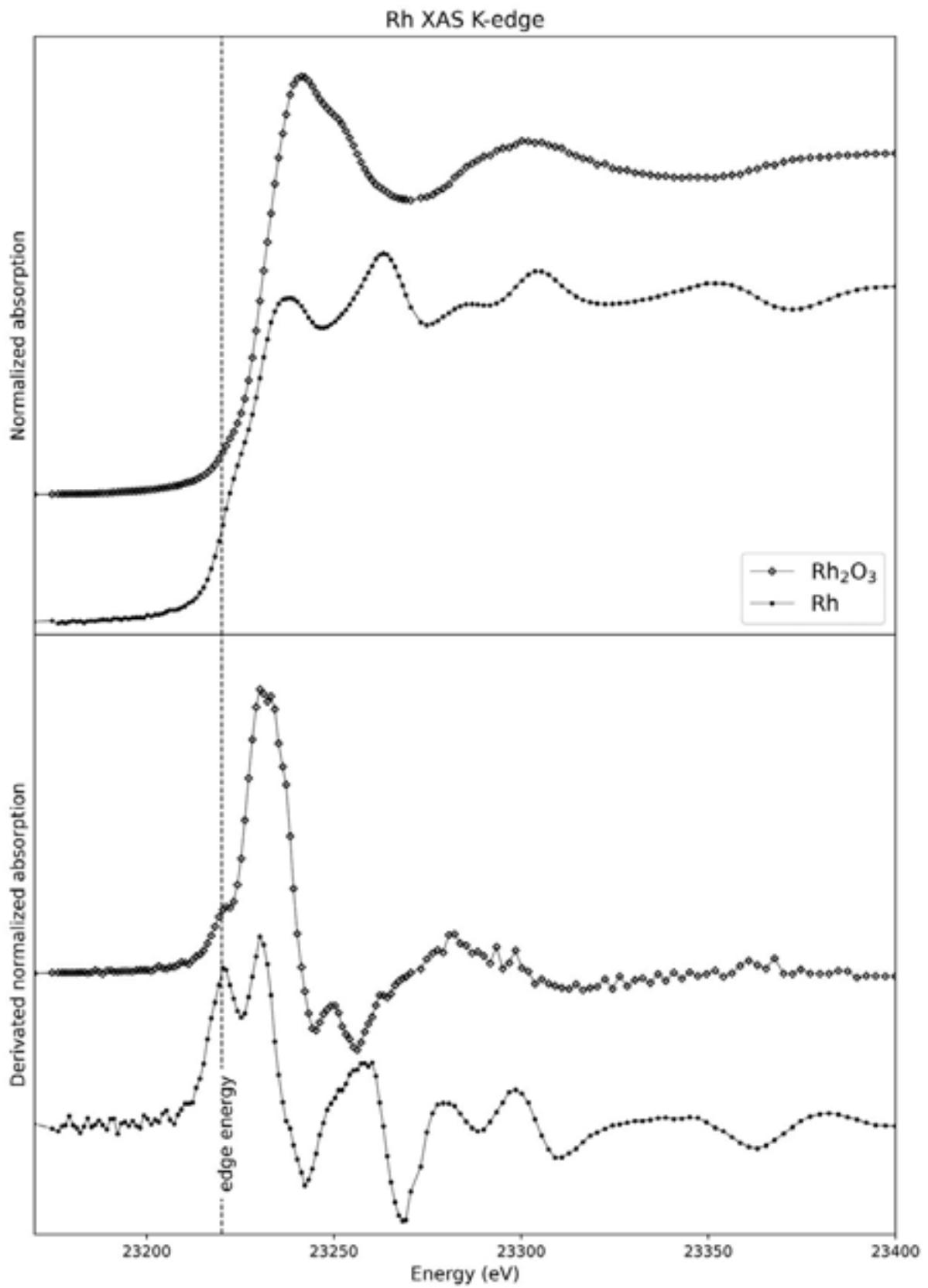
Z=45**Rh****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	23 220	20 216	22 724
Natural width	5.77	7.9	8.06

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	4.88	3.06
Si220	7.99	1.34

XAS Reference spectra



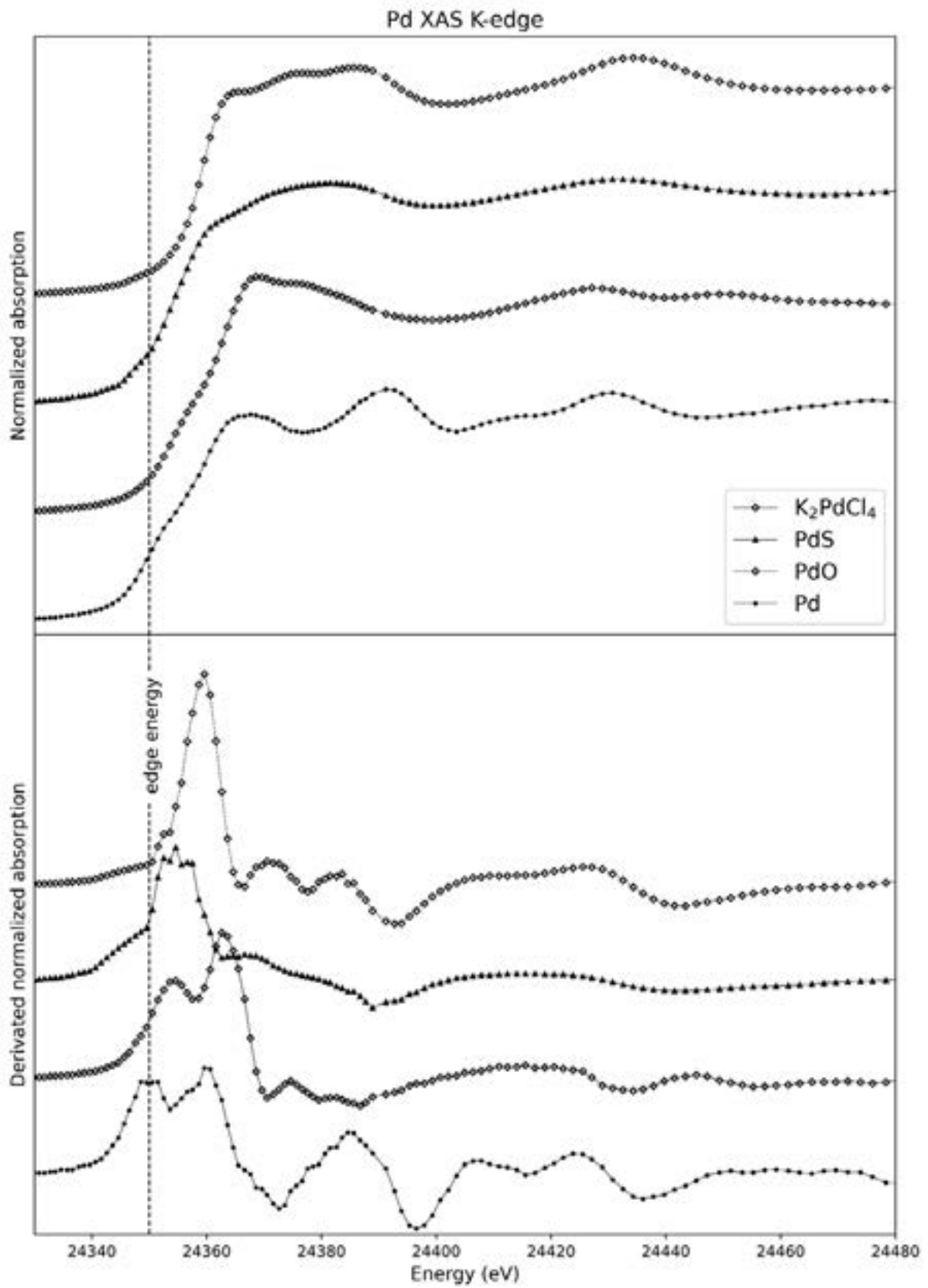
Z=46**Pd****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	24 350	21 177	23 818
Natural width	6.24	8.49	8.62

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	4.66	3.21
Si220	7.62	1.41

XAS Reference spectra



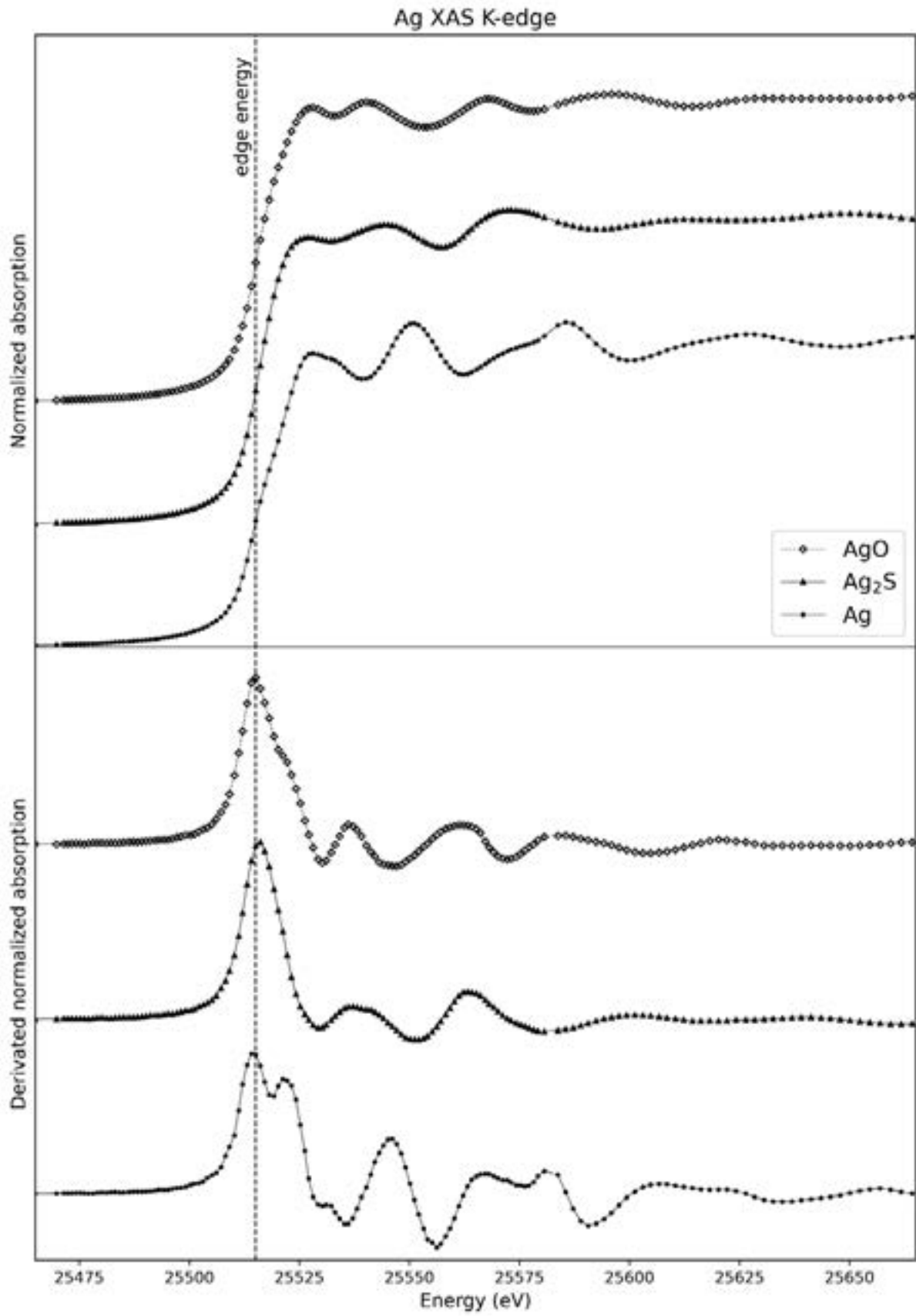
Z=47**Ag****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	25 515	22 163	24 941
Natural width	3.52	9.16	9.24

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	4.44	3.36
Si220	7.26	1.47

XAS Reference spectra



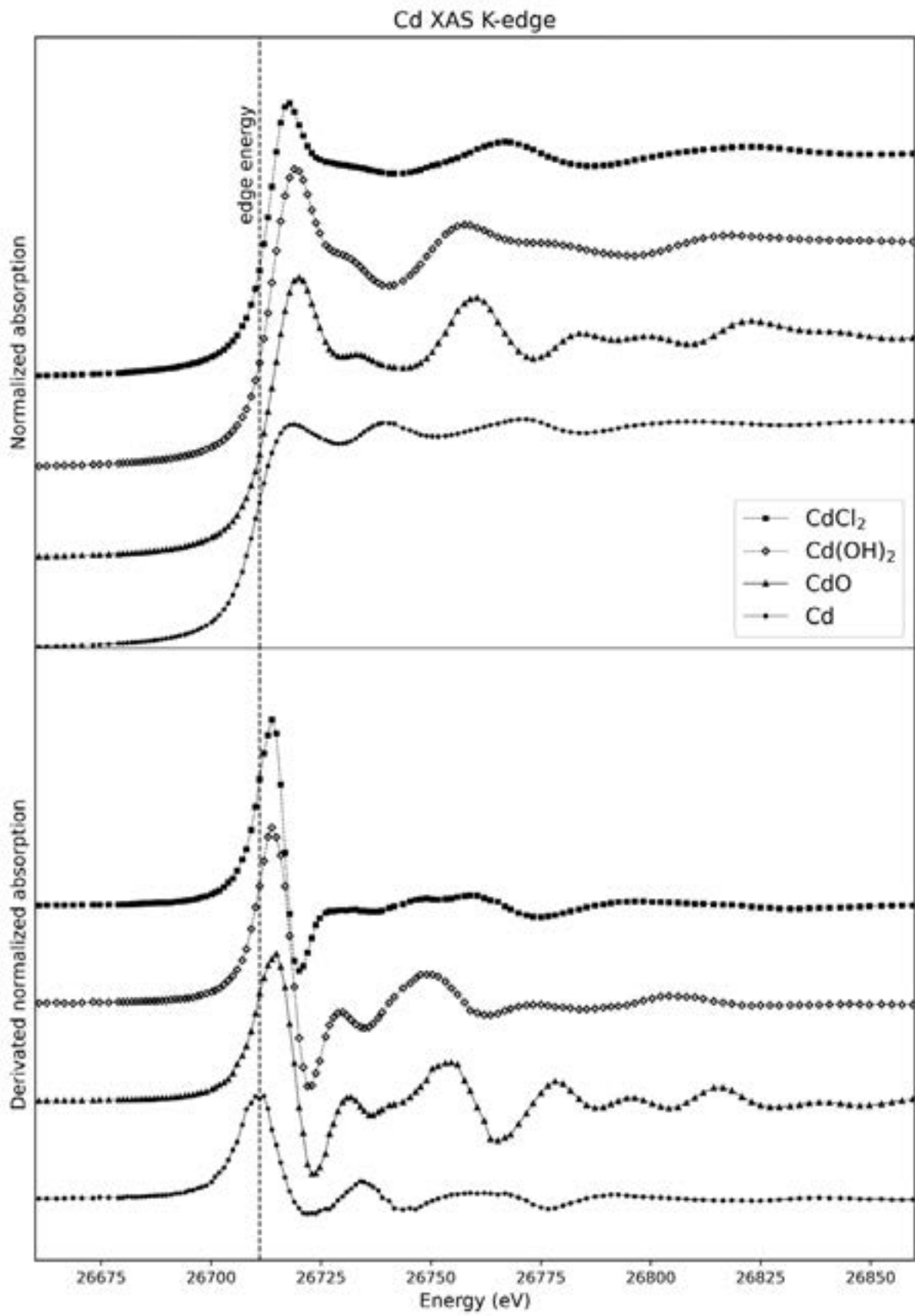
Z=48**Cd****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	26 711	23 173	26 093
Natural width	7.28	9.79	10.06

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	4.24	3.52
Si220	6.94	1.54

XAS Reference spectra



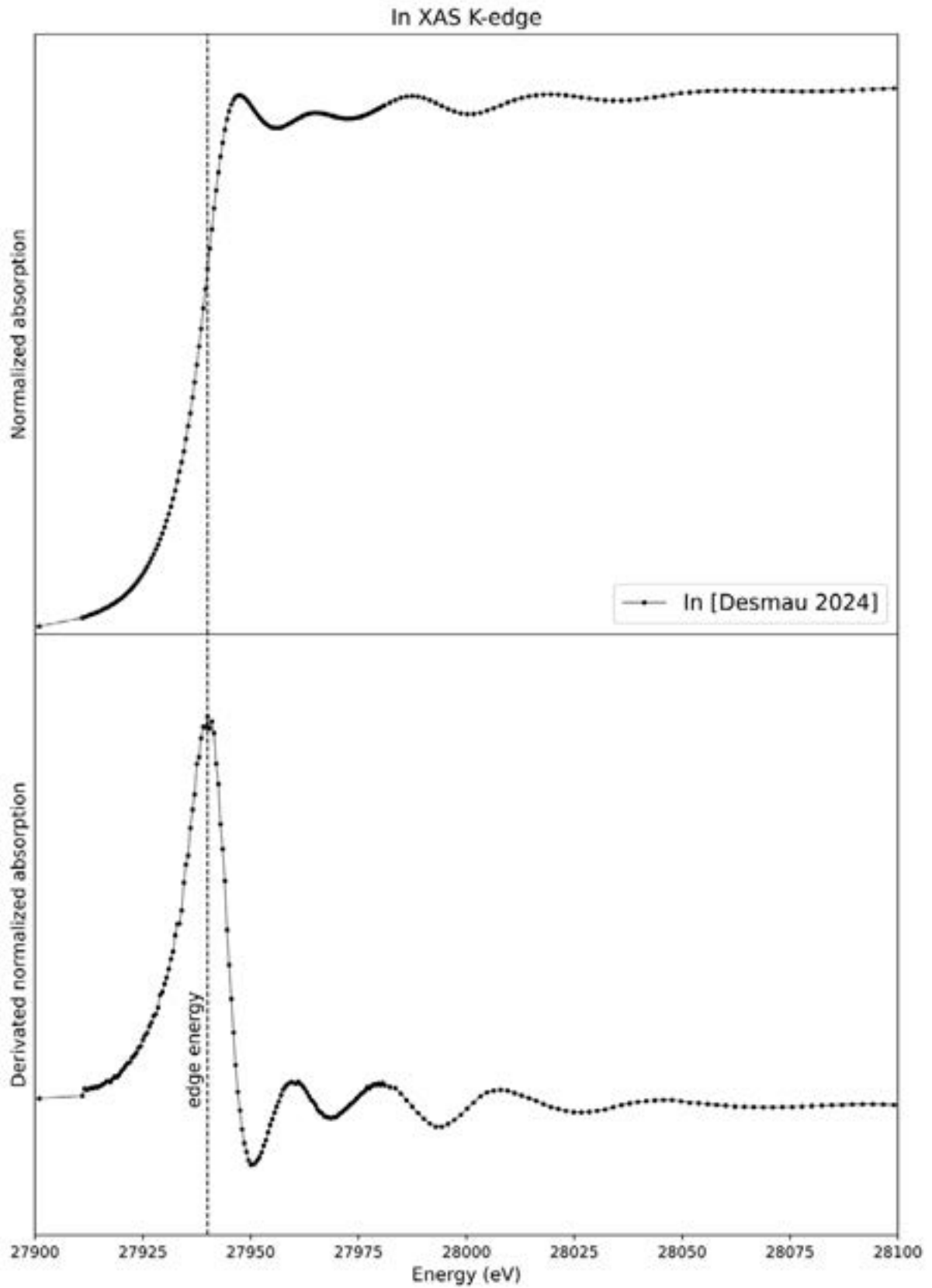
Z=49**In****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	27 940	24 210	27 247.7
Natural width	7.91	10.56	10.67

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	4.06	3.68
Si220	6.64	1.61

XAS Reference spectra



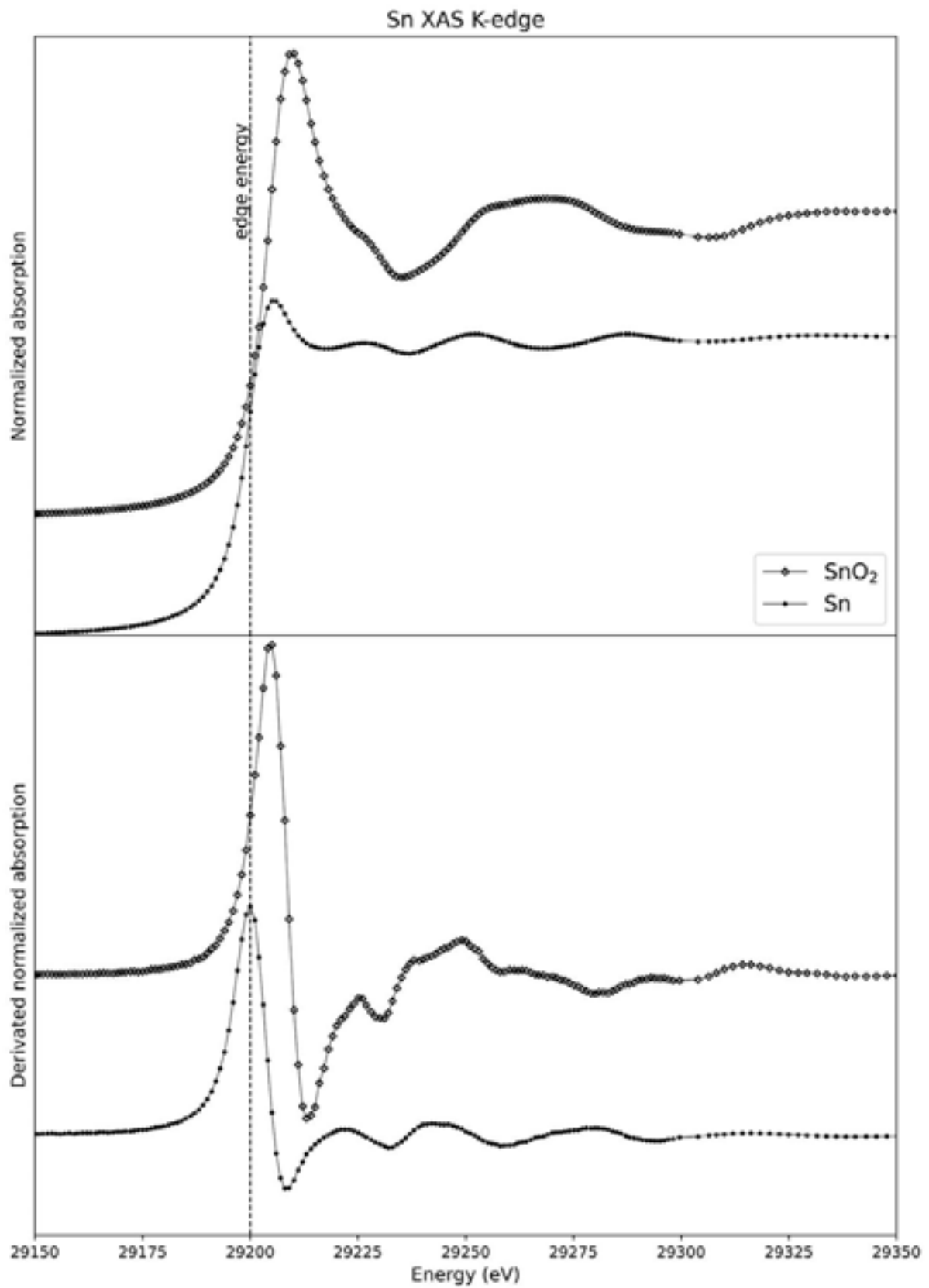
Z=50**Sn****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	29 200	25 271	28 485.4
Natural width	8.49	11.2	11.8

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	3.88	3.84
Si220	6.35	1.69

XAS Reference spectra



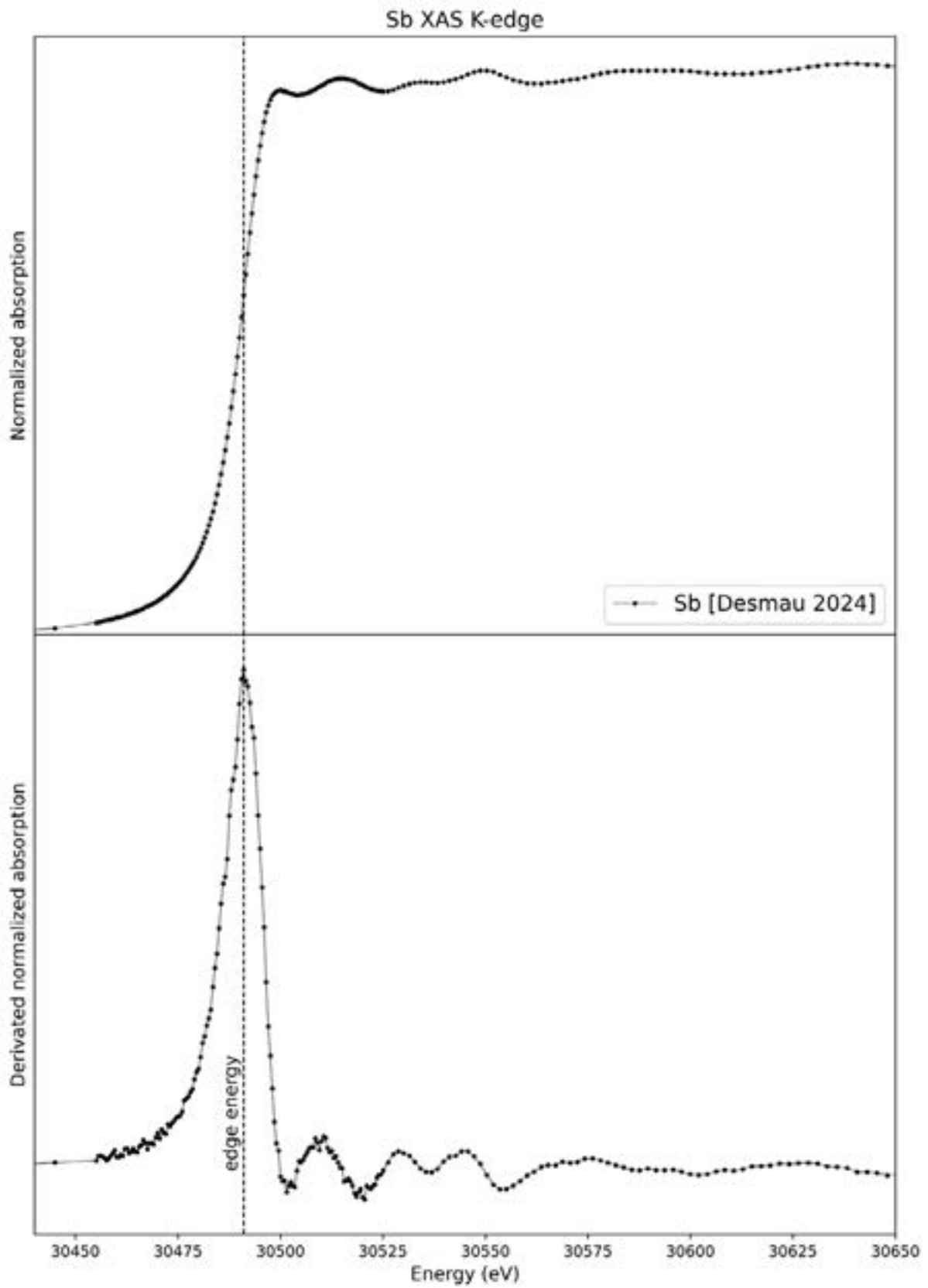
Z=51**Sb****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	30 491	26 359	29 724.6
Natural width	9.16	12.0	12.35

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	3.72	4.01
Si220	6.08	1.76

XAS Reference spectra



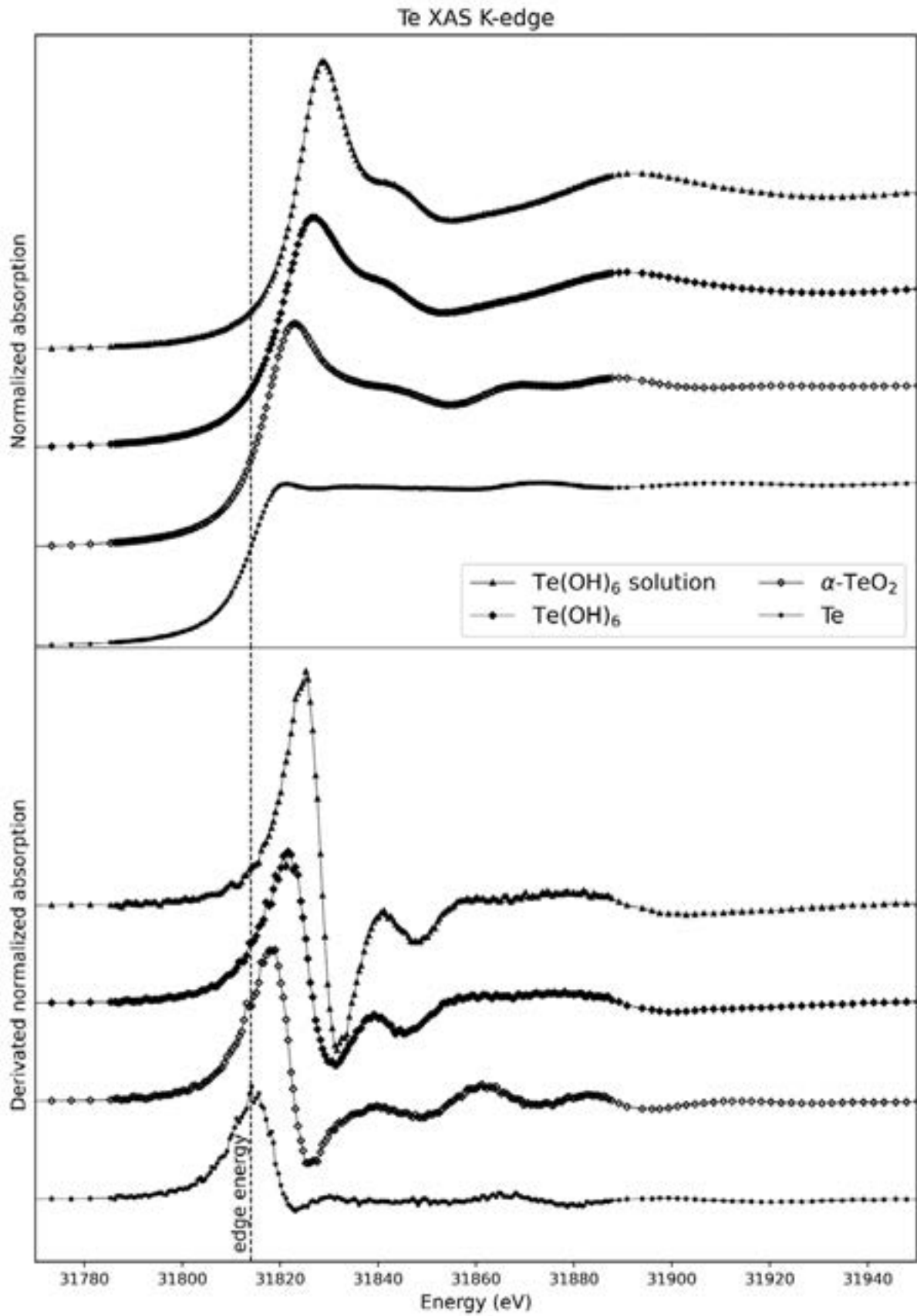
Z=52**Te****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	31 814	27 473	30 993.2
Natural width	9.89	12.8	13.3

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	3.56	4.18
Si220	5.52	1.84

XAS Reference spectra



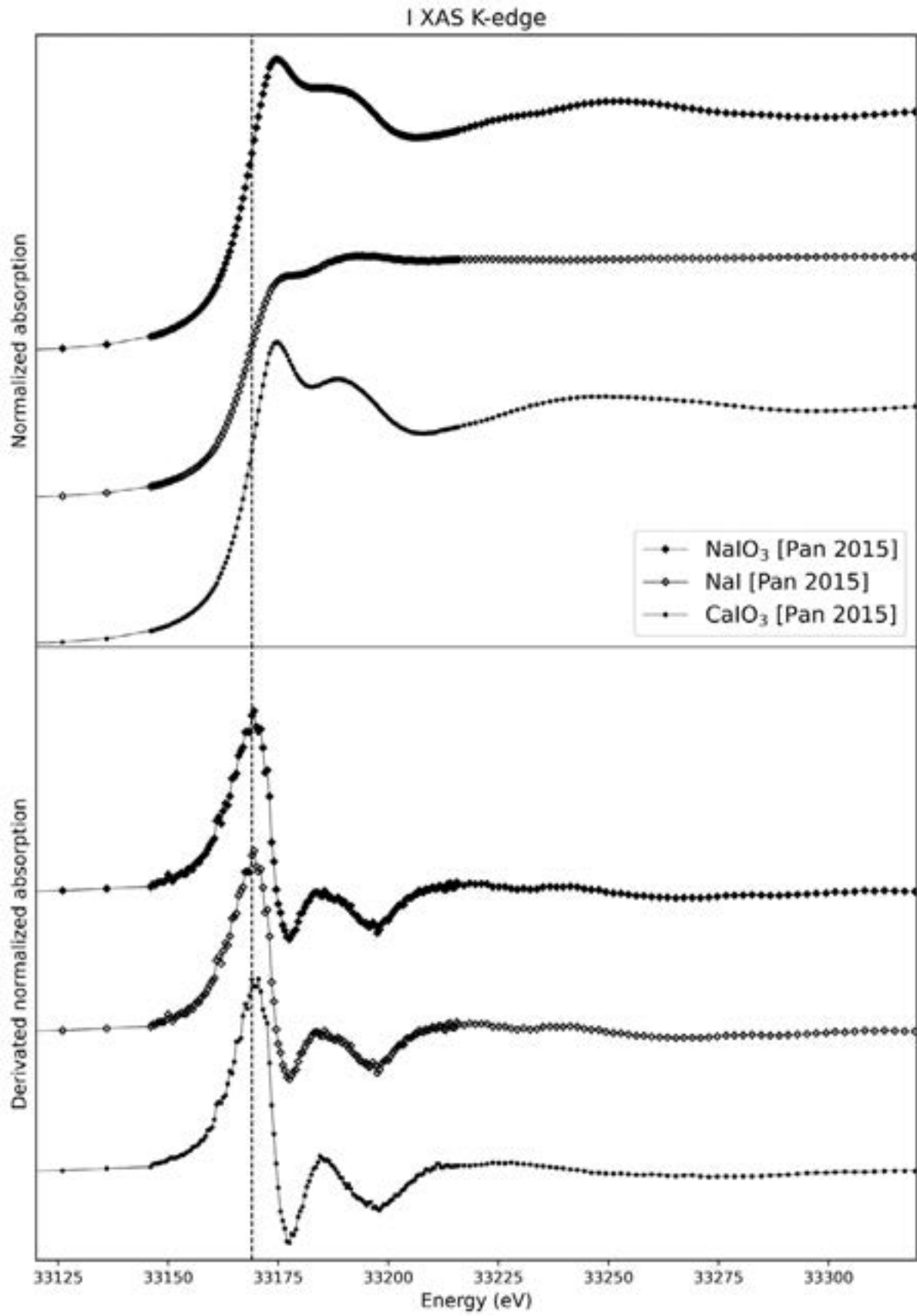
Z=53**I****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	33 169	28 612	32 294
Natural width	10.6	13.7	14.3

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	3.42	4.36
Si220	5.59	1.91

XAS Reference spectra



Z=54**Xe****K-edge****Characteristic energies and natural width (eV)**

	K-edge	Emission lines	
		$K_{\alpha 1}$	$K_{\beta 1}$
Energies	34 561	29 775	33 620.4
Natural width	11.4	14.6	15.3

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	3.28	4.54
Si220	5.36	1.99

XAS Reference spectra

Z=55**Cs****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	5 012	4 286	4 619
Natural width	3.25	3.27	3.33

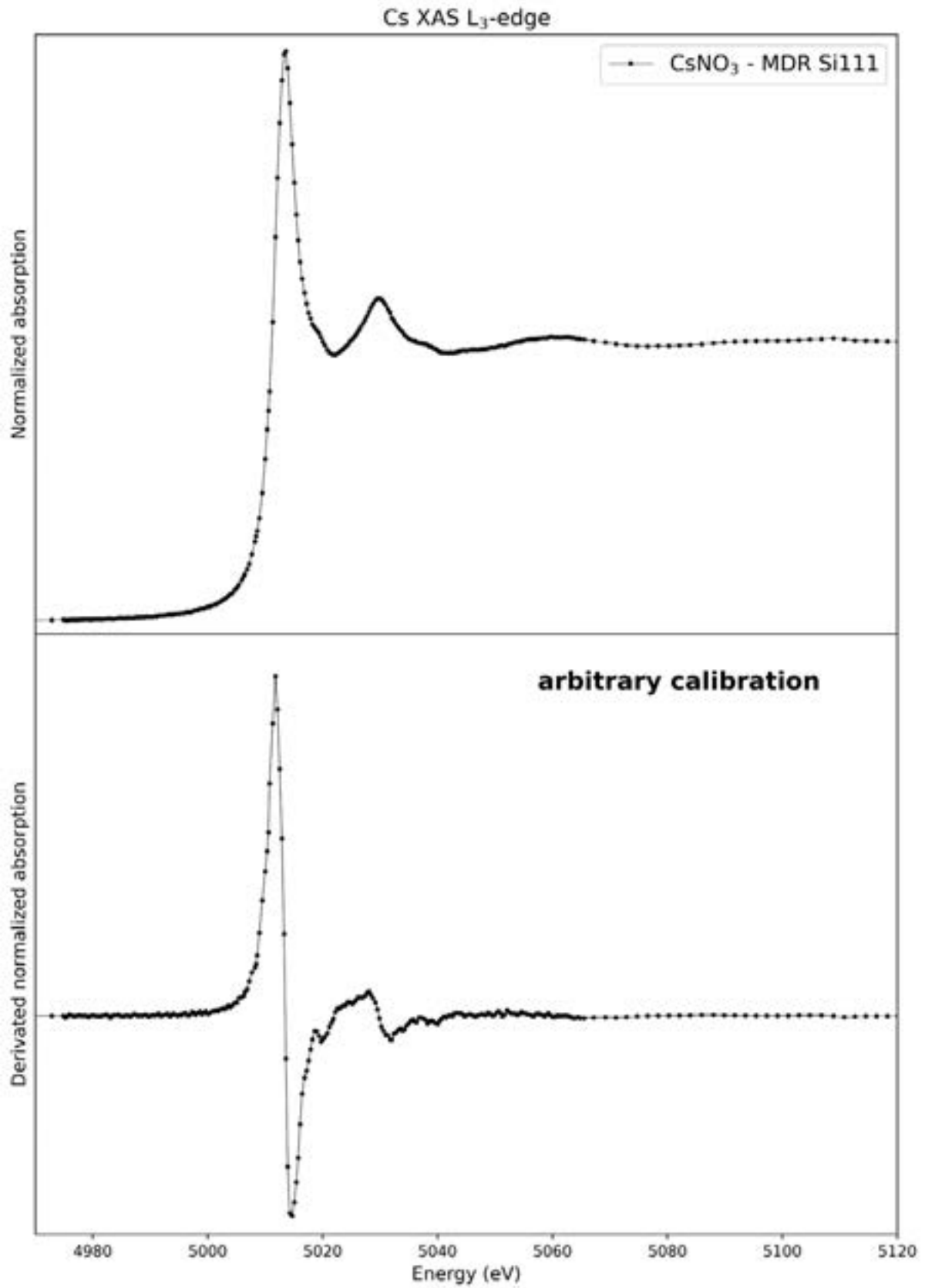
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	23.23	0.68
Si220	40.10	0.30

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si311	62.0
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si400	81.3

XAS Reference spectra



Z=56**Ba****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	5 247	4 466.5	4 828.3
Natural width	3.32	3.39	3.45

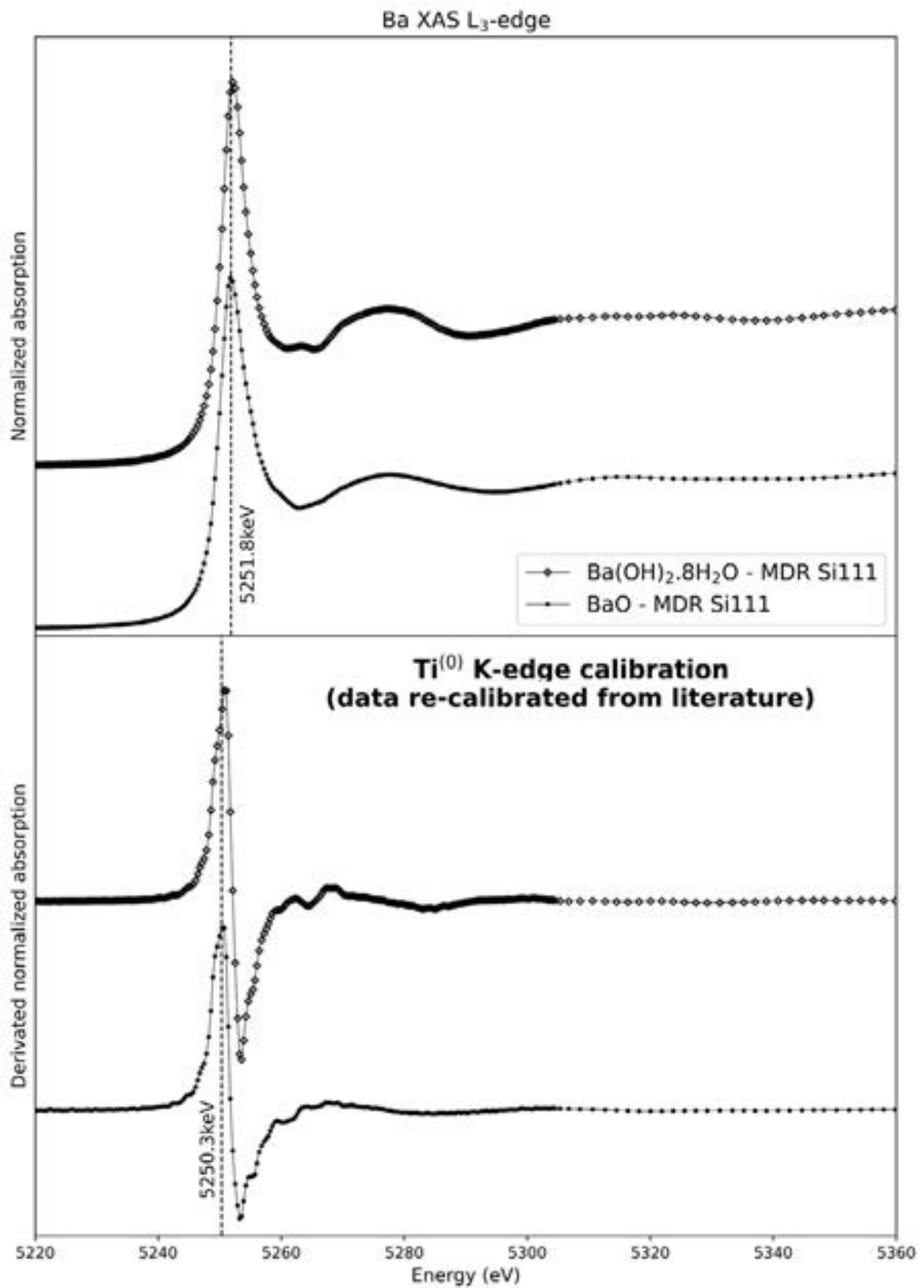
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	22.13	0.71
Si220	37.97	0.32

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge400	78.9
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge331	81.6

XAS Reference spectra



Z=57**La****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	5 483	4 647.0	5 038.0
Natural width	3.41	3.55	3.59

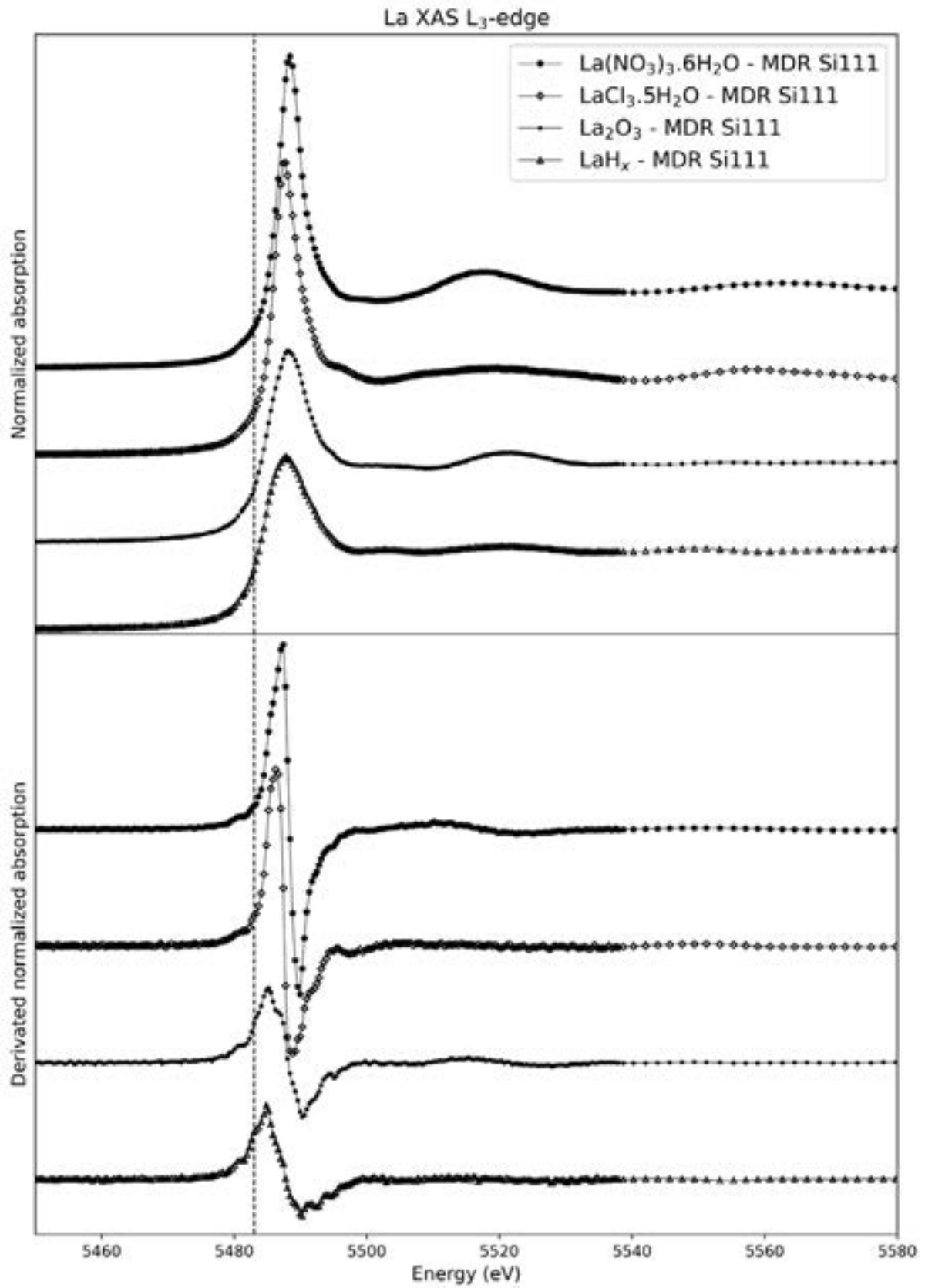
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	21.14	0.75
Si220	36.07	0.33

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si400	79.3
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si331	81.0

XAS Reference spectra



Z=58**Ce****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	5 723	4 839.2	5 261.6
Natural width	3.48	3.70	3.73

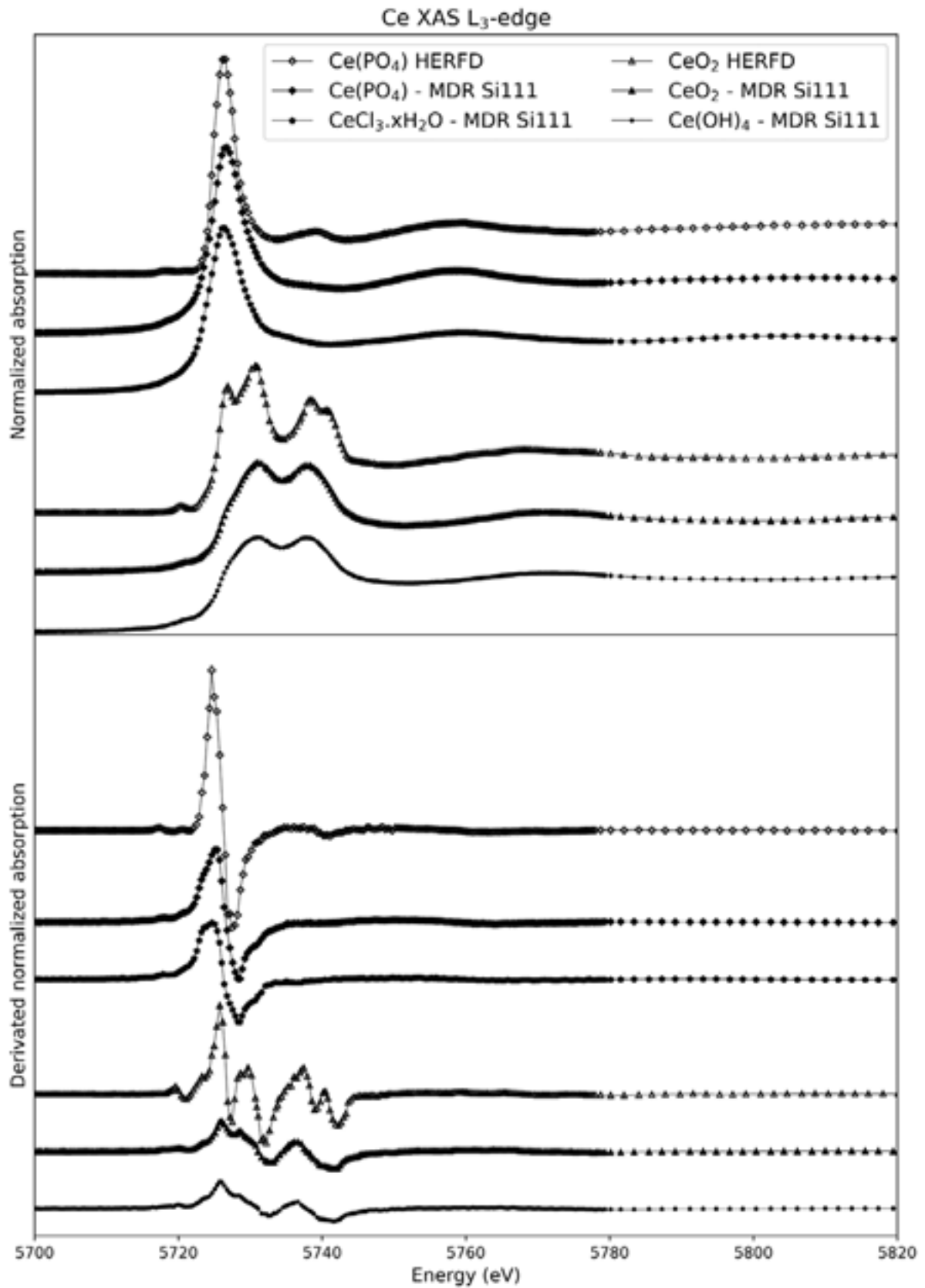
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	20.21	0.78
Si220	34.34	0.34

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge331	80.7
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si331	71

XAS Reference spectra



Z=59**Pr****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	5 964	5 035.2	5 491.7
Natural width	3.60	3.82	3.87

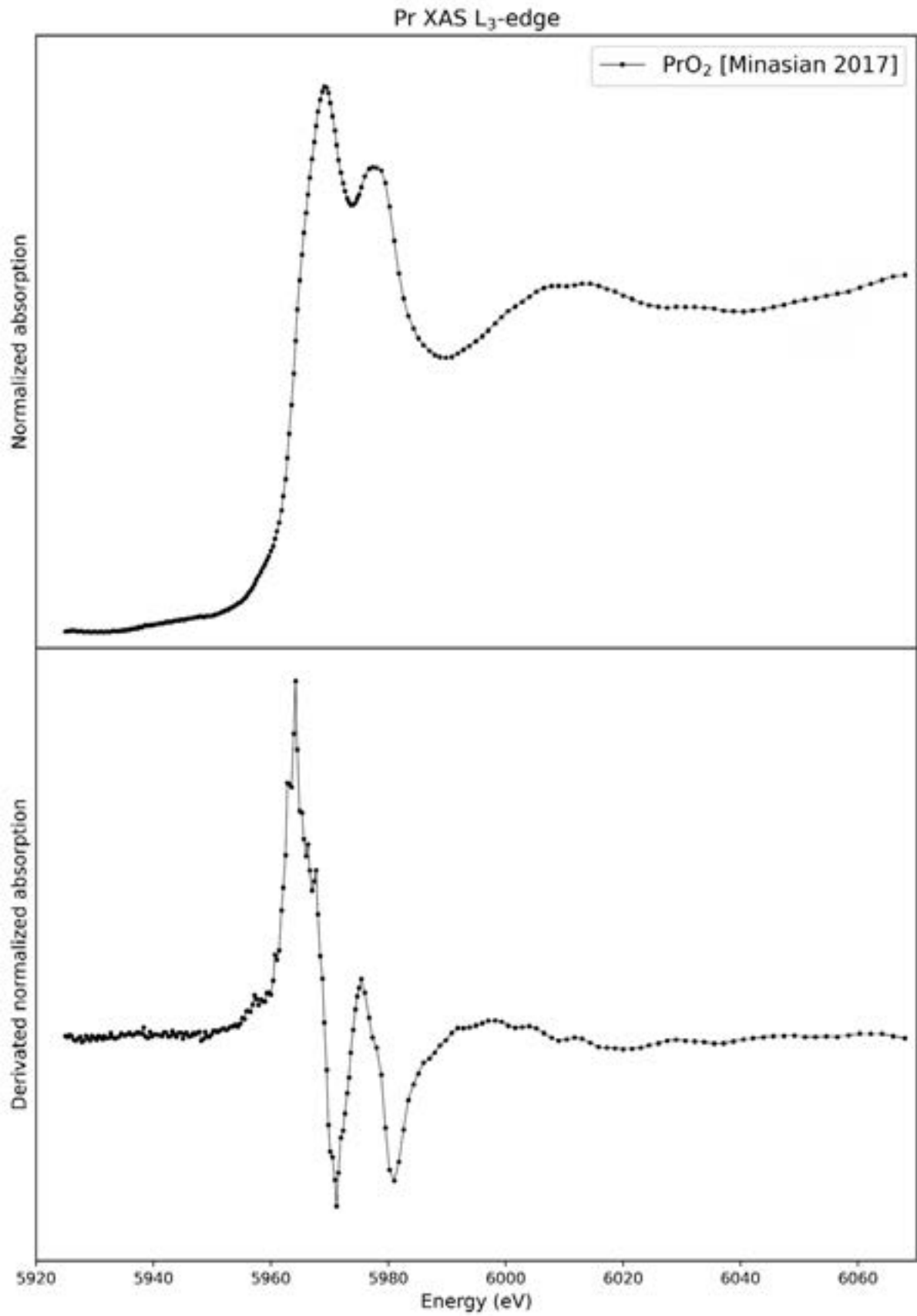
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	19.36	0.81
Si220	32.78	0.36

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si331	81.2
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge422	77.8

XAS Reference spectra



Z=60**Nd****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	6 208	5 227.6	5 718.7
Natural width	3.65	3.93	4.00

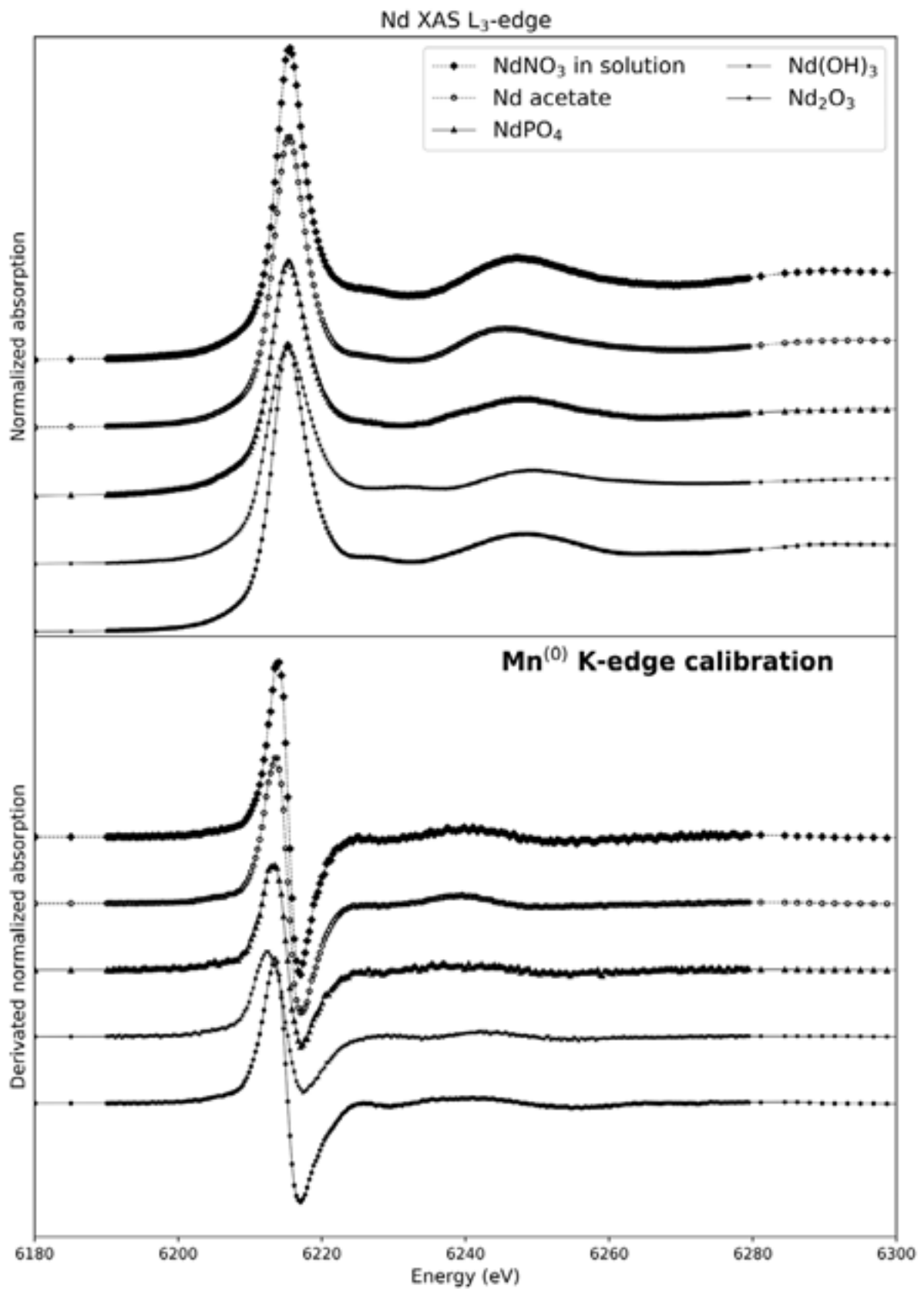
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	18.57	0.84
Si220	31.33	0.37

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si331	72.1
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge333	84.6

XAS Reference spectra



Z=61**Pm****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	6 459	5 432.0	5 961.0
Natural width	3.75	4.03	4.17

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	17.82	0.87
Si220	29.99	0.39

Crystal Analyzer Spectrometer parameters

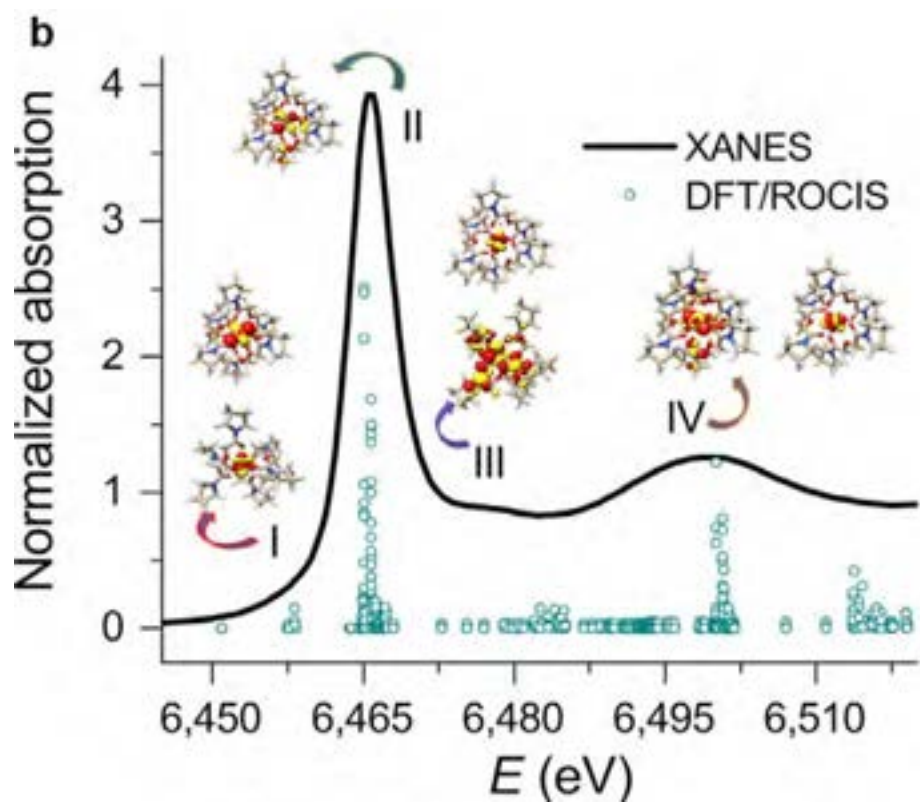
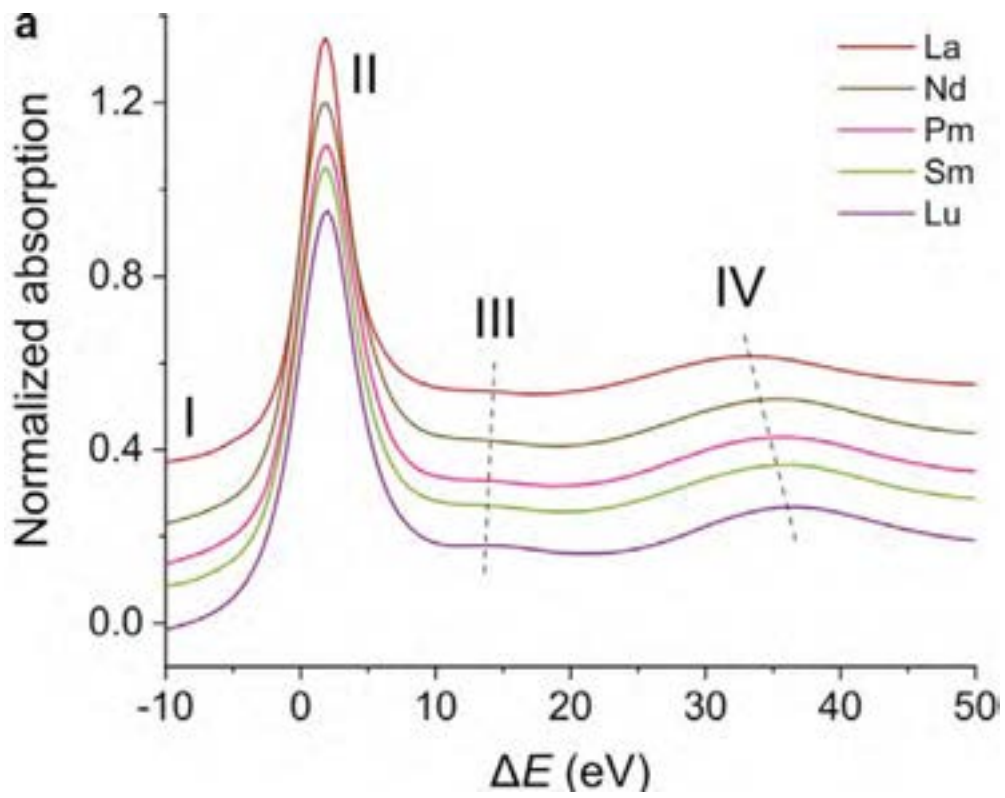
L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge422	81.2
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si333	84.3

Data from Driscoll et al. [Driscoll 2024].

(a) La^{III}, Nd^{III}, Sm^{III} and Lu^{III} spectra are compared to the Pm^{III} data. The plot is presented as a function of ΔE (the difference between the photon energy E and the peak in the first derivative of the data E_0).

(b) Experimental (black line) and simulated (circles) XANES spectra of Pm(PyDGA)₃³⁺ complexes in solution, with the representative orbitals participating in the core electron excitations.

XAS Reference spectra



Z=62**Sm****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	6 716	5 632.6	6 201.1
Natural width	3.86	4.13	4.33

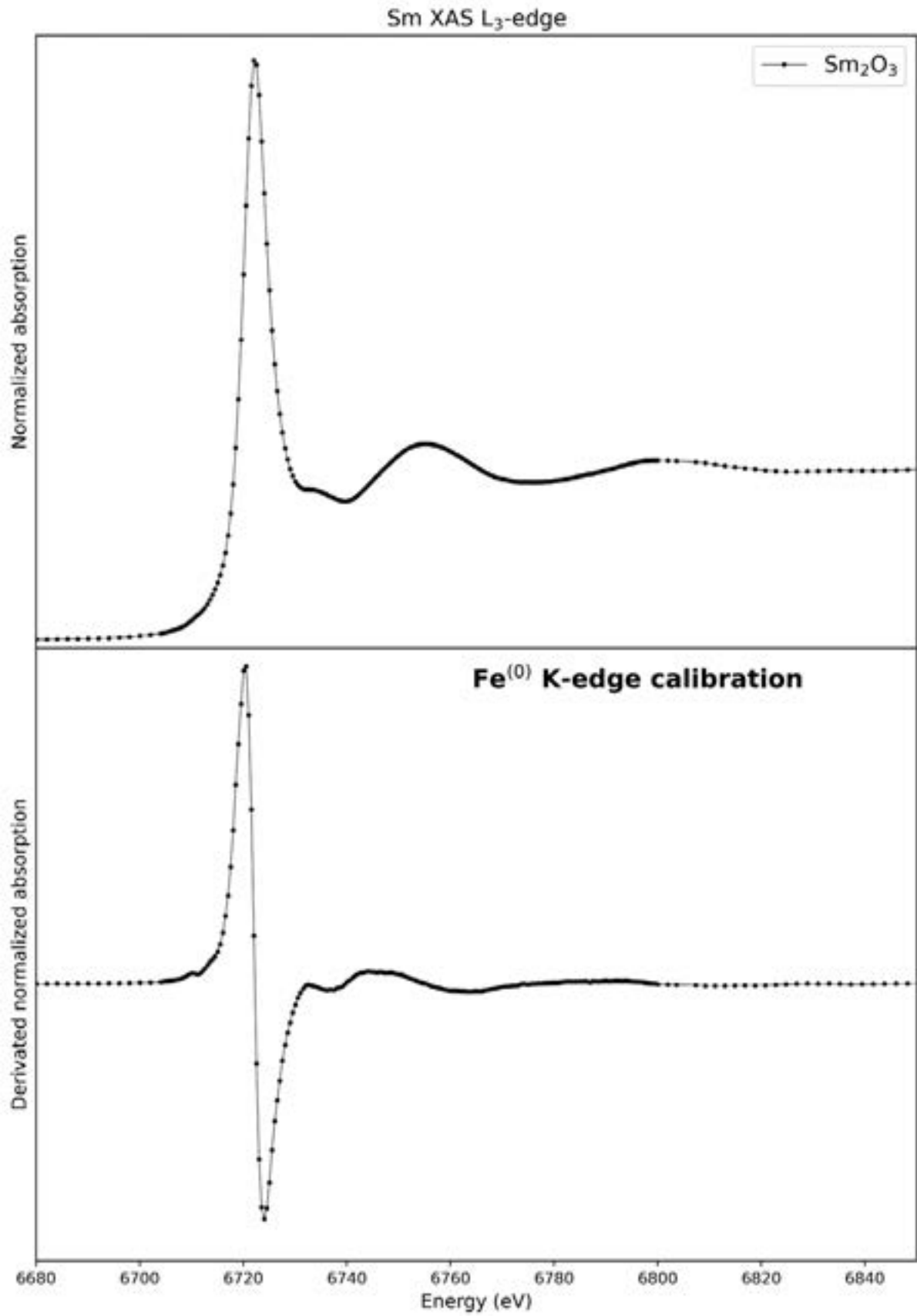
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	17.12	0.91
Si220	28.73	0.40

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si422	83.1
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge440	88.3

XAS Reference spectra



Z=63**Eu****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	6 977	5 849.5	6 458.4
Natural width	3.91	4.30	4.48

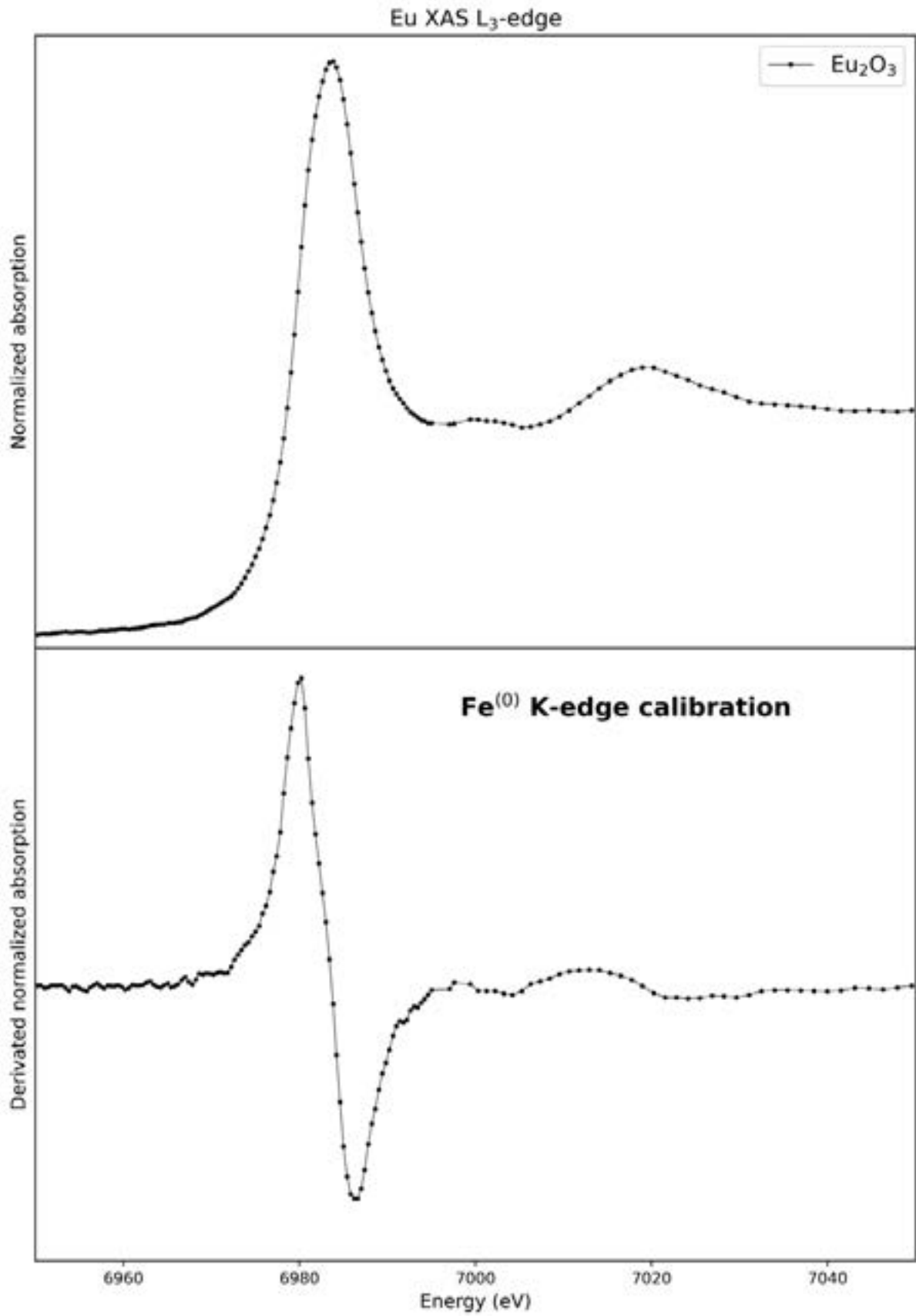
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	16.46	0.94
Si220	27.56	0.42

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge333	76.7
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si440	89.1

XAS Reference spectra



Z=64**Gd****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	7 243	6 053.4	6 708.1
Natural width	4.01	4.46	4.63

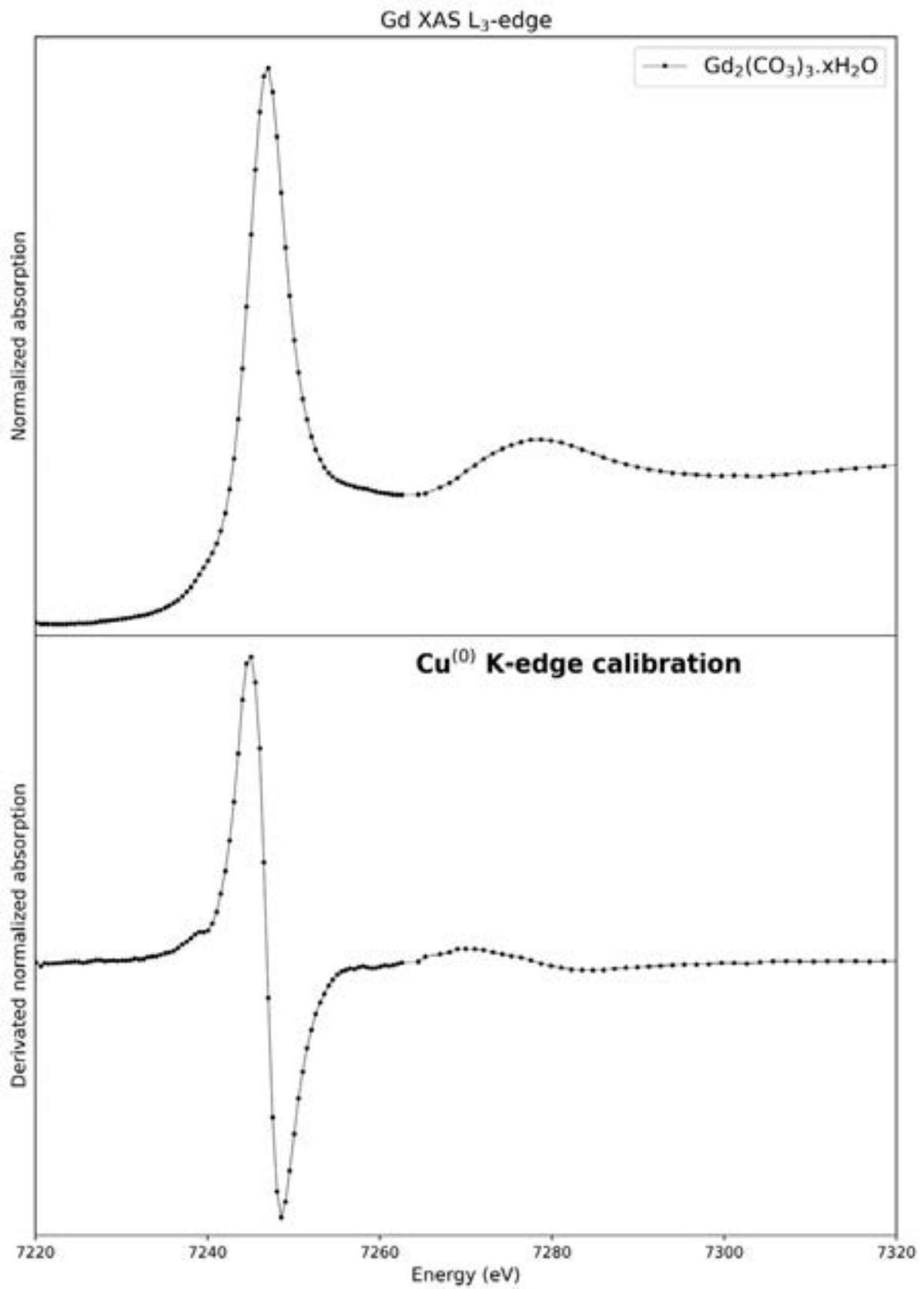
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	15.84	0.98
Si220	26.47	0.43

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si333	78.5
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si440	74.3

XAS Reference spectra



Z=65**Tb****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	7 514	6 272.9	6 975.1
Natural width	4.12	4.64	4.83

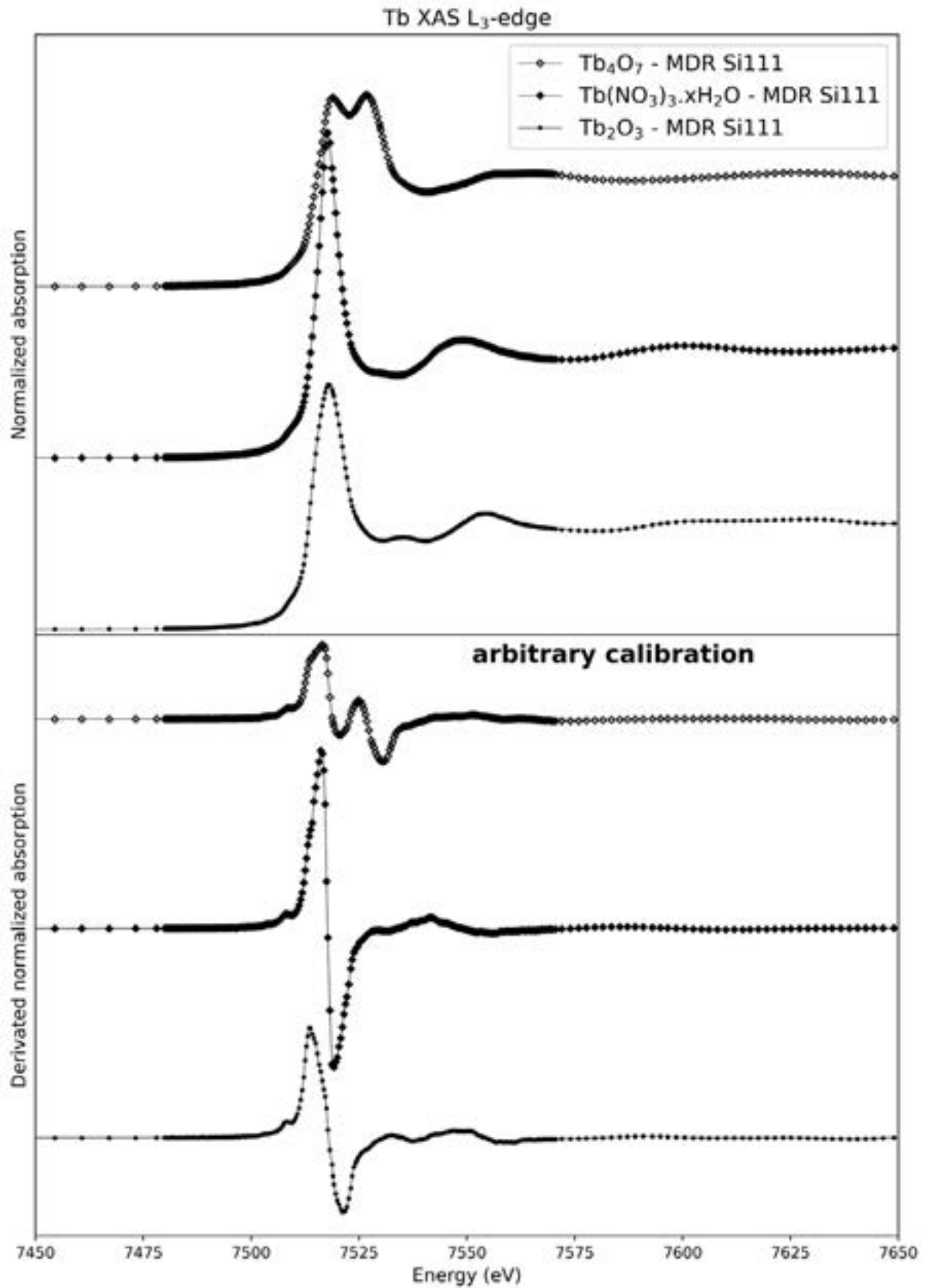
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	15.26	1.01
Si220	25.45	0.45

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge440	81.1
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge620	83.5

XAS Reference spectra



Z=66 Dy L-edges

Characteristic energies and natural width (eV)

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	7 790	6 498	7 248
Natural width	4.17	4.81	5.03

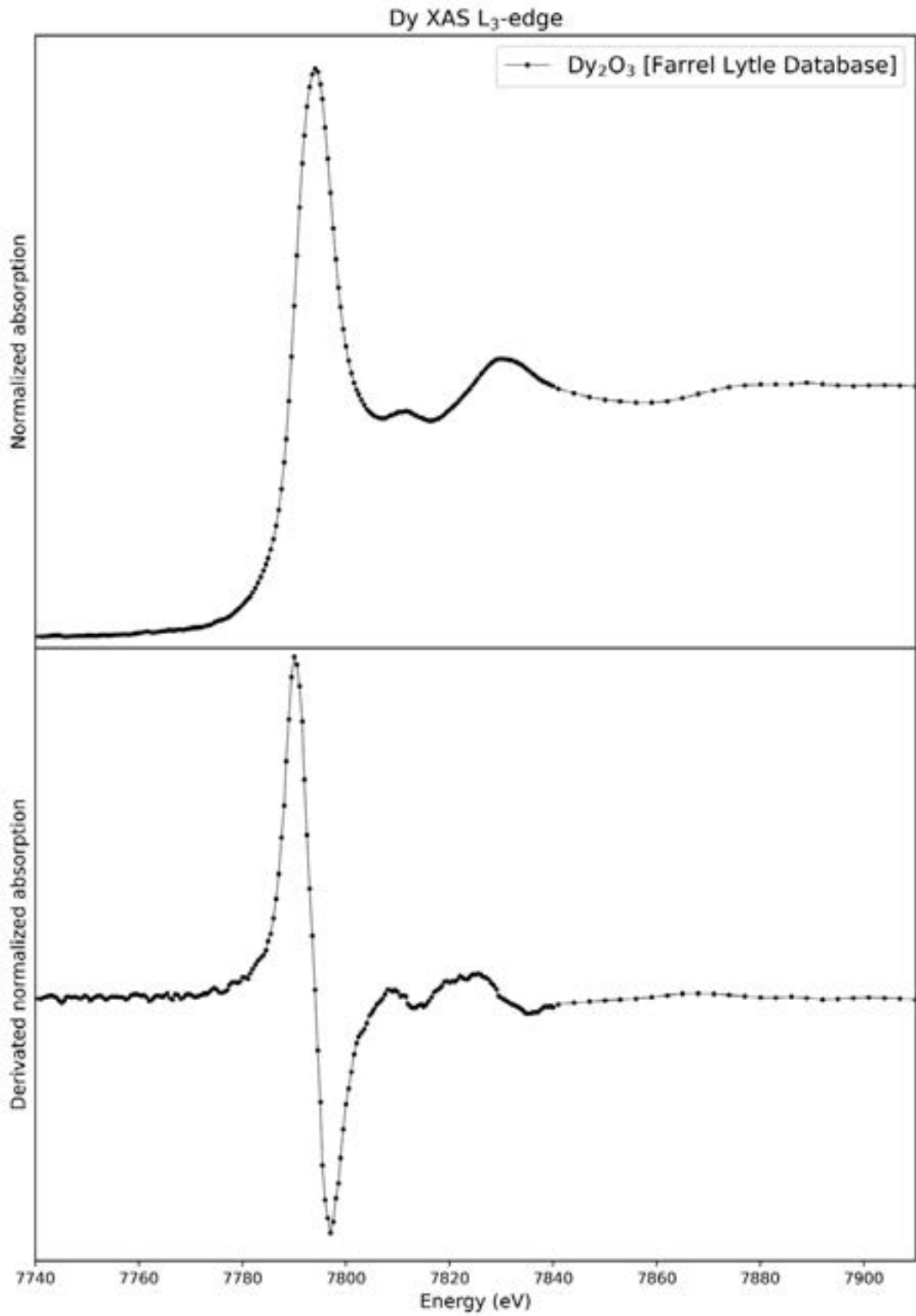
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	14.70	1.05
Si220	24.48	0.46

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si440	83.6
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si620	84.9

XAS Reference spectra



Z=67**Ho****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	8 071	6 720	7 526
Natural width	4.26	4.99	5.24

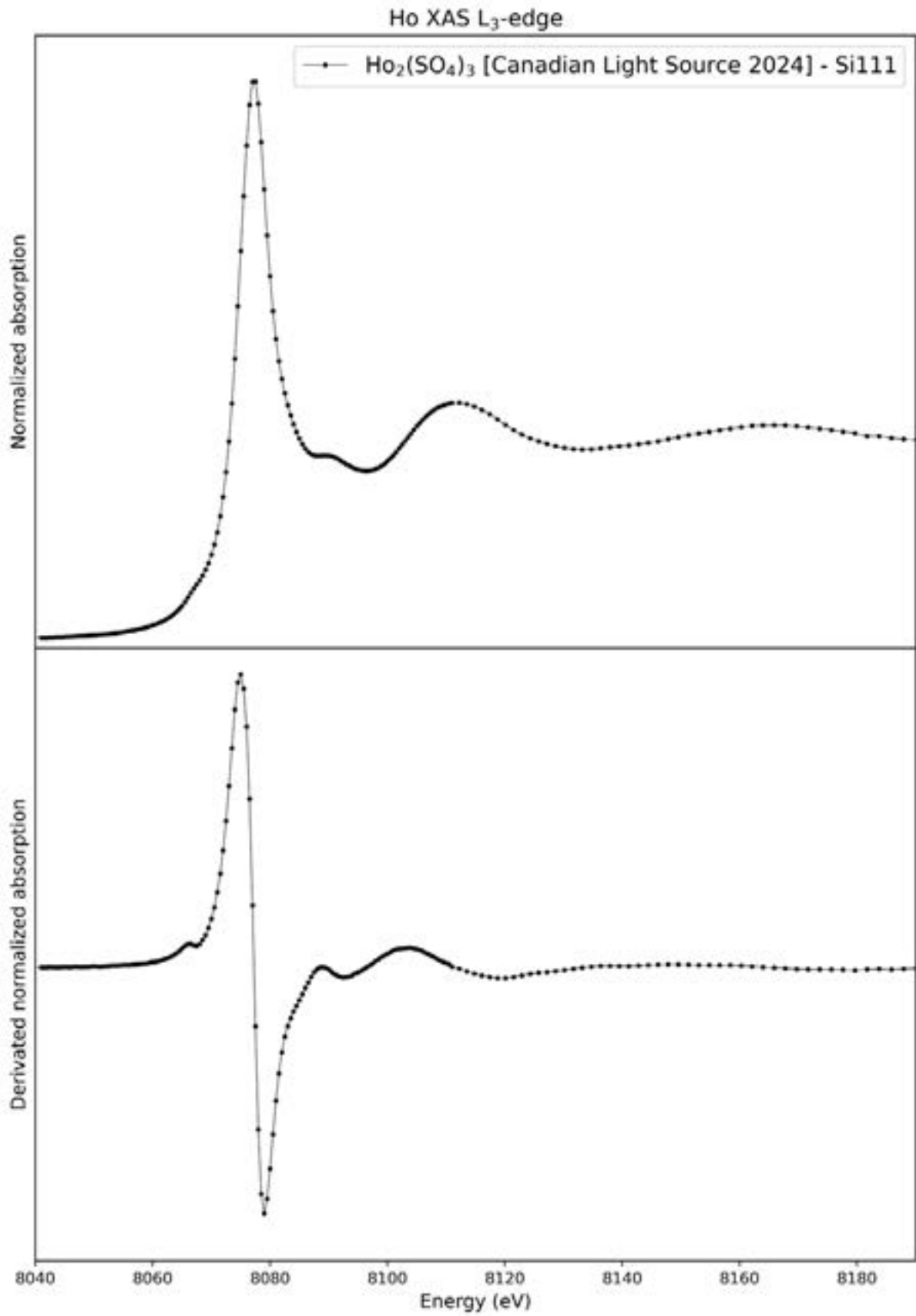
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	14.18	1.08
Si220	23.58	0.48

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si531	74.7
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si620	73.6

XAS Reference spectra



Z=68**Er****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	8 358	6 949	7 811
Natural width	4.35	5.17	5.45

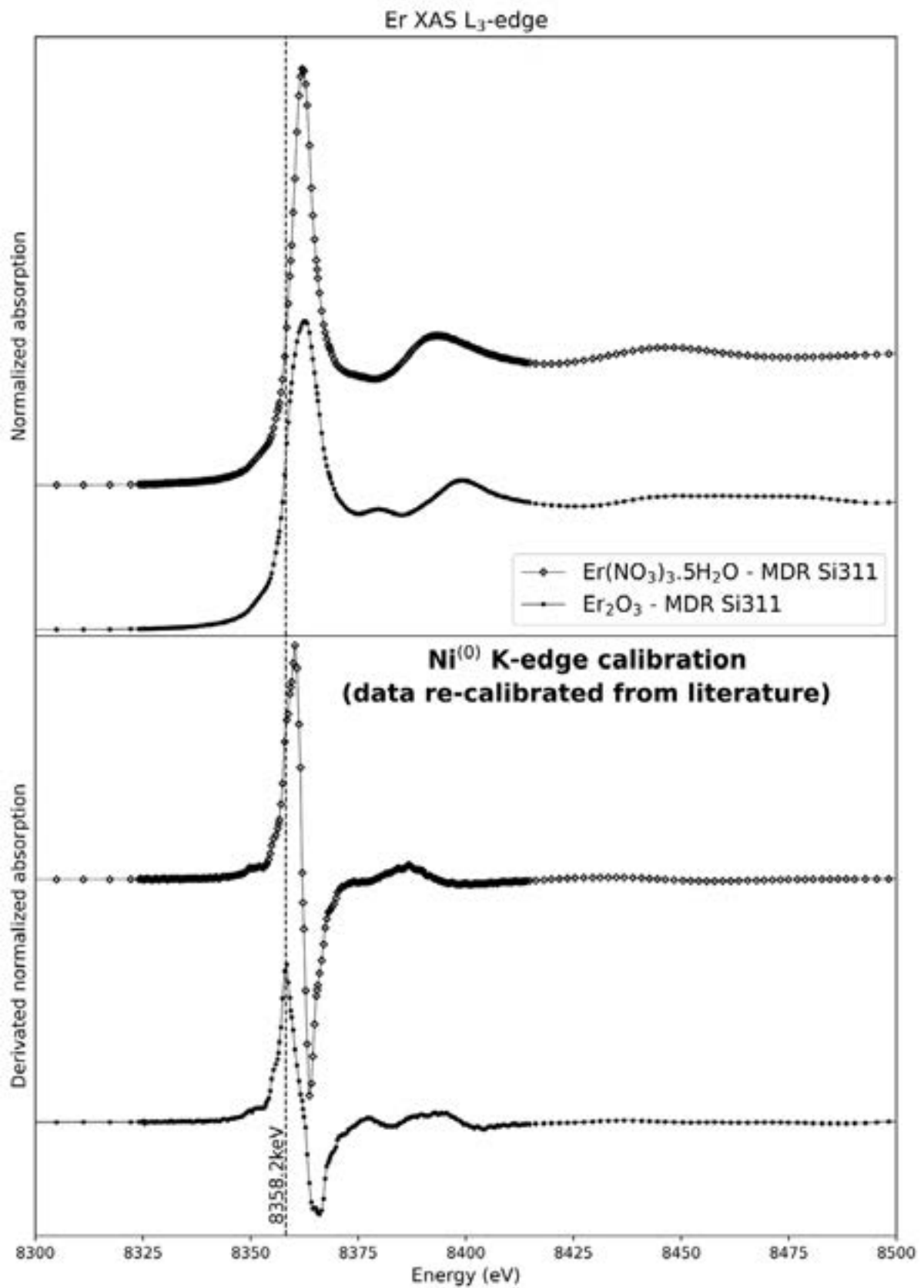
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	13.68	1.12
Si220	22.72	0.49

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge620	85.7
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge444	76.4

XAS Reference spectra



Z=69**Tm****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	8 648	7 180	8 102
Natural width	4.48	5.29	6.675

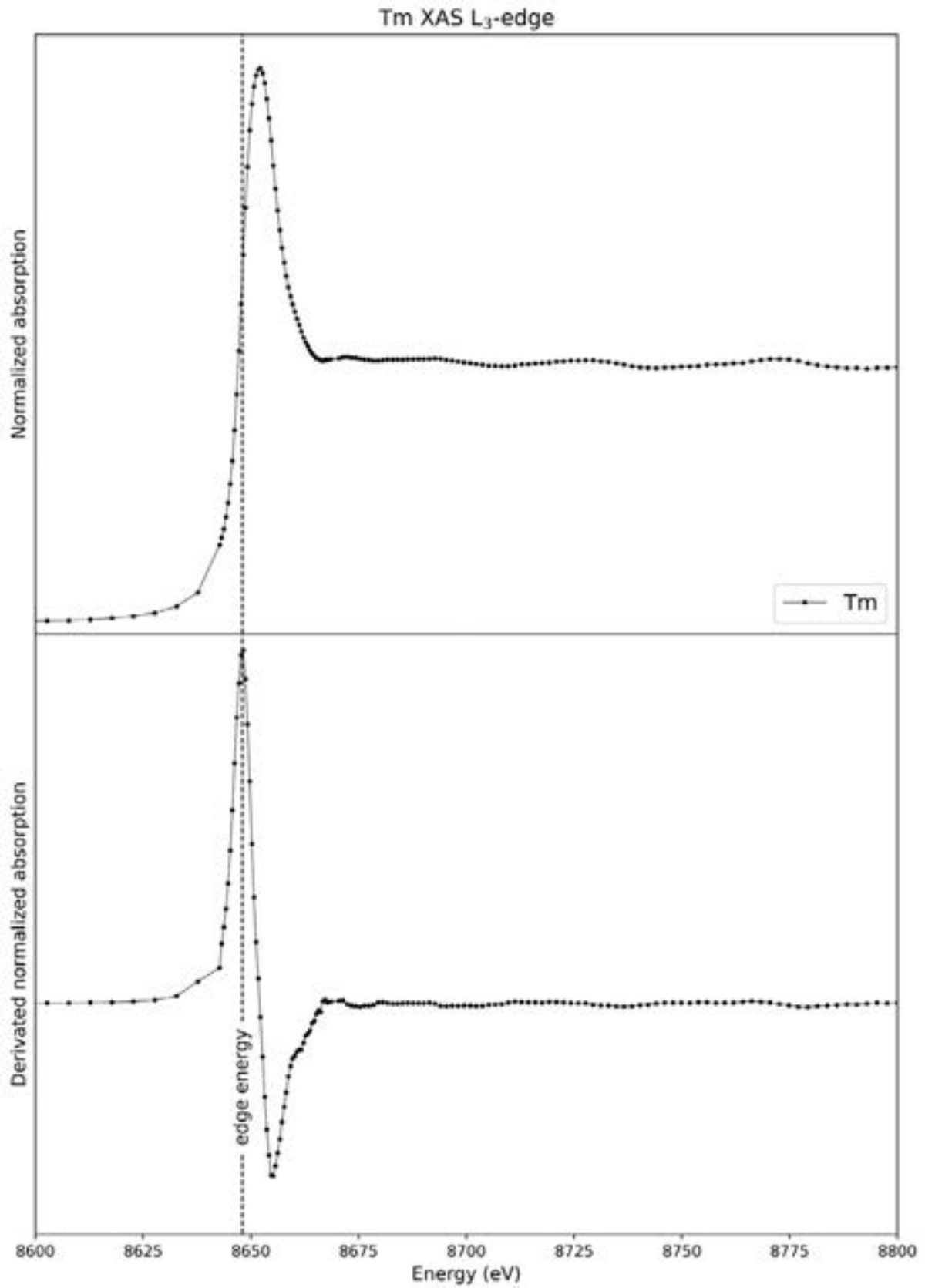
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	13.21	1.16
Si220	21.92	0.51

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge620	74.8
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si444	77.4

XAS Reference spectra



Z=70**Yb****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	8 944	7 416	8 402
Natural width	4.40	5.4	5.9

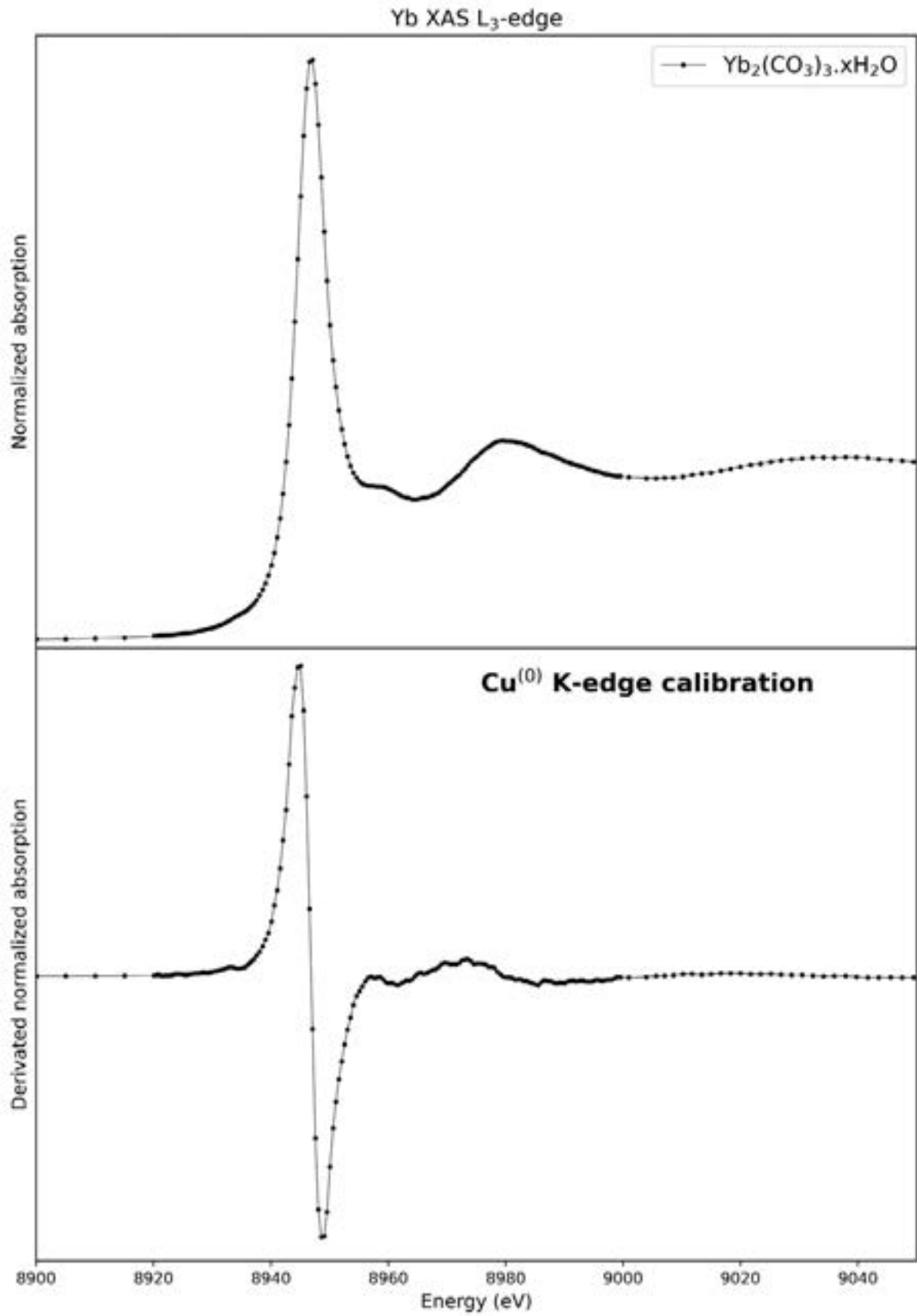
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	12.77	1.20
Si220	21.16	0.53

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si620	76.8
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si551	76.0

XAS Reference spectra



Z=71**Lu****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	9 244	7 655	8 710
Natural width	4.68	5.62	6.13

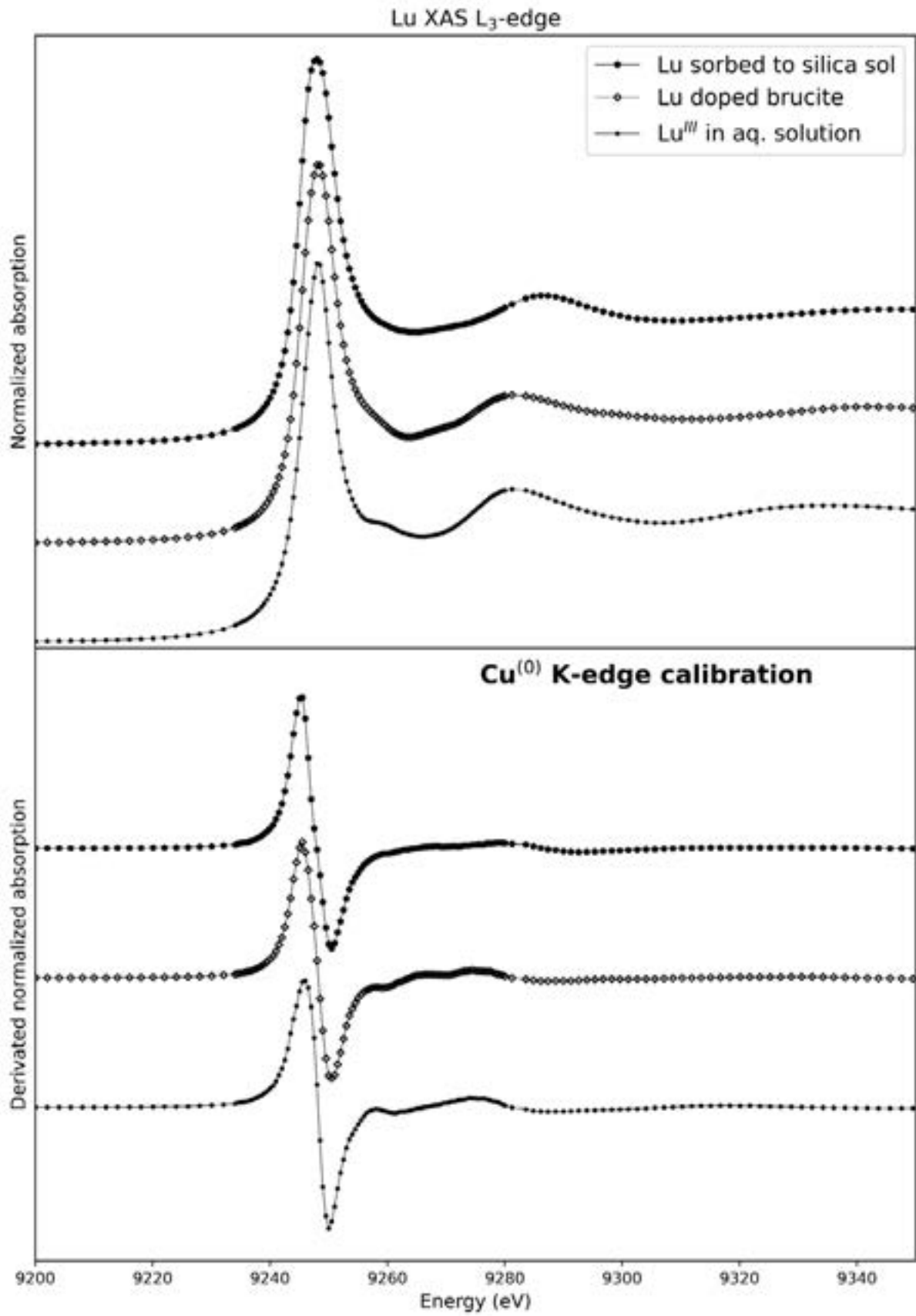
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	12.35	1.24
Si220	20.44	0.55

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge844	82.6
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si551	69.4

XAS Reference spectra



Z=72**Hf****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	9 561	7 899	9 023
Natural width	4.80	5.83	6.36

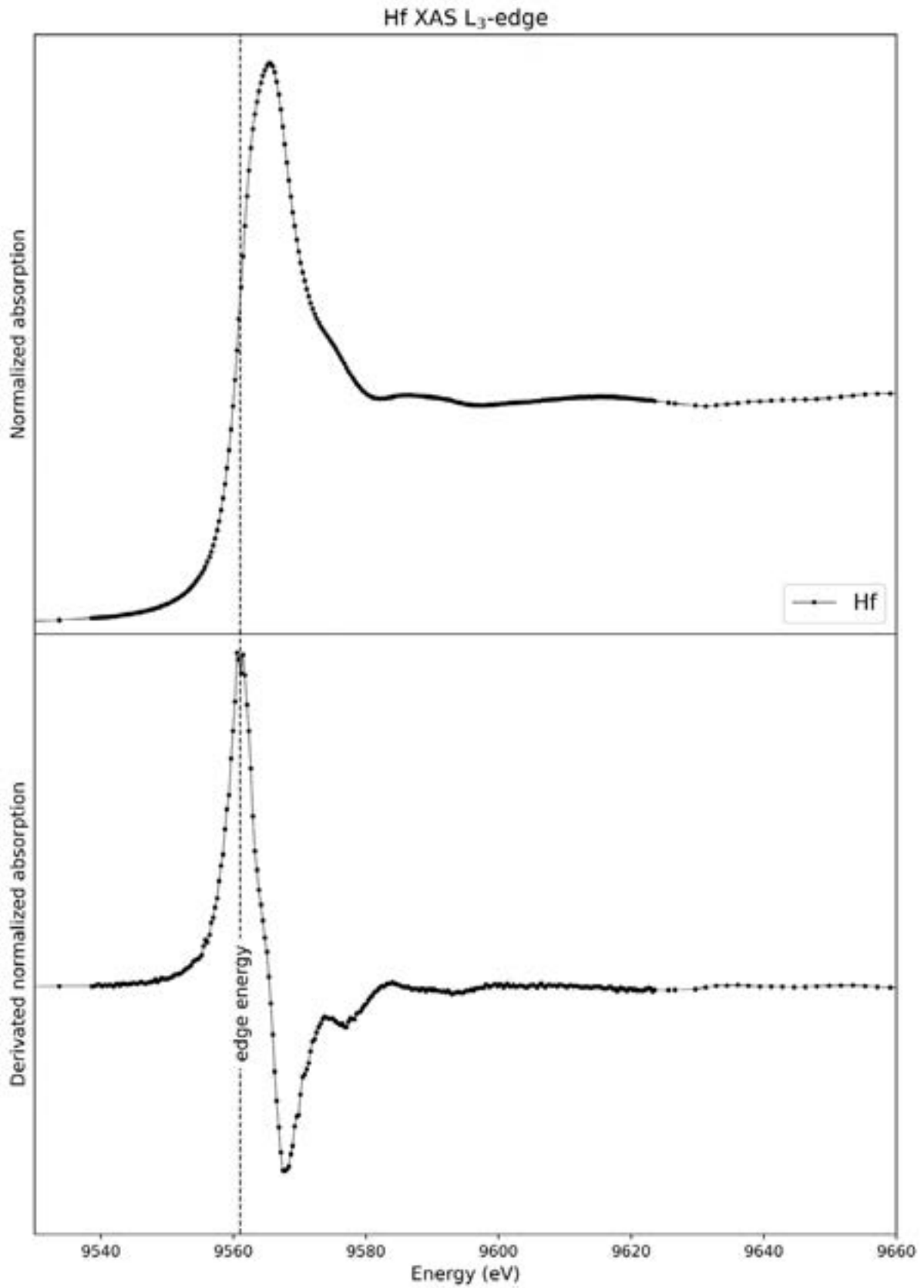
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	11.93	1.28
Si220	19.73	0.56

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge444	74.0
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge733	83.7
Ge800	76.3

XAS Reference spectra



Z=73**Ta****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	9 881	8 146	9 343
Natural width	4.88	6.17	6.63

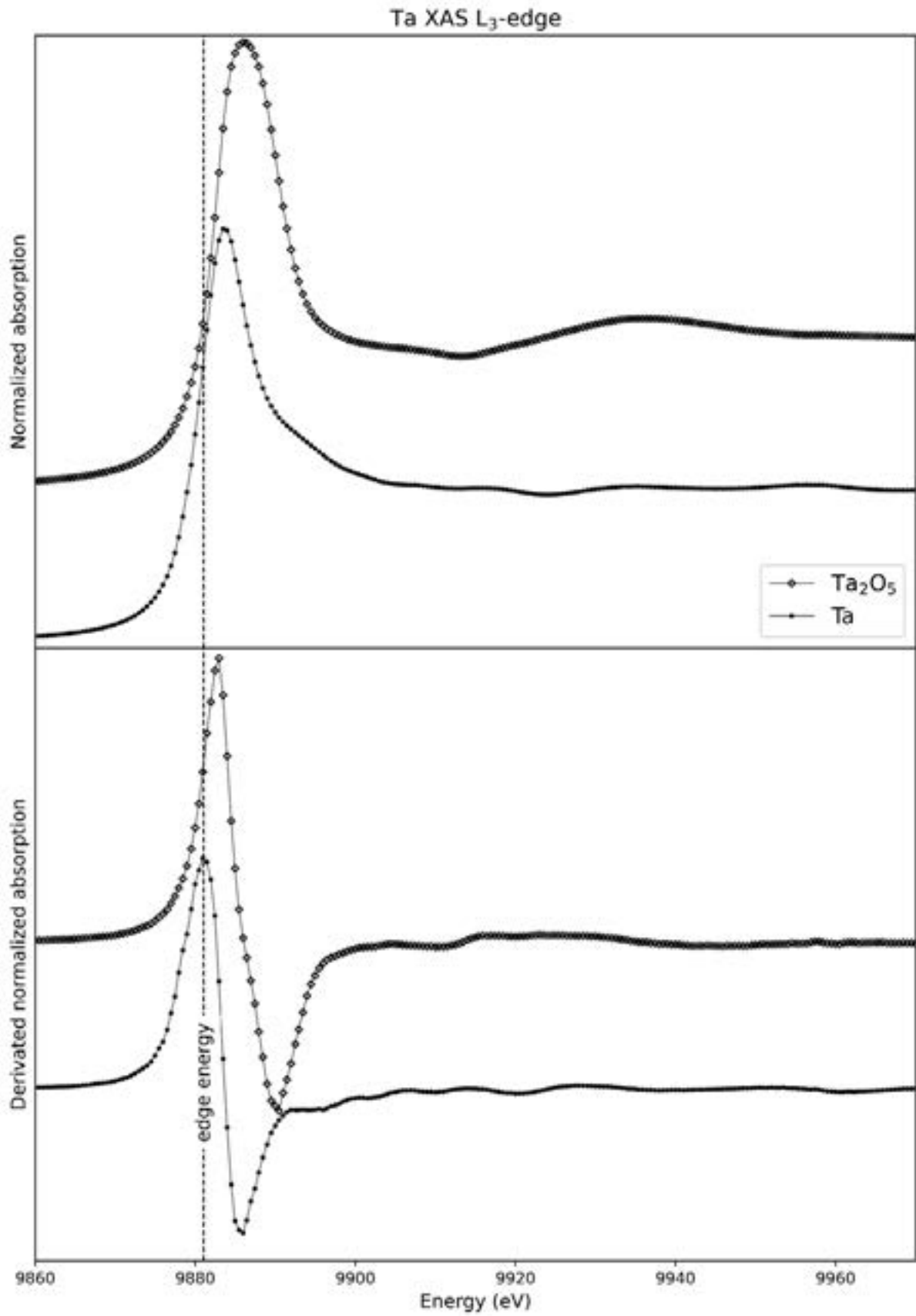
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	11.54	1.32
Si220	19.07	0.58

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si444	76.1
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge660	84.3

XAS Reference spectra



Z=74**W****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	10 207	8 398	9 672
Natural width	4.98	6.5	6.9

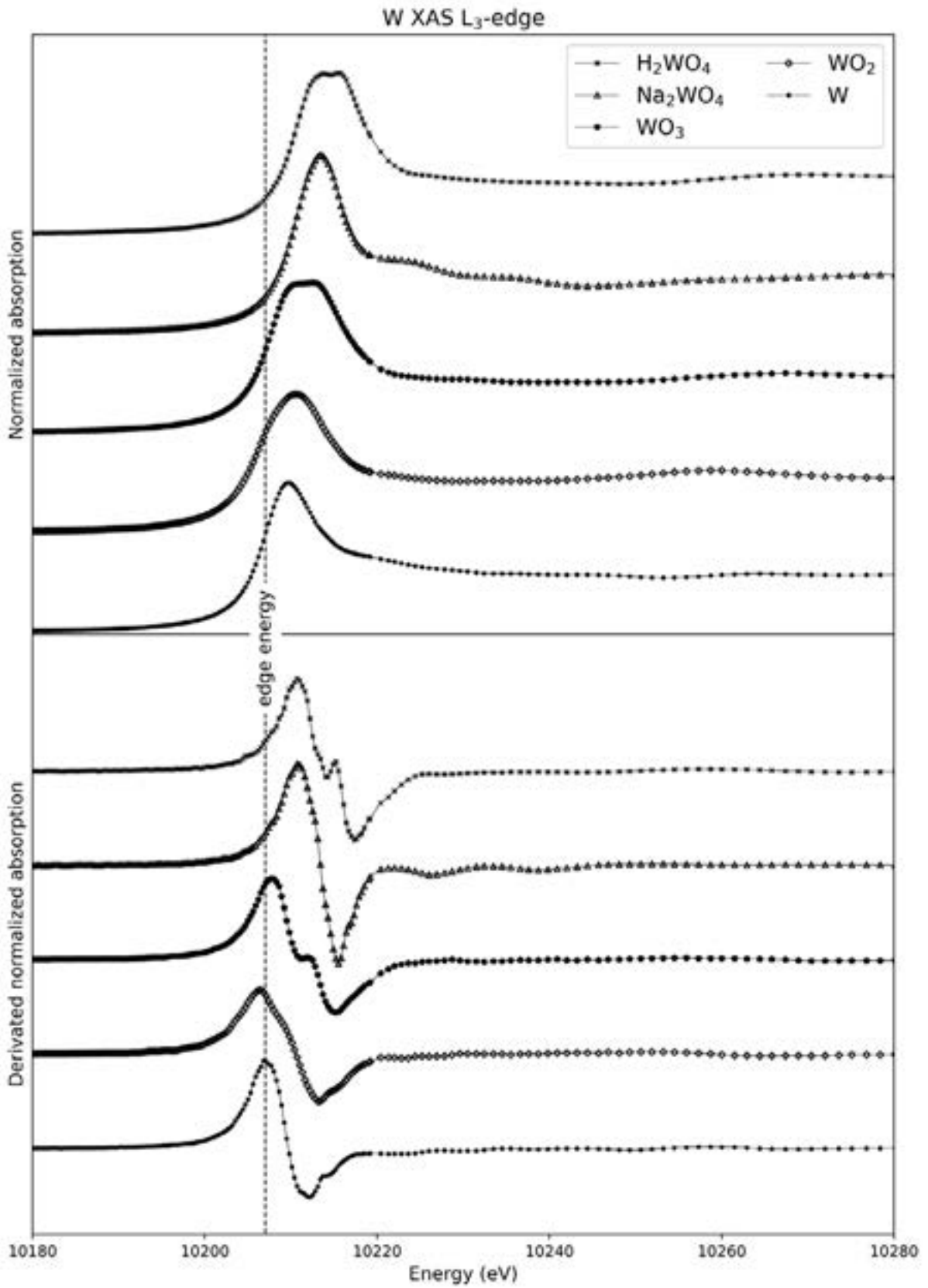
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	11.17	1.36
Si220	18.44	0.60

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si551	76.1
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge555	78.8

XAS Reference spectra



Z=75**Re****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	10 535	8 652	10 010
Natural width	5.04	6.77	7.16

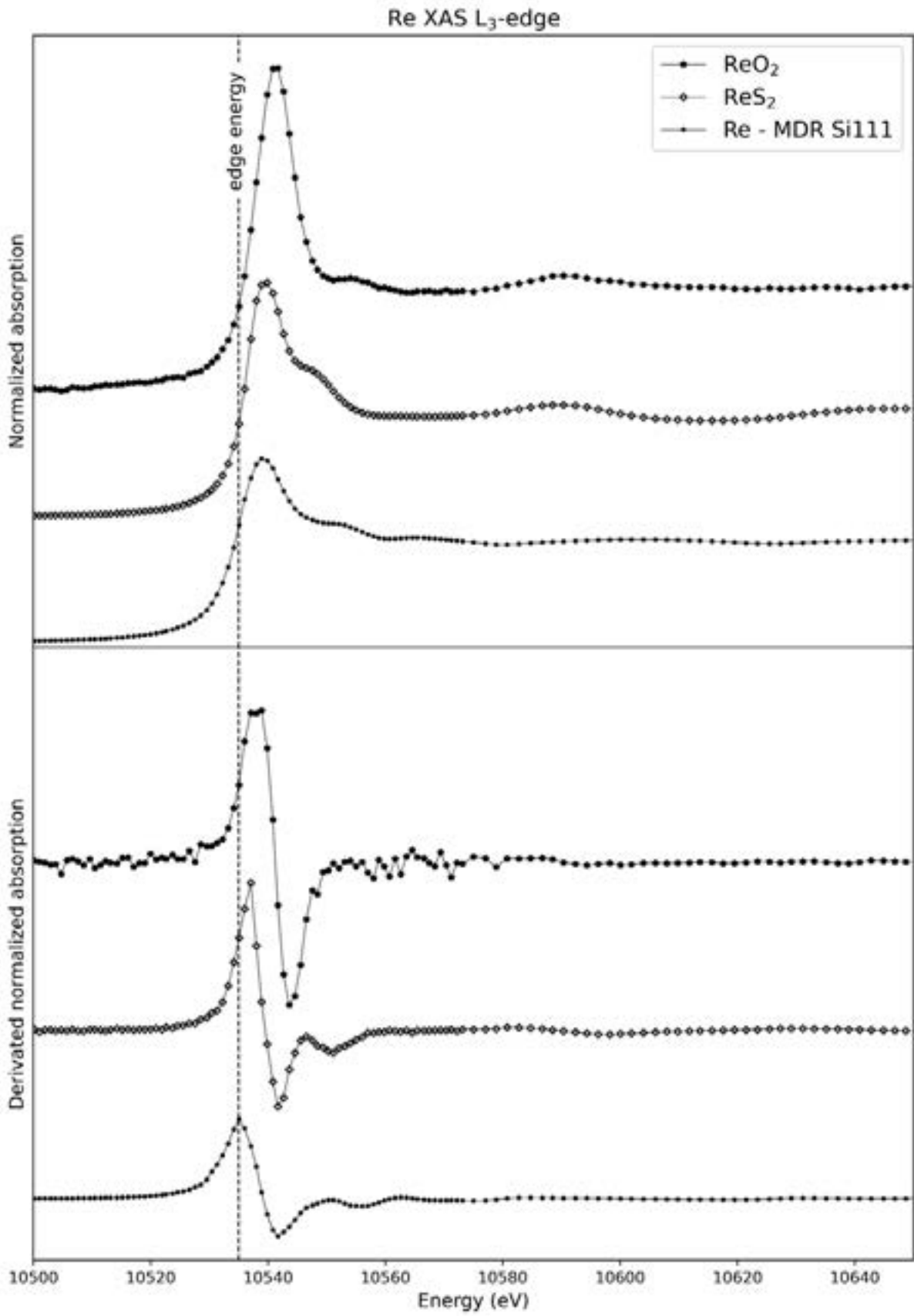
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	10.82	1.41
Si220	17.85	0.62

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si642	80.9
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si555	90.9

XAS Reference spectra



Z=76**Os****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	10 871	8 911	10 354
Natural width	5.16	7.04	7.42

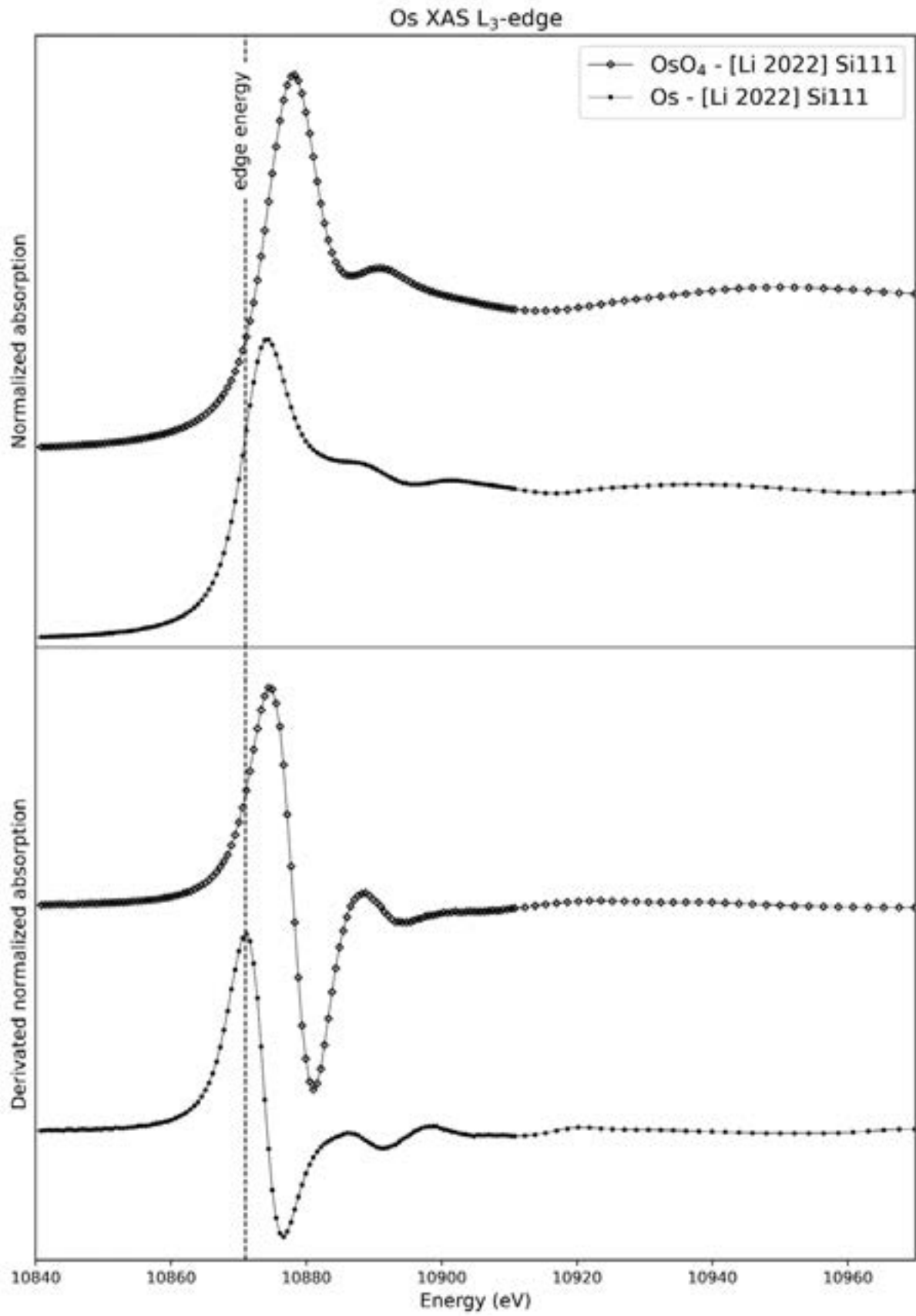
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	10.48	1.45
Si220	17.28	0.64

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge800	79.6
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si555	72.7

XAS Reference spectra



Z=77**Ir****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	11 215	9 175	10 708
Natural width	5.25	7.32	7.71

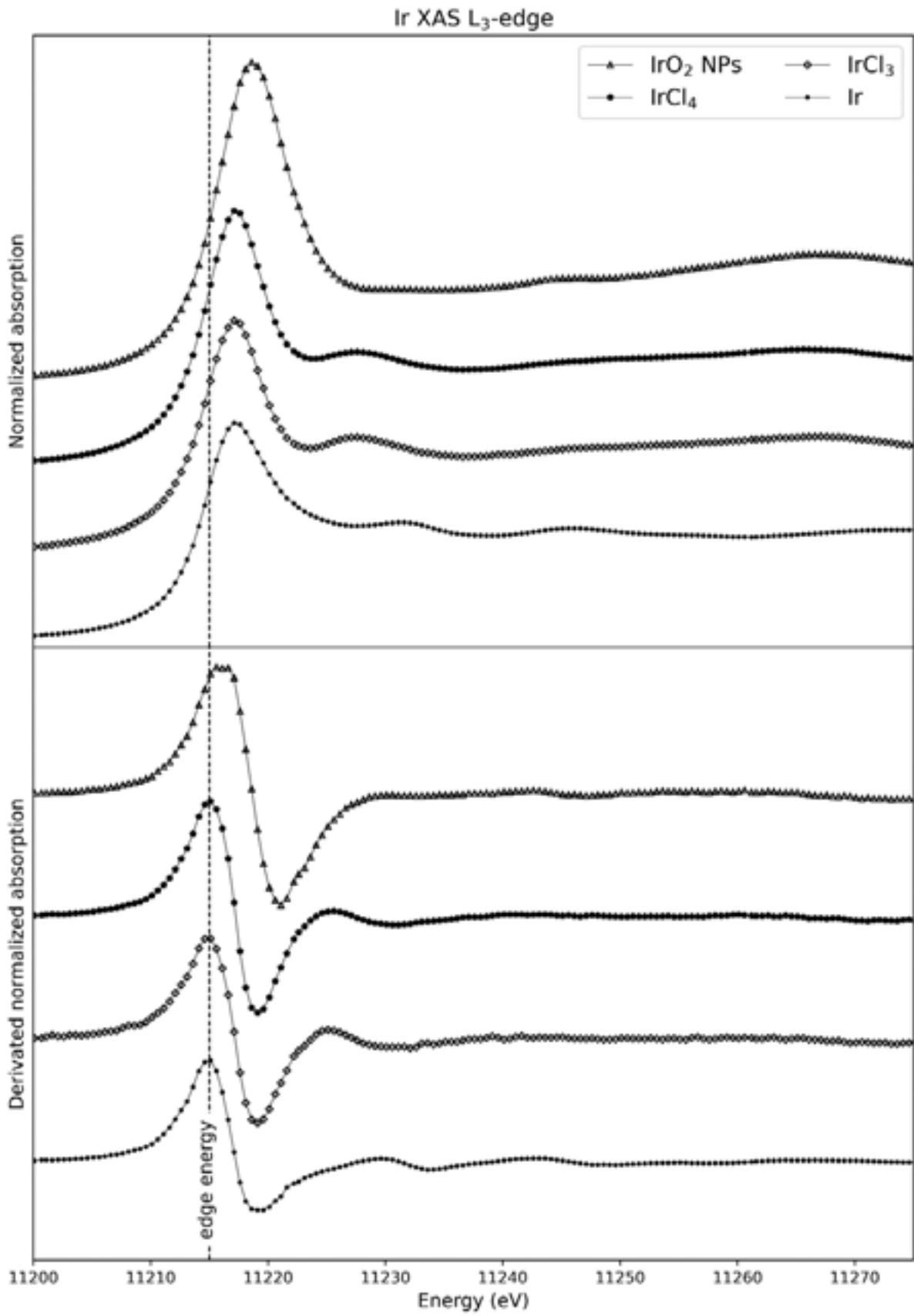
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	10.15	1.49
Si220	16.73	0.66

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si800	84.4
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge931	77.4
Si555	67.4

XAS Reference spectra



Z=78**Pt****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	11 564	9 442	11 071
Natural width	5.31	7.6	8.0

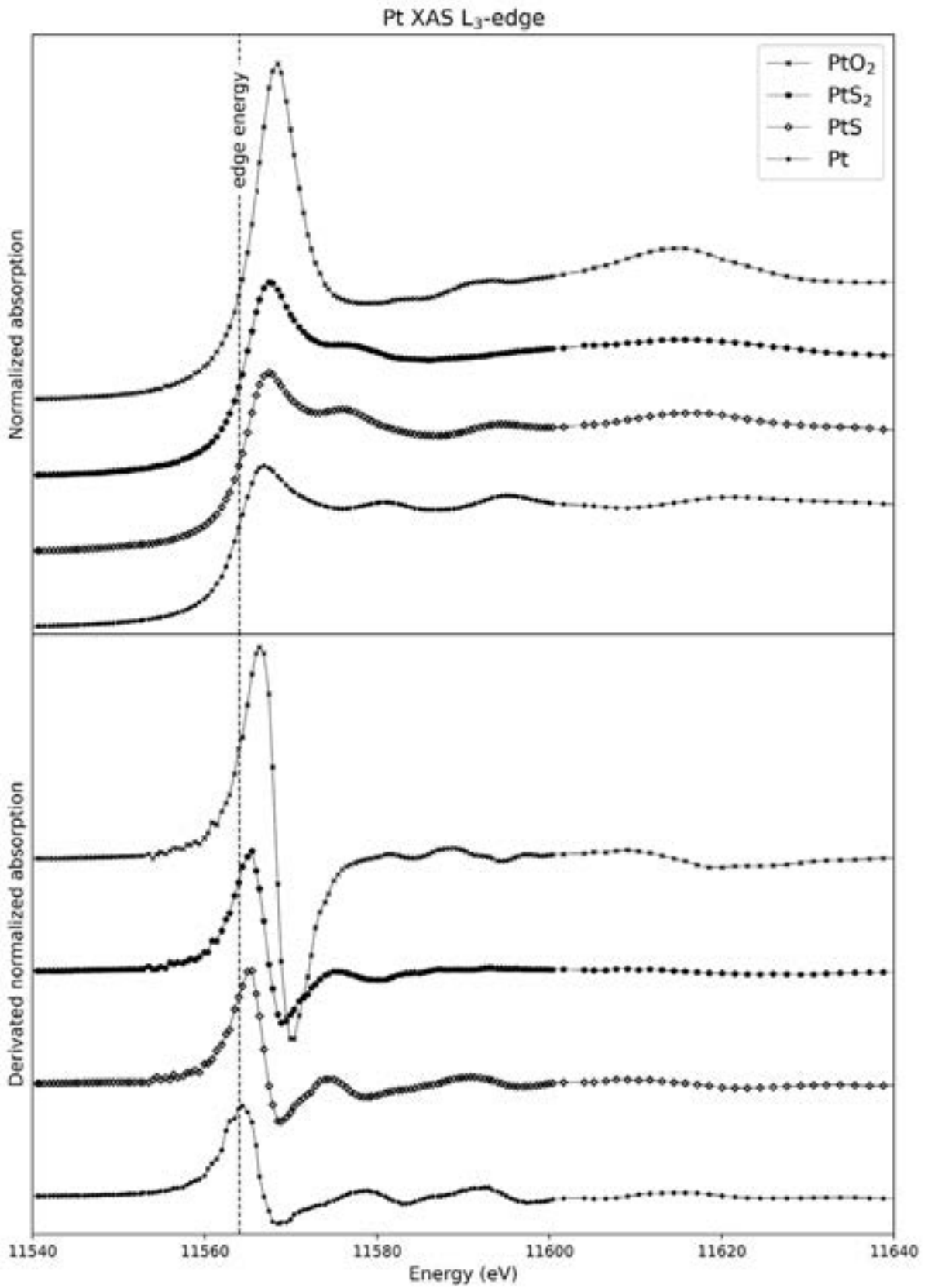
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	9.84	1.54
Si220	16.21	0.68

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge660	80.0
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si931	79.6
Ge844	77.8

XAS Reference spectra



Z=79**Au****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	11 919	9 713	11 443
Natural width	5.41	7.85	8.35

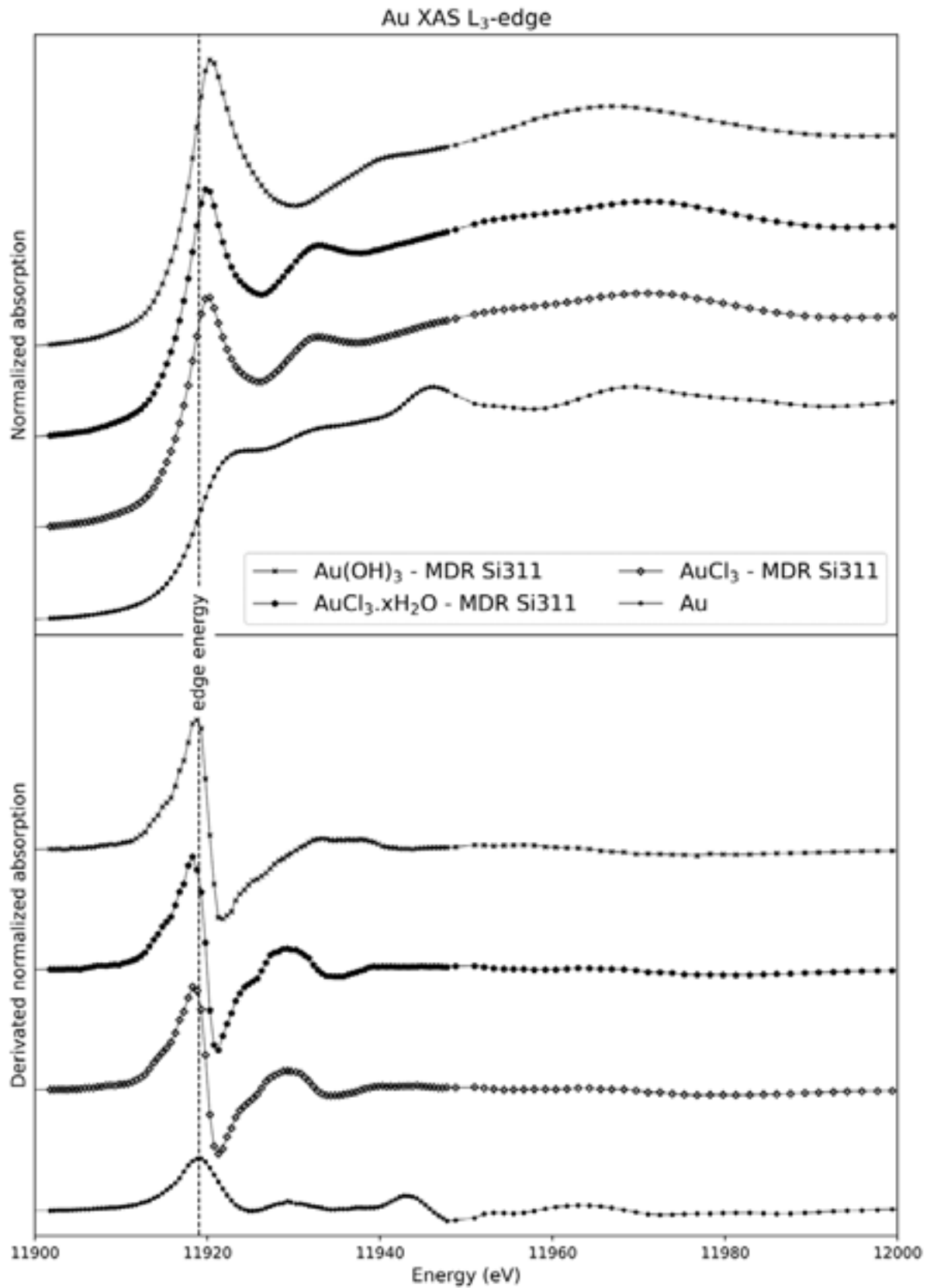
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	9.55	1.59
Si220	15.72	0.70

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si660	85.7
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si755	83.0
Si844	77.8

XAS Reference spectra



Z=80**Hg****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	12 284	9 989	11 824
Natural width	5.50	8.1	8.7

2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	9.26	1.63
Si220	15.24	0.72

Crystal Analyzer Spectrometer parameters

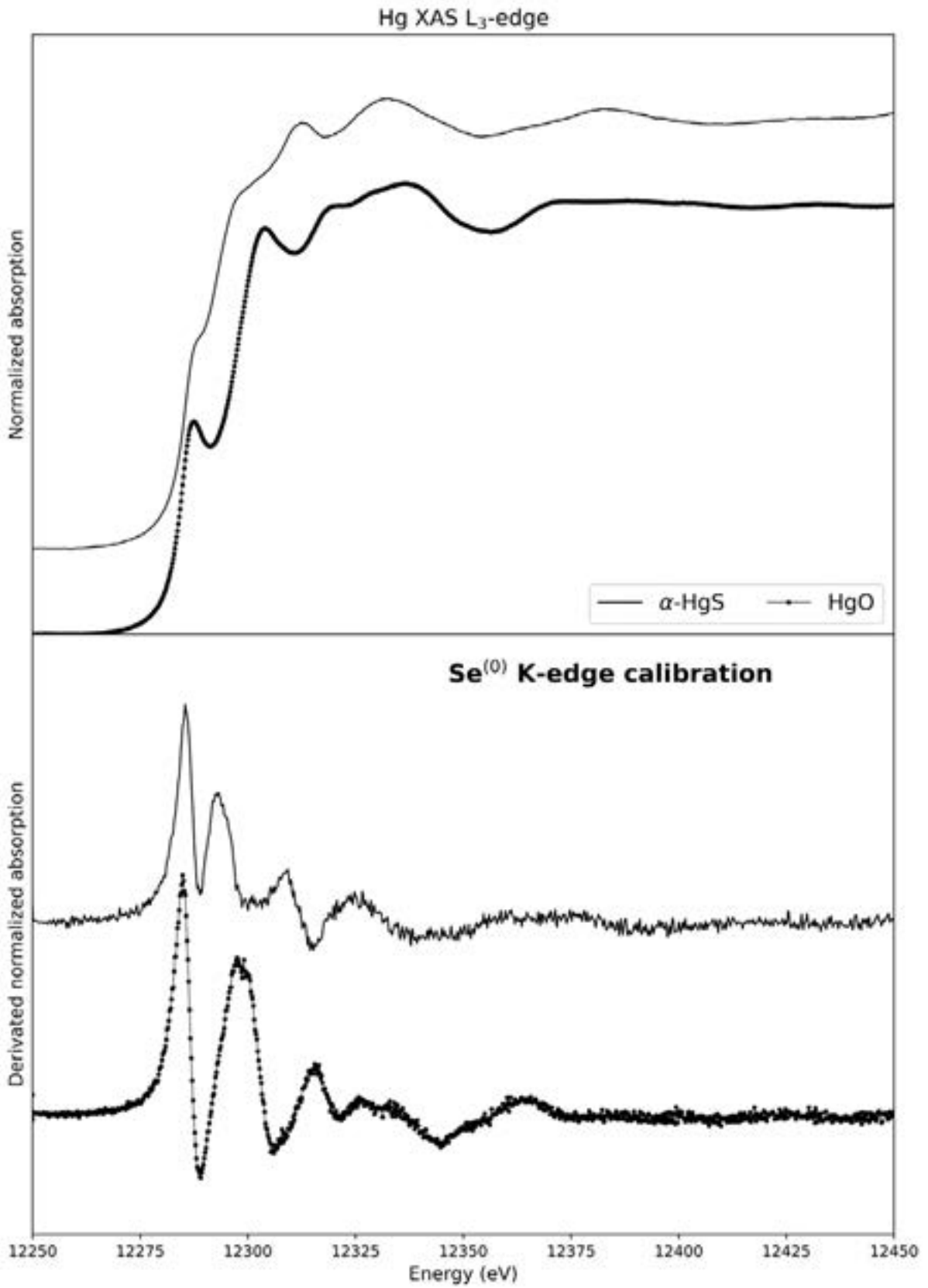
L _{α1} emission line	
Crystals	Bragg Angle (°)
Si555	81.7
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si951	87.0

Edges positions (eV)

Calibration	Hg ⁽⁰⁾	HgCl ₂	α-HgS	HgO
Au ⁽⁰⁾ L _{III} -edge		12 284.4 ^(a)	12 284.6 ^(a)	12 283.6 ^(a)
Hg ⁽⁰⁾ L _{III} -edge	12 284.0 ^(b)	12 284.5 ^(b)	12 284.6 ^(b)	
Se ⁽⁰⁾ K-edge			12 285.4	12 284.9

(a) [Riddle 2002] - (b) from [Colombo 2013]

XAS Reference spectra



Z=81**Tl****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	12 658	10 269	12 213
Natural width	5.65	8.46	9.03

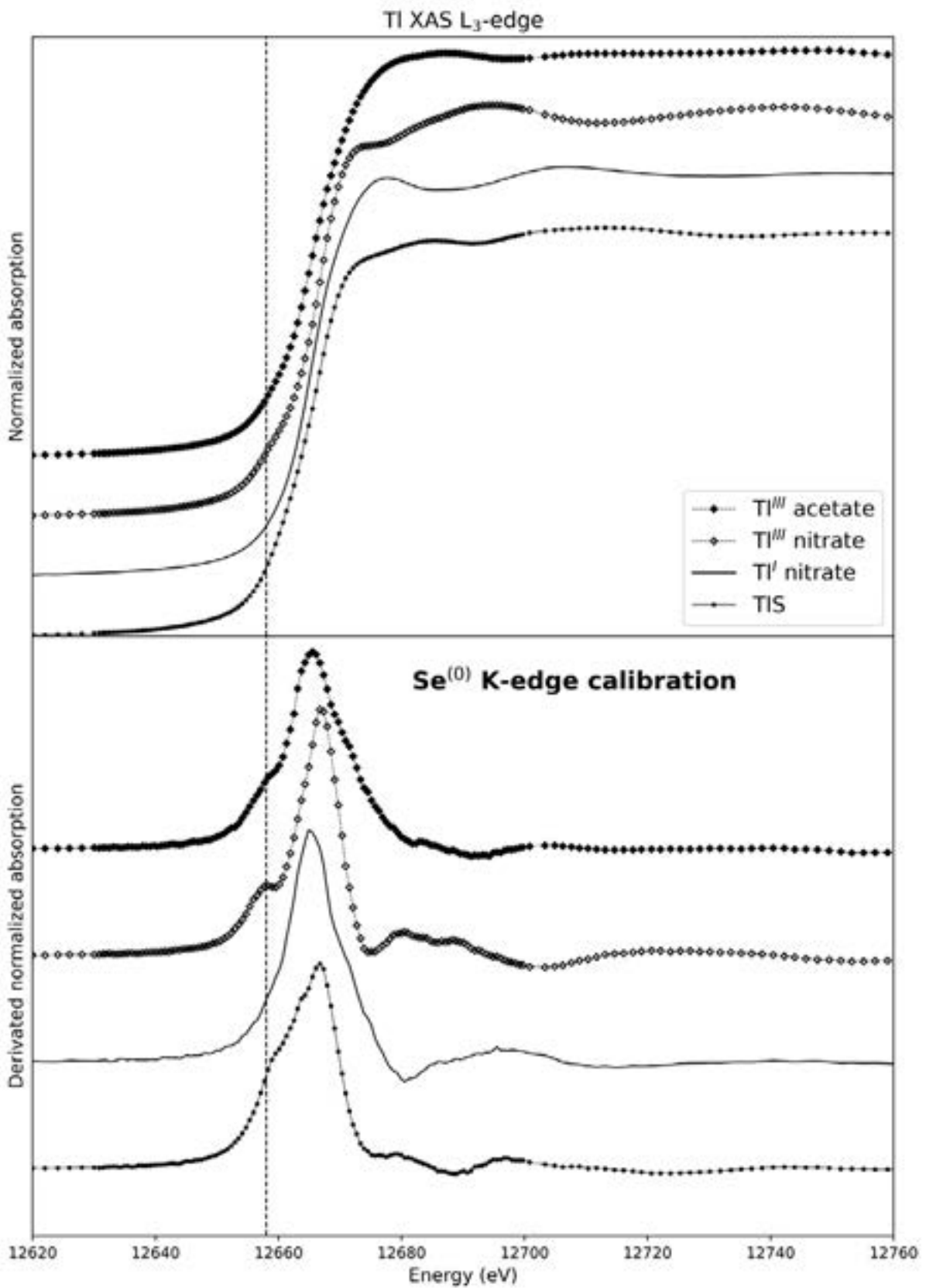
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	8.99	1.68
Si220	14.78	0.74

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si555	74.3
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si951	75.2

XAS Reference spectra



Z=82**Pb****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	13 035	10 551	12 601
Natural width	5.81	8.82	9.35

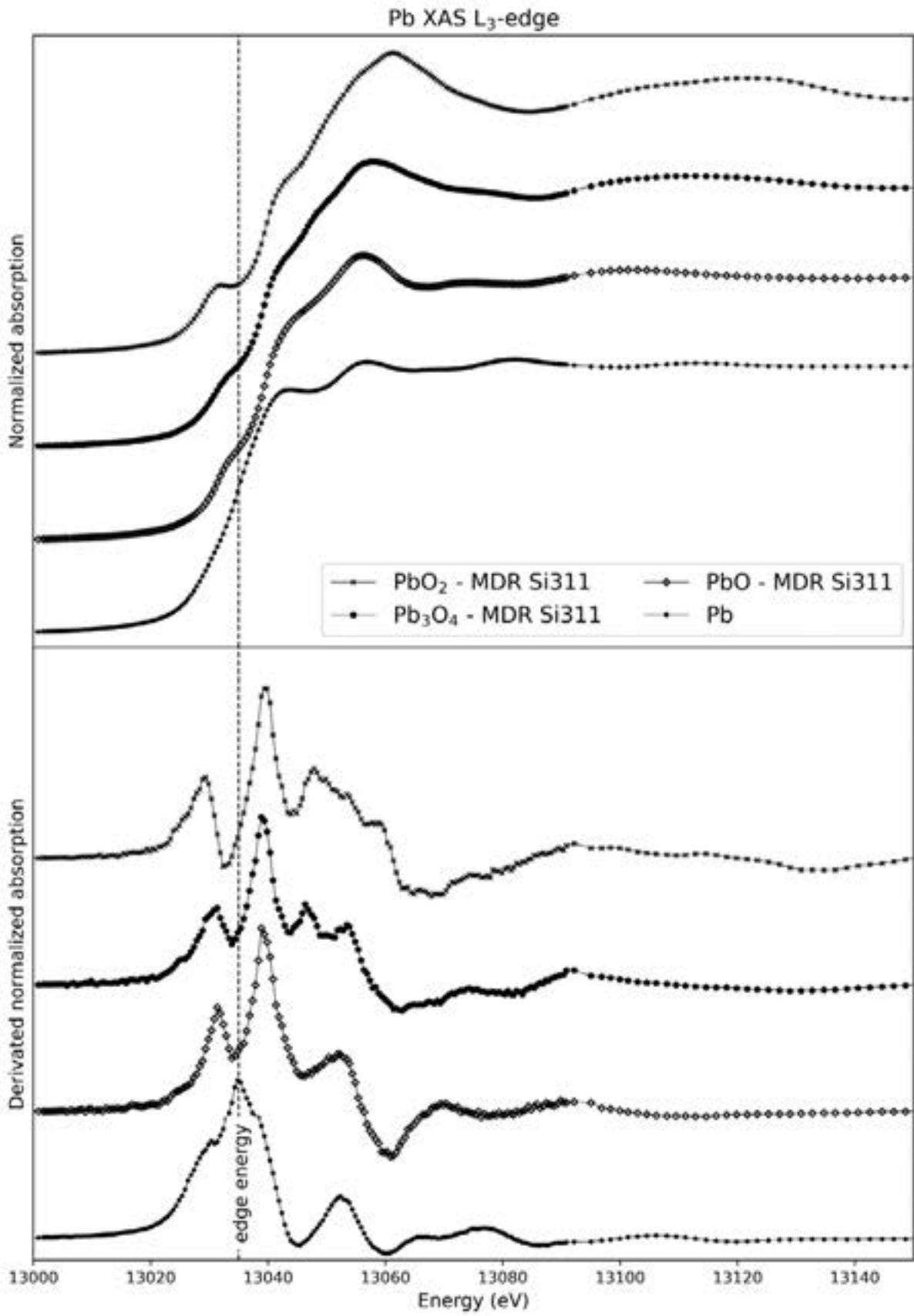
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	8.72	1.73
Si220	14.34	0.76

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Si555	69.5
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge880	79.3

XAS Reference spectra



Z=83**Bi****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	13 419	10 839	13 023
Natural width	5.98	9.16	9.73

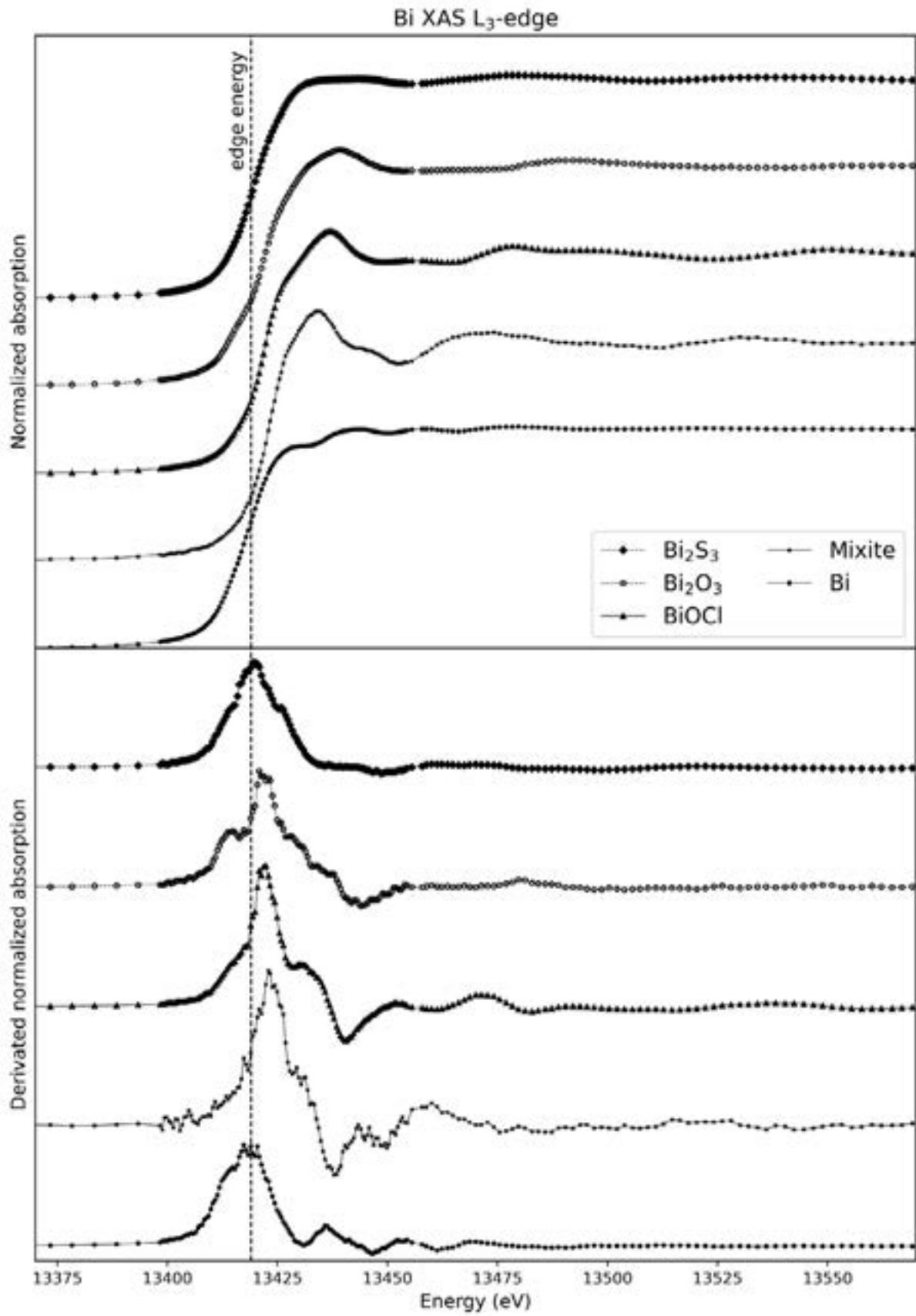
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	8.47	1.78
Si220	13.92	0.78

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge844	82.1
L _{β1} emission line	
Crystals	Bragg Angle (°)
Si880	82.6

XAS Reference spectra



Z=92**U****L-edges****Characteristic energies and natural width (eV)**

	L ₃ -edge	Emission lines	
		L _{α1} (L ₃ -M ₅)	L _{β1} (L ₂ -M ₄)
Energies	17 166	13 614	17 220
Natural width	7.43	12.4	13.5

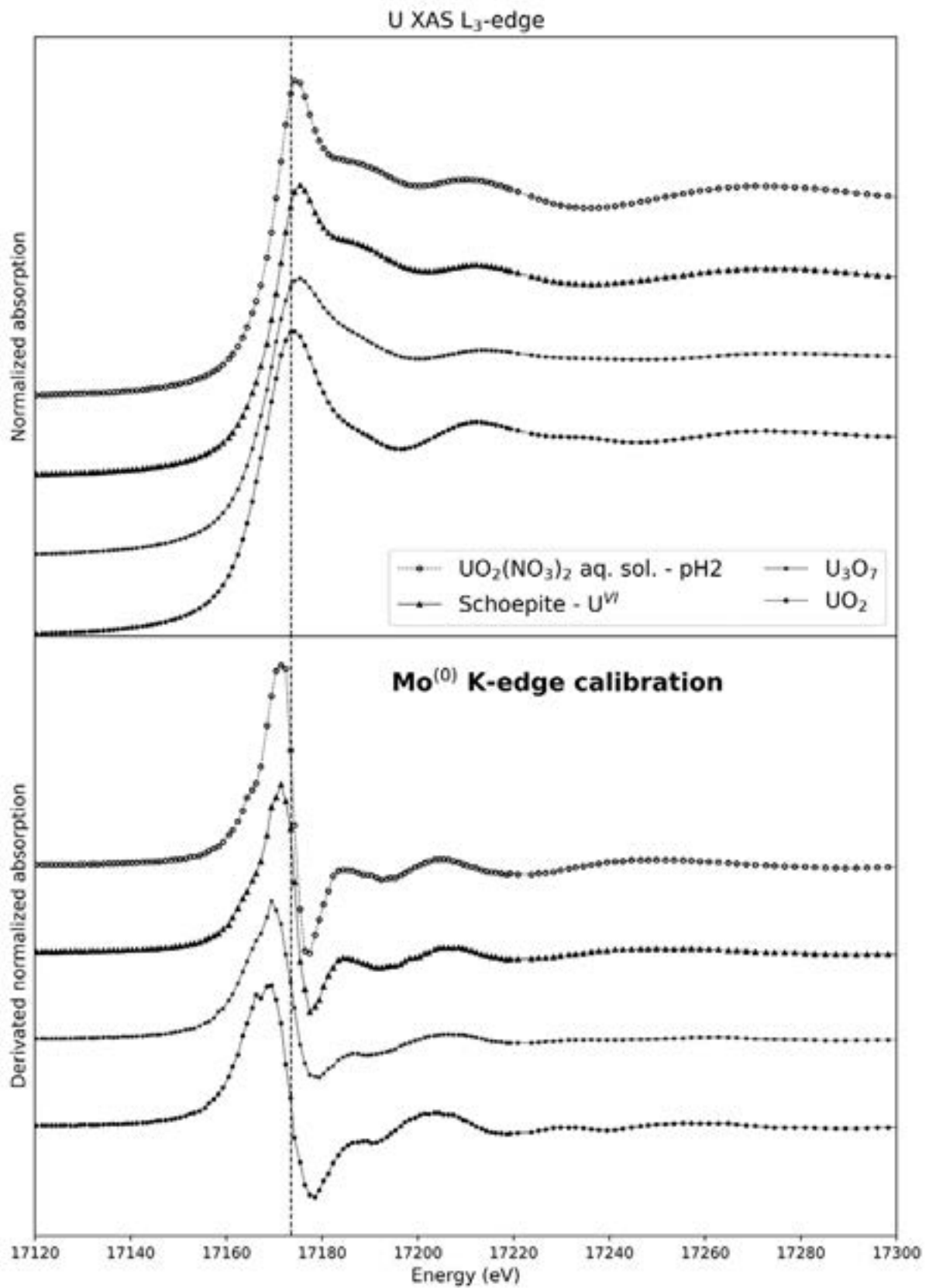
2-crystal monochromator parameters

Crystals	Bragg Angle (°)	Darwin Width (eV)
Si111	6.61	2.27
Si220	10.84	1.00

Crystal Analyzer Spectrometer parameters

L _{α1} emission line	
Crystals	Bragg Angle (°)
Ge777	77.4
L _{β1} emission line	
Crystals	Bragg Angle (°)
Ge999	82.7

XAS Reference spectra



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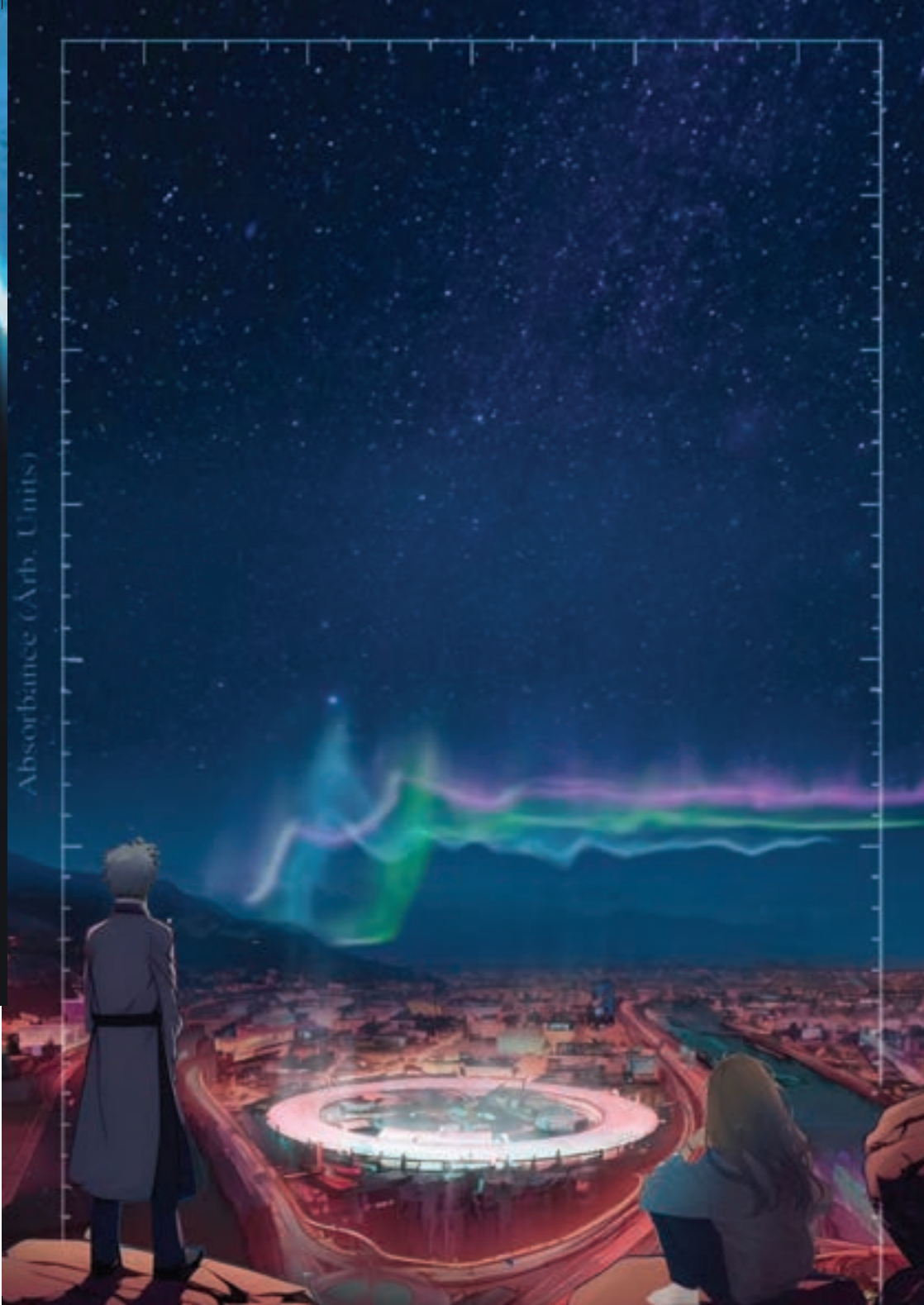
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Absorbance (Arb. Units)



1	1.0078	H	Hydrogen	2	4.0026	He	Helium
3	6.9410	Li	Lithium	5	10.811	B	Boron
4	9.0122	Be	Beryllium	6	12.011	C	Carbon
11	22.990	Na	Sodium	7	14.007	N	Nitrogen
12	24.305	Mg	Magnesium	8	16.000	O	Oxygen
19	39.098	K	Potassium	9	18.998	F	Fluorine
20	40.078	Ca	Calcium	10	20.180	Ne	Neon
21	44.956	Sc	Scandium	13	26.982	Al	Aluminum
22	47.882	Ti	Titanium	14	28.086	Si	Silicon
23	50.942	V	Vanadium	15	30.974	P	Phosphorus
24	51.996	Cr	Chromium	16	32.065	S	Sulfur
25	54.938	Mn	Manganese	17	35.453	Cl	Chlorine
26	55.945	Fe	Iron	18	39.948	Ar	Argon
27	58.933	Co	Cobalt	19	39.948	K	Potassium
28	58.933	Ni	Nickel	20	40.078	Ca	Calcium
29	63.927	Cu	Copper	21	68.926	Zn	Zinc
30	63.927	Ni	Nickel	22	68.926	Ga	Gallium
31	69.923	Zn	Zinc	23	72.640	Ge	Germanium
32	72.640	Ga	Gallium	24	72.640	As	Arsenic
33	74.922	Se	Selenium	25	74.922	Se	Selenium
34	78.972	Br	Bromine	26	78.972	Br	Bromine
35	78.972	Br	Bromine	27	78.972	Kr	Krypton
36	83.904	Kr	Krypton	28	83.904	Kr	Krypton
37	85.468	Rb	Rubidium	29	85.468	Kr	Krypton
38	87.62	Sr	Strontium	30	87.62	Kr	Krypton
39	88.906	Y	Yttrium	31	88.906	Kr	Krypton
40	90.907	Zr	Zirconium	32	90.907	Kr	Krypton
41	90.907	Zr	Zirconium	33	90.907	Kr	Krypton
42	90.907	Zr	Zirconium	34	90.907	Kr	Krypton
43	90.907	Zr	Zirconium	35	90.907	Kr	Krypton
44	90.907	Zr	Zirconium	36	90.907	Kr	Krypton
45	90.907	Zr	Zirconium	37	90.907	Kr	Krypton
46	90.907	Zr	Zirconium	38	90.907	Kr	Krypton
47	90.907	Zr	Zirconium	39	90.907	Kr	Krypton
48	90.907	Zr	Zirconium	40	90.907	Kr	Krypton
49	90.907	Zr	Zirconium	41	90.907	Kr	Krypton
50	90.907	Zr	Zirconium	42	90.907	Kr	Krypton
51	90.907	Zr	Zirconium	43	90.907	Kr	Krypton
52	90.907	Zr	Zirconium	44	90.907	Kr	Krypton
53	90.907	Zr	Zirconium	45	90.907	Kr	Krypton
54	90.907	Zr	Zirconium	46	90.907	Kr	Krypton
55	132.91	Ba	Barium	47	132.91	Ba	Barium
56	137.33	La	Lanthanum	48	137.33	Ba	Barium
57	138.91	Ce	Cerium	49	138.91	Ba	Barium
58	140.12	Pr	Praseodymium	50	140.12	Ba	Barium
59	140.91	Nd	Neodymium	51	140.91	Ba	Barium
60	141.90	Pm	Promethium	52	141.90	Ba	Barium
61	144.24	Sm	Samarium	53	144.24	Ba	Barium
62	150.36	Eu	Europium	54	150.36	Ba	Barium
63	151.96	Gd	Gadolinium	55	151.96	Ba	Barium
64	157.25	Tb	Terbium	56	157.25	Ba	Barium
65	162.50	Dy	Dysprosium	57	162.50	Ba	Barium
66	167.26	Ho	Holmium	58	167.26	Ba	Barium
67	168.93	Er	Erbium	59	168.93	Ba	Barium
68	168.93	Er	Erbium	60	168.93	Ba	Barium
69	168.93	Er	Erbium	61	168.93	Ba	Barium
70	168.93	Er	Erbium	62	168.93	Ba	Barium
71	168.93	Er	Erbium	63	168.93	Ba	Barium
72	168.93	Er	Erbium	64	168.93	Ba	Barium
73	168.93	Er	Erbium	65	168.93	Ba	Barium
74	168.93	Er	Erbium	66	168.93	Ba	Barium
75	168.93	Er	Erbium	67	168.93	Ba	Barium
76	168.93	Er	Erbium	68	168.93	Ba	Barium
77	168.93	Er	Erbium	69	168.93	Ba	Barium
78	168.93	Er	Erbium	70	168.93	Ba	Barium
79	168.93	Er	Erbium	71	168.93	Ba	Barium
80	168.93	Er	Erbium	72	168.93	Ba	Barium
81	168.93	Er	Erbium	73	168.93	Ba	Barium
82	168.93	Er	Erbium	74	168.93	Ba	Barium
83	168.93	Er	Erbium	75	168.93	Ba	Barium
84	168.93	Er	Erbium	76	168.93	Ba	Barium
85	168.93	Er	Erbium	77	168.93	Ba	Barium
86	168.93	Er	Erbium	78	168.93	Ba	Barium
87	223	Fr	Francium	88	223	Ra	Radium
88	226	Ra	Radium	89	227	Ac	Actinium
89	227	Ac	Actinium	90	227	Ac	Actinium

58	140.12	Ce	Cerium	68	168.93	Er	Erbium
59	140.91	Nd	Neodymium	69	168.93	Er	Erbium
60	141.90	Pm	Promethium	70	168.93	Er	Erbium
61	144.24	Sm	Samarium	71	168.93	Er	Erbium
62	150.36	Eu	Europium	72	168.93	Er	Erbium
63	151.96	Gd	Gadolinium	73	168.93	Er	Erbium
64	157.25	Tb	Terbium	74	168.93	Er	Erbium
65	162.50	Dy	Dysprosium	75	168.93	Er	Erbium
66	167.26	Ho	Holmium	76	168.93	Er	Erbium
67	168.93	Er	Erbium	77	168.93	Er	Erbium
68	168.93	Er	Erbium	78	168.93	Er	Erbium
69	168.93	Er	Erbium	79	168.93	Er	Erbium
70	168.93	Er	Erbium	80	168.93	Er	Erbium
71	168.93	Er	Erbium	81	168.93	Er	Erbium
72	168.93	Er	Erbium	82	168.93	Er	Erbium
73	168.93	Er	Erbium	83	168.93	Er	Erbium
74	168.93	Er	Erbium	84	168.93	Er	Erbium
75	168.93	Er	Erbium	85	168.93	Er	Erbium
76	168.93	Er	Erbium	86	168.93	Er	Erbium
77	168.93	Er	Erbium	87	168.93	Er	Erbium
78	168.93	Er	Erbium	88	168.93	Er	Erbium
79	168.93	Er	Erbium	89	168.93	Er	Erbium
80	168.93	Er	Erbium	90	168.93	Er	Erbium
81	168.93	Er	Erbium	91	168.93	Er	Erbium
82	168.93	Er	Erbium	92	168.93	Er	Erbium
83	168.93	Er	Erbium	93	168.93	Er	Erbium
84	168.93	Er	Erbium	94	168.93	Er	Erbium
85	168.93	Er	Erbium	95	168.93	Er	Erbium
86	168.93	Er	Erbium	96	168.93	Er	Erbium
87	168.93	Er	Erbium	97	168.93	Er	Erbium
88	168.93	Er	Erbium	98	168.93	Er	Erbium
89	168.93	Er	Erbium	99	168.93	Er	Erbium
90	168.93	Er	Erbium	100	168.93	Er	Erbium

K-edge / Z from 1 to 54



L_{III}-edge / Z from 55 to 95

