ASTRO-H

INSTRUMENT CALIBRATION REPORT
NATURAL LINE SHAPES
OF SXS ONBOARD CALIBRATION SOURCES
ASTH-SXS-CALDB-LINEFIT

Version 0.2

19 October 2016

ISAS/ GSFC

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CHANGE RECORD PAGE (1 of 1)

DOCUMENT TITLE: Natural Line Shapes of SXS Onboard Calibration Sources			
ISSUE	DATE	PAGES AFFECTED	DESCRIPTION
Version 0.1	March 2016	All	First Release
Version 0.2	Oct 2016	All	Fix minor errors in Mn Kα and Mg Kα lineshapes; correct center of mass values for three line complexes

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Introduction

1.1 Purpose

This document describes the natural line shapes of the characteristic x-ray radiation produced by the SXS onboard calibration sources. These include Mn Kα and Kβ lines from the ^{55}Fe sources on the filter wheel and the small source directed at the calibration pixel, Cr and Cu lines produced by the direct modulated x-ray source (MXS), and Al and Mg lines produced by the indirect (fluorescent) MXS. These complexes will be used to calibrate the SXS energy scale and to monitor the SXS line-spread function.

1.2 Scientific Impact

The natural line shapes described in this CALDB file are used by the task `sxsgain` while fitting the calibration lines to determine the SXS gain scale as a function of time.

2 Release CALDB 20161122

Filename	Valid data	Release data	CALDB Vrs	Comments
ah_gen_linefit_20140101v002.fits	2014-01-01	20161122	005	Minor corrections to Mn Kα and Mg Kα lineshapes and center of mass values for three line complexes

2.1 Data Description and Data Analysis

Please see Section 3.1 for an overview.

2.2 Results

The CALDB file contains the parameters used to calculate each line complex (E_0, FWHM, and amplitude) and the center of mass value for each line complex. Tables 1–3 provide the updated/corrected values contained in CALDB 20161122; the full set of original parameters is provided in Section 3.2.

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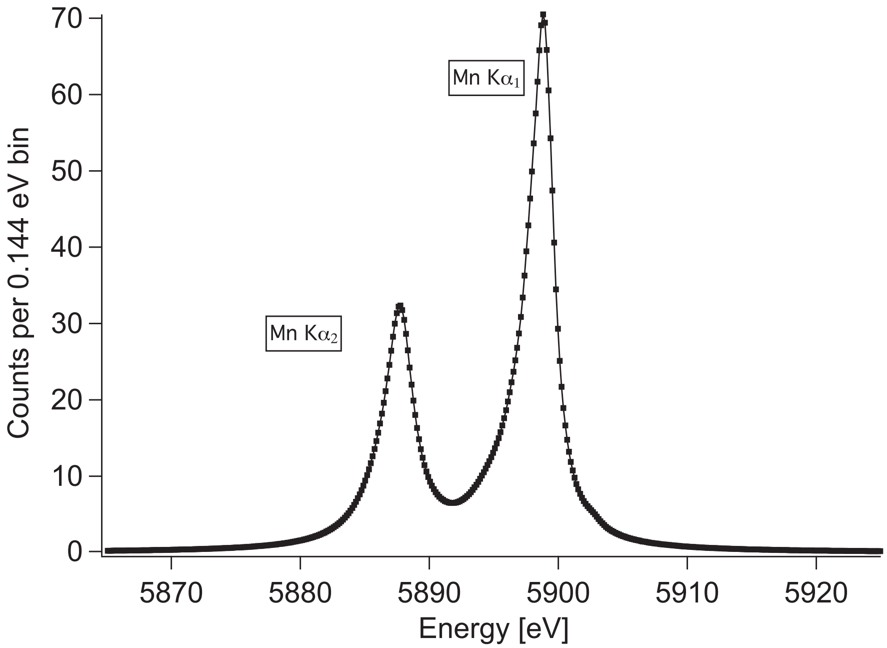
Extension 1: Mn Kα complex – Produced by the ^{55}Fe sources

Eight-Lorentzian model based on re-fit of Holzer's deconvolved spectrum: The seven-Lorentzian model from Holzer et al. (1997) had a few errors that were discussed by Holzer and Porter (private communication, 1997). The modifications include the addition of $K\alpha_{16}$ line (row 6 in Table 1); a change in the intensity of the $K\alpha_{15}$ line (row 5; the intensity given in Holzer et al. (1997) is wrong by a factor of ten), and change of the intensity of the $K\alpha_{22}$ line (row 8) to 0.1 (fixing a typo). In the previous version of the CALDB we provided the Holzer et al. (1997) data plus those corrections (see Table 4). But in fact we should have been using the below table instead, based upon a full re-fit of Holzer's deconvolved spectrum. The fit was performed by F. S. Porter on 11/30/2014, and the resulting natural line shape has been used by the GSFC calorimeter group since then.



	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	5898.882	1.7145	0.784	0.3523
2	5897.898	2.0442	0.263	0.1409
3	5894.864	4.4985	0.067	0.07892
4	5896.566	2.6616	0.095	0.06624
5	5899.444	0.97669	0.071	0.01818
6	5902.712	1.5528	0.011	0.004475
7	5887.772	2.3604	0.369	0.2283
8	5886.528	4.2168	0.1	0.1106

Table 1 Lorentzian coefficients for the Mn Kα complex.

Mn Kα center of mass = 5894.40 eV

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Extension 9: Mg Kα_{12} – Produced by the indirect (fluorescent) MXS

Line positions from Schweppe et al. (1994). Literature values for Ka_1 and Ka_2 line widths range from 0.33 to 0.54 eV FWHM (see Schweppe et al. (1994), Perkins et al. (1991), and Klauber (1992)); here we use the line widths referenced in Schweppe et al.

	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	1253.69	0.36	1	0.666667
2	1253.44	0.36	0.5	0.333333

Table 2 Lorentzian coefficients for Mg Kα_{12} complex

Mg Kα center of mass = 1253.6 eV

Center of Mass Updates:

Finally, we provide updates to a few of the center of mass values, which had minor errors in the previous release of the CALDB. In previous versions of `sxsgain` these values were used in calculating the effective temperature; in the current version of `sxsgain` these values are not used (the center of mass for the given binning is calculated internal to the task), but we provide the values in the CALDB file header for reference.

Line Complex	Center of Mass [eV]	Extension	Comments
Mn Kα	5894.40	1	This is the center of mass value for the updated line shape provided in Table 1. The center of mass value for the line shape provided in CALDB 20160310 (Table 4) was also incorrect. Using that line-shape, the value should have been 5894.37 eV (not 5894.62 eV).
Mn Kβ	6486.38	2	
Cu Kβ	8904.75	6	

Table 3 Corrected center of mass values for the line complexes that required updates compared to CALDB 20160310. These values are provided as keywords in the appropriate extension.

2.3 Changes from last release

This version has minor changes to the Mn Kα (Extension 1) and Mg Kα (Extension 9) line-shape tables. In addition, we have corrected the center of mass values for Mn Kα, Mn Kβ and Cu Kβ line complexes.

3 Release CALDB 20160310

Filename	Valid data	Release data	CALDB Vrs	Comments
ah_gen_linefit_20140101v001.fits	2014-01-01	20160310	001	original filename: LineShapes_v2.pdf

3.1 Data Description and Data Analysis

The line shapes are derived from the literature; corresponding references are given in Section 3.2.

Each line complex is described as a sum of Lorentzians, or, in a few cases, as a single Lorentzian. The individual Lorentzians are given by A/(1+(2*(E–E_0)/FWHM)^2), where A is the amplitude, E_0 is the centroid in eV, and FWHM is the full-width-at-half-maximum width in eV.

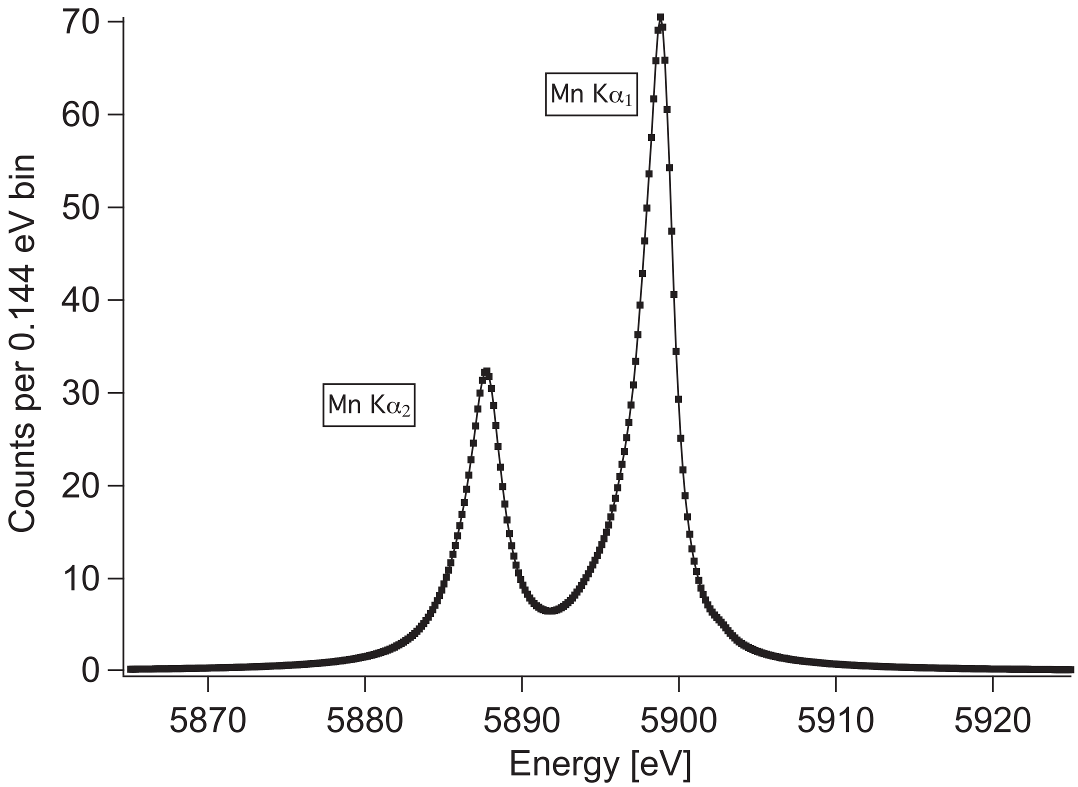
3.2 Results

The CALDB file contains the parameters used to calculate each line complex (E_0, FWHM, and amplitude). There is a separate extension for each line complex. For most complexes we also provide an “Area” column that provides the relative areas contributed by each Lorentzian component, for reference.

The following pages list the line complexes in the order given in the CALDB file.

Extension 1: Mn Kα complex – Produced by the ^{55}Fe sources

Eight-Lorentzian model: seven-Lorentzian model from Holzer et al. (1997) with modifications based on Holzer and Porter (private communication, 1997). The modifications include the addition of $K\alpha_{16}$ line (row 6 in Table 4); a change in the intensity of the $K\alpha_{15}$ line (row 5; the intensity given in Holzer et al. (1997) is wrong by a factor of ten), and change of the intensity of the $K\alpha_{22}$ line (row 8) to 0.1 (fixing a typo).



	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	5898.853	1.715	0.790	0.353
2	5897.867	2.043	0.264	0.141
3	5894.829	4.499	0.068	0.079
4	5896.532	2.663	0.096	0.066
5	5899.417	0.969	0.0714	~0.05
6	5902.712	1.5528	0.0106	
7	5887.743	2.361	0.372	0.229
8	5886.495	4.216	0.1	0.110

Table 4 Lorentzian coefficients for the Mn Kα complex.

Mn Kα center of mass = 5894.62 eV

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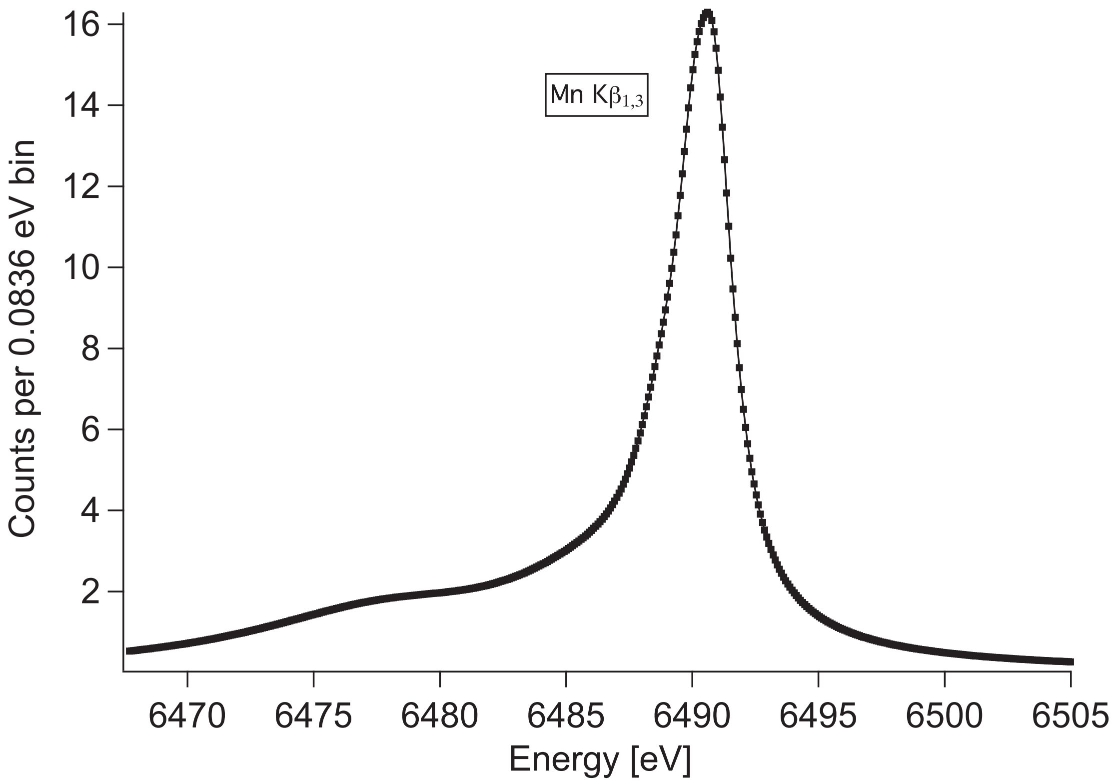
Extension 2: Mn Kβ complex – Produced by the ^{55}Fe sources

Five-Lorentzian model from Holzer et al. (1997).



	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	6490.89	1.83	0.608	0.254
2	6486.31	9.4	0.109	0.234
3	6477.73	13.22	0.077	0.234
4	6490.06	1.81	0.397	0.164
5	6488.83	2.81	0.176	0.114

Table 5 Lorentzian coefficients for the Mn Kβ complex

Mn Kβ center of mass = 6486.37 eV

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Extension 3: Cr Kα complex – Produced by the direct MXS

Seven-Lorentzian model from Holzer et al. (1997).
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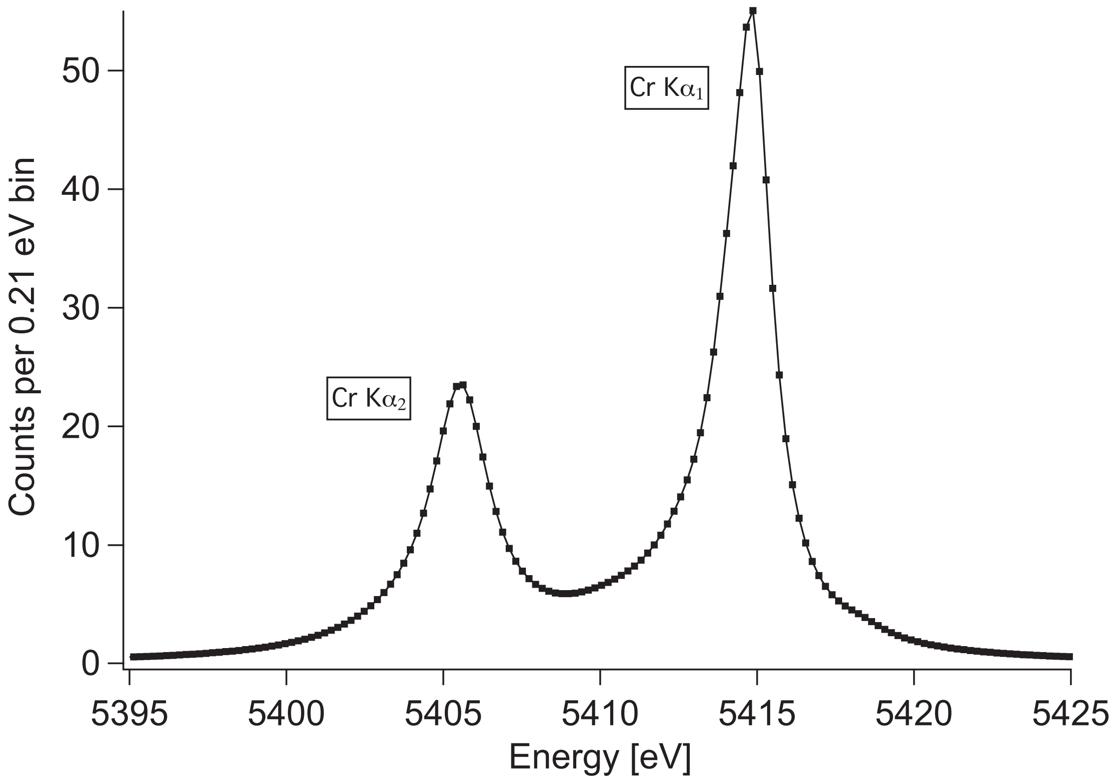


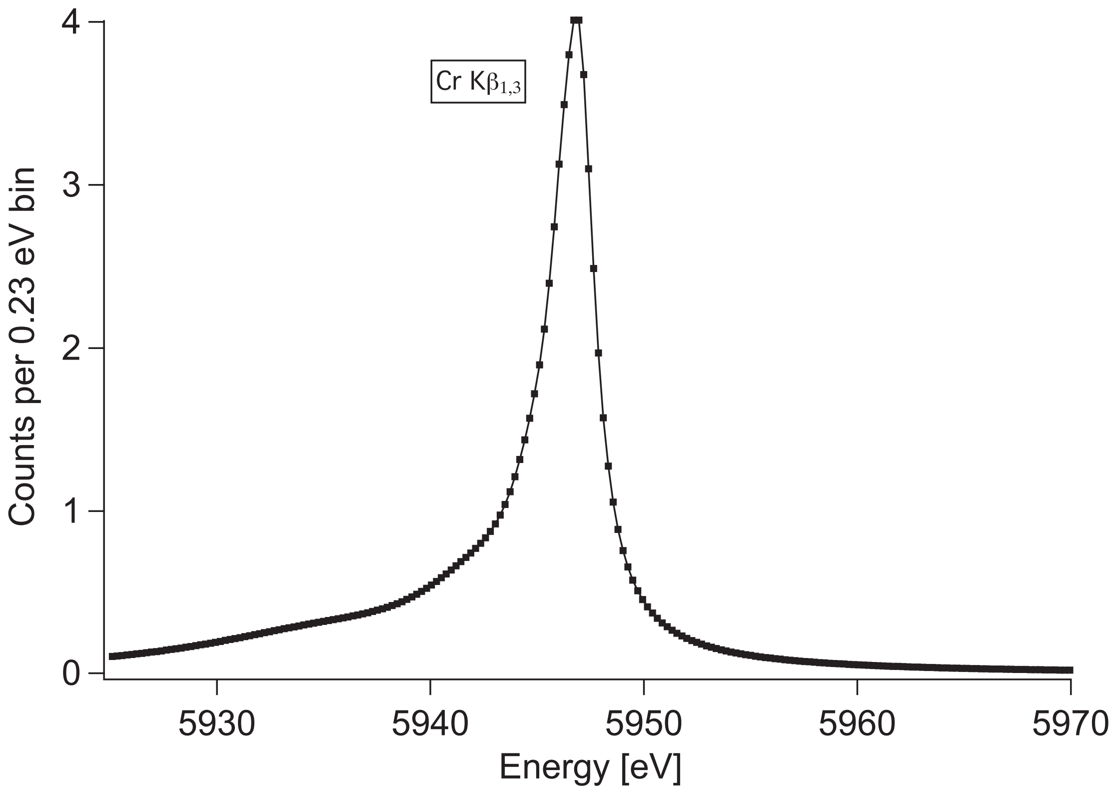
	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	5414.874	1.457	0.822	0.378
2	5414.099	1.760	0.237	0.132
3	5412.745	3.138	0.085	0.084
4	5410.583	5.149	0.045	0.073
5	5418.304	1.988	0.015	0.009
6	5405.551	2.224	0.386	0.271
7	5403.986	4.740	0.036	0.054

Table 6 Lorentzian coefficients for Cr Kα complex

Cr Kα center of mass = 5411.20 eV

Extension 4: Cr Kβ complex – Produced by the direct MXS

Five-Lorentzian model from Holzer et al. (1997).



	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	5947.00	1.70	0.670	0.307
2	5935.31	15.98	0.055	0.236
3	5946.24	1.90	0.337	0.172
4	5942.04	6.69	0.082	0.148
5	5944.93	3.37	0.151	0.137

Table 7 Lorentzian coefficients for Cr Kβ complex

Cr Kβ center of mass = 5943.09 eV

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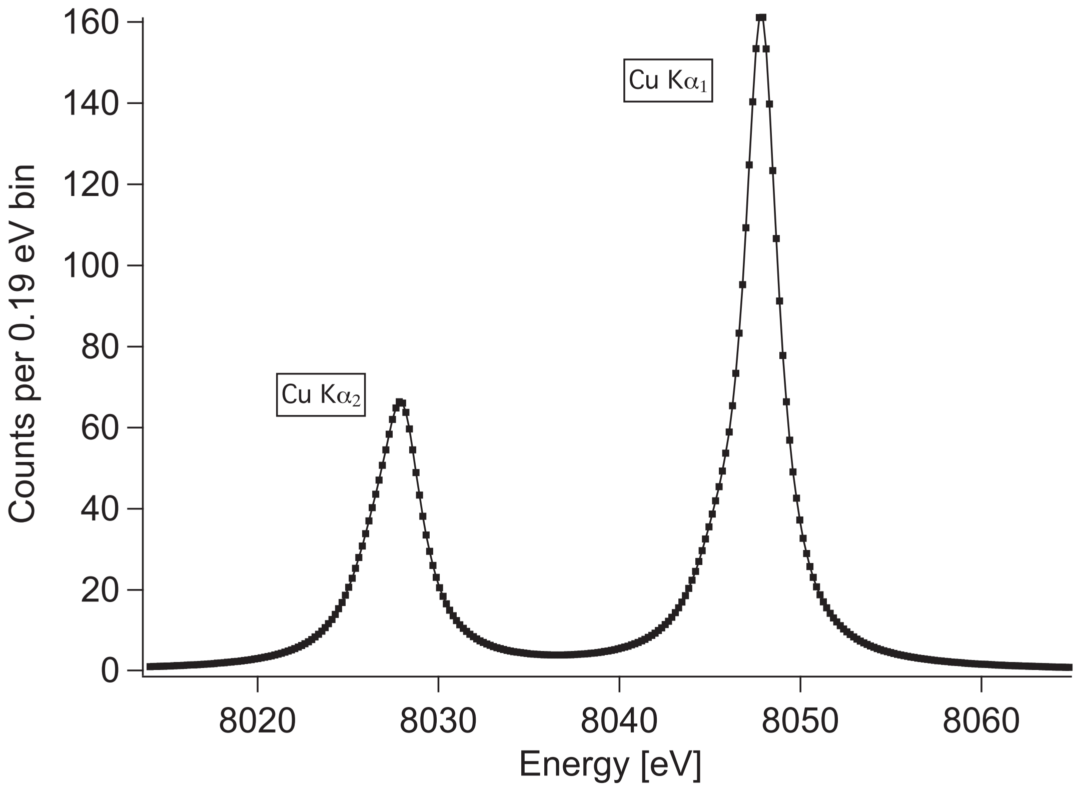
Extension 5: Cu Kα complex – Produced by the direct MXS

Four-Lorentzian model from Holzer et al. (1997).



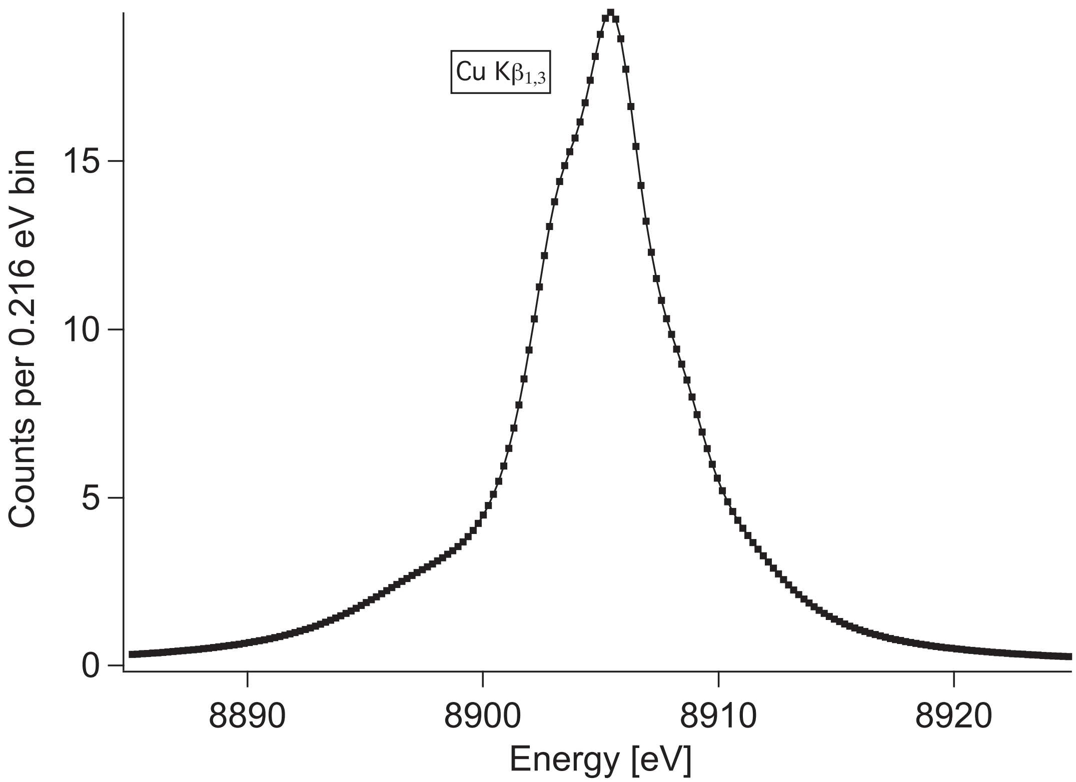
	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	8047.837	2.285	0.957	0.579
2	8045.367	3.358	0.090	0.080
3	8027.993	2.666	0.334	0.236
4	8026.504	3.571	0.111	0.105

Table 8 Lorentzian coefficients for Cu Kα complex

Cu Kα center of mass = 8040.72 eV

Extension 6: Cu Kβ complex – Produced by the direct MXS

Five-Lorentzian model from Holzer et al. (1997).



	E_0 [eV]	FWHM [eV]	Amplitude	Area
1	8905.532	3.52	0.757	0.485
2	8903.109	3.52	0.388	0.248
3	8908.462	3.55	0.171	0.110
4	8897.387	8.08	0.068	0.100
5	8911.393	5.31	0.055	0.055

Table 9 Lorentzian coefficients for Cu Kβ complex

Cu Kβ center of mass = 8904.76 eV

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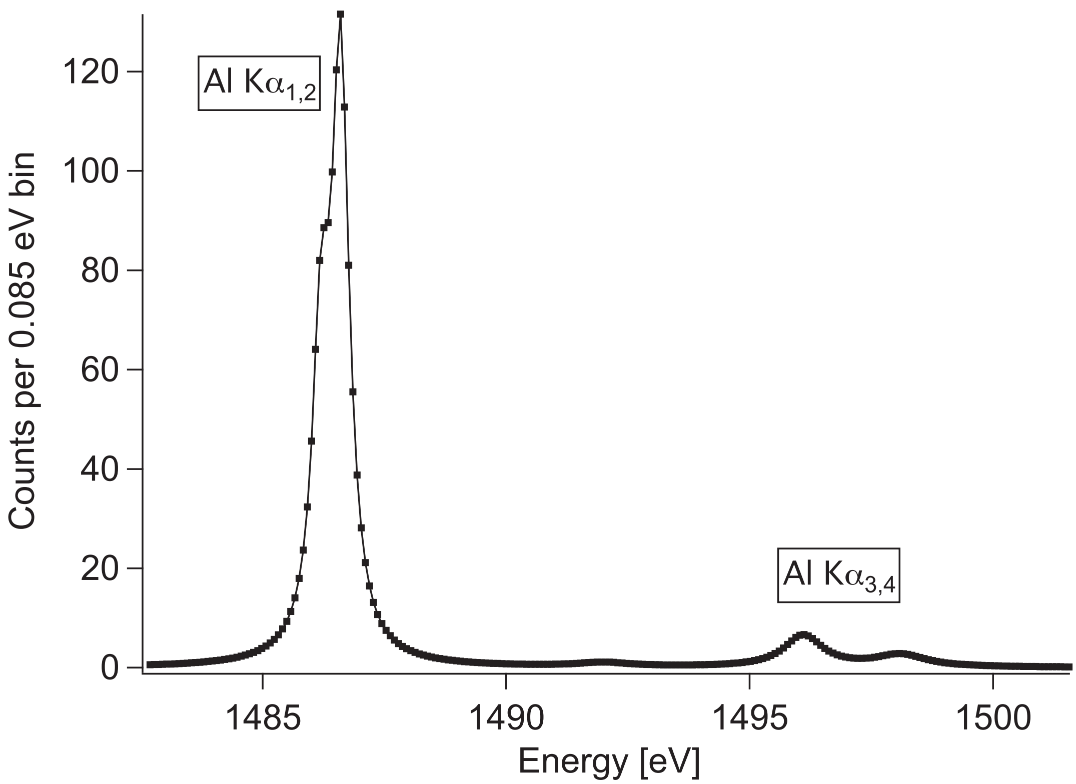
Extension 7: Al Kα complex – Produced by the indirect (fluorescent) MXS

Line positions from Fischer and Baun (1965). Line widths for Al $K\alpha_1$ and $K\alpha_2$ (rows 1 and 2) from Krause and Oliver (1979); widths for Al $K\alpha_3$ and $K\alpha_4$ (rows 4 and 5) from Nordfors (1955).



	E_0 [eV]	FWHM [eV]	Amplitude
1	1486.9	0.43	1
2	1486.5	0.43	0.5
3*	1496.4	0.96	0.05375
4*	1498.4	1.252	0.04121
5*	1492.3	1.34	0.03851

Table 10 Lorentzian coefficients for Al Kα complex

Al Kα12 center of mass = 1486.77 eV

* The literature values of the non-diagram lines (Kα', $K\alpha_3$, $K\alpha_4$) are given for reference only. Because these lines change based on details of the x-ray generator, the lines produced by the MXS will likely be slightly different from the values in Table 10. If fitting for gain or line-spread function parameters, we suggest using $K\alpha_{12}$ only (rows 1 and 2).

Extension 8: Al Kβ complex – Produced by the indirect (fluorescent) MXS

Line positions from Bearden et al. (1967).

	E_0 [eV]	FWHM [eV]	Amplitude
1	1557.4	0.5*	1

Table 11 Lorentzian coefficient for Al Kβ complex

Extension 9: Mg $K\alpha_{12}$ – Produced by the indirect (fluorescent) MXS

Line position and width from Schweppe et al. Because $K\alpha_1$ and $K\alpha_2$ are only 0.25 eV apart, we model them as a single Lorentzian.

	E_0 [eV]	FWHM [eV]	Amplitude
1	1253.6	0.36	1

Table 12 Lorentzian coefficients for Mg $K\alpha_{12}$ complex

Not incorporated in CALDB file: Mg Kβ – Produced by the indirect (fluorescent) MXS

Line positions from Bearden et al. (1967).

	E_0 [eV]	FWHM [eV]	Amplitude
1	1302.2	0.4*	1

Table 13 Lorentzian coefficients for Mg Kβ complex

*Note: there is no reference for this width, so this is our best estimate based on the width of Mg Kα.

3.3 Final Remarks

This is the first official release of this document.

4 References

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[8] J. Schweppe, R.D. Deslattes, T. Mooney, and C.J. Powell. *Electron Spectrosc. Relat. Phenom.,* **67,** 463 (1994).

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