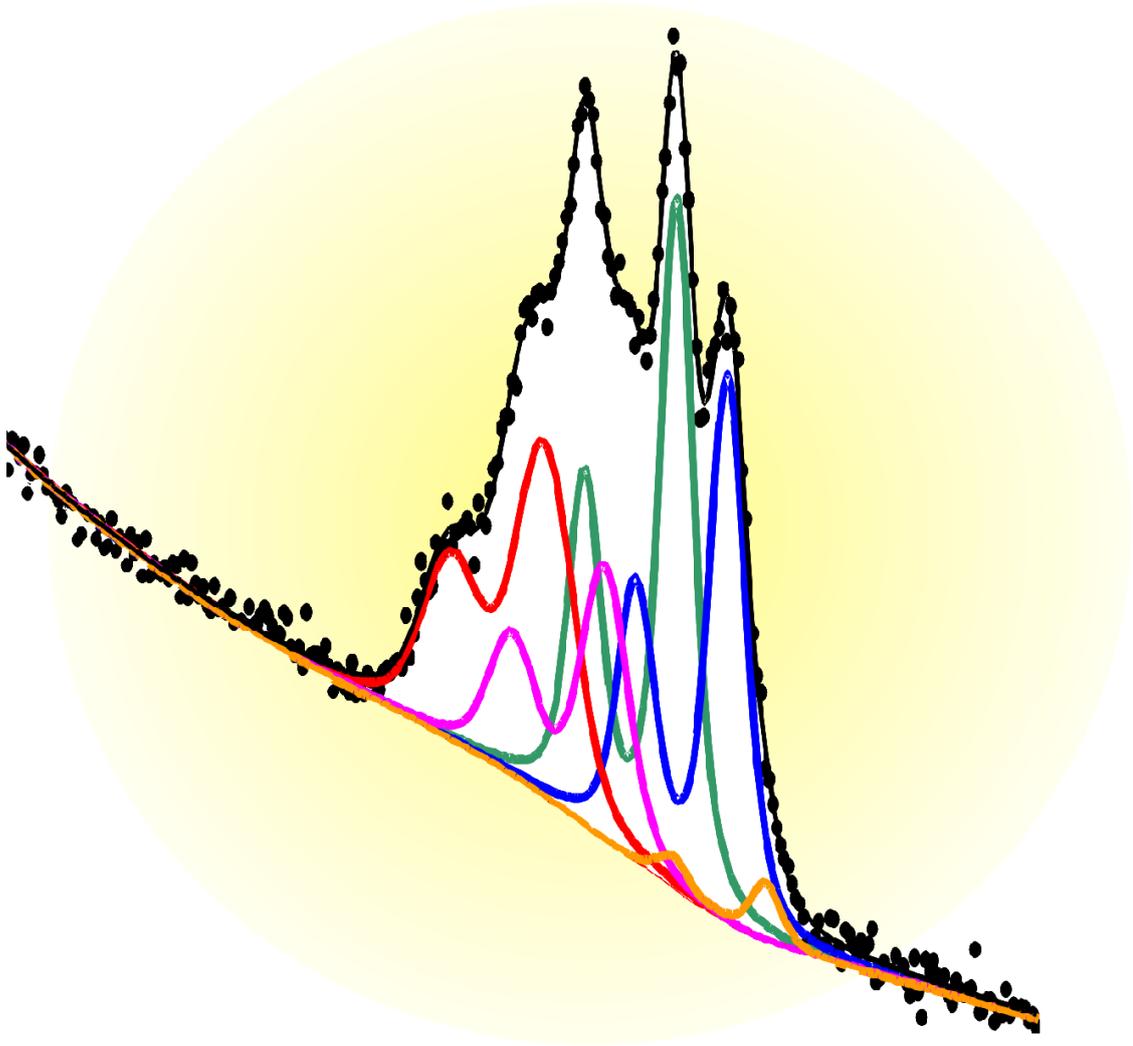


# unifit FOR WINDOWS



Line Positions and Data Formats

Version 2024



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Unifit for Windows

Data Formats

Version 2024

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## Content

<b>1</b>	<b>Line positions .....</b>	<b>8</b>
<b>2</b>	<b>Auger Parameters .....</b>	<b>48</b>
<b>3</b>	<b>Experimental Files .....</b>	<b>53</b>
3.1	XPS Data .....	53
3.1.1	ESCALAB Eclipse (*.TAP;*.TXT) .....	53
3.1.2	ESCALB/K-ALPHA Avantage (*.AVG).....	61
3.1.3	ESCA3 (*.TAP).....	63
3.1.4	BESSY (*.*).....	64
3.1.5	VSI (*.GPH).....	65
3.1.6	HHUD (*.DAT).....	67
3.1.7	CAF (*.CAF).....	68
3.1.8	KRATOS (*.CIL) .....	68
3.1.9	PHI-5400/PHI-5600 (*.INF), (*.ASC) .....	69
3.1.10	PHI-545/590 .....	74
3.1.10.1	Single Region (*.TXT).....	74
3.1.10.2	Multiregion (*.TXT) .....	74
3.1.10.3	Profile (*.TXT).....	75
3.1.11	PHI-1600/1600C .....	77
3.1.11.1	Standard Format, Version 1 (*.csv).....	77
3.1.11.2	Standard Format, Version 2 (*.csv).....	79
3.1.11.3	Parameter Dependent Measurement (Depth Profile) (*.CSV) .....	80
3.1.12	VGX-900 (*.1) .....	82
3.1.13	VAMAS.....	83
3.1.13.1	Standard Format (*.VMS;*.NPL) .....	83
3.1.13.2	Parameter Dependent Measurement (Depth Profile) (*.VMS) .....	91
3.1.13.3	Multipoint Measurement (Area Scan) (*.VMS).....	98
3.1.14	NPL (*.NPL) .....	106
3.1.15	SPECSLAB (*.EXP) .....	108
3.1.16	VSW-Tübingen (*.DAT).....	122
3.1.17	VGS2000 (*.XPS).....	123
3.1.18	ScientaSES-Signals (*.txt) .....	124
3.1.19	ScientaSES-Spectra (*.txt) .....	126
3.1.20	PHI Spectrometer .....	127
3.1.20.1	Multiregion Measurements (*.spe).....	127
3.1.20.2	PHI Spectrometer/Profile (*.pro) .....	159
3.1.20.3	PHI Spectrometer/Angle Resolved Profile (*.ang) .....	181
3.1.2321		
0.4	PHI Spectrometer/Mapping (*.map) .....	188
3.1.21	Focus CSA (*.dat) .....	193
3.1.22	Croissant (*.pesp).....	195
3.1.23	SSI-XPS (*.mrs).....	196
3.1.24	SPECS Phoibos225/Prodigy (*.xy).....	201
3.1.25	Energy-Intensity (*.dat).....	206

3.1.26	HTW-Berlin (*.dat) .....	208
3.2	XAS Data .....	209
3.2.1	NEXAFS (*.dat) .....	209
3.2.2	BESSY-EMP/2 (*.*) .....	209
3.2.3	MAXlab Scan Zeiss (*.sp7) .....	210
3.2.4	Lausanne-NanoLab (*.txt) .....	211
3.2.5	SPECS Prodigy (*.xy) .....	212
3.2.6	Photon Energy/Intensity (*.dat) .....	215
3.3	AES Data .....	216
3.3.1	VAMAS (*.vms) .....	216
3.3.2	PHI Spectrometer .....	221
3.3.2.1	Multiregion Measurements (*.spe) .....	221
3.3.2.2	PHI Spectrometer/Profile (*.pro) .....	223
3.3.2.3	PHI Spectrometer/Mapping (*.map) .....	224
3.4	RAMAN Data .....	225
3.4.1	S_I VistaControl (*.tvf) .....	225
3.4.2	S_I VistaControl XY Multipoint/Batch Parameter Measurement (*.csv) .....	225
3.4.3	RRUFF (*.txt) .....	228
3.4.4	EMCCD LabRam HR800 (.txt) .....	229
3.4.5	EMCCD LabRam HR800 Mapping WN decreasing (.txt) .....	229
3.4.6	EMCCD LabRam HR800 Mapping WN increasing (.txt) .....	229
<b>4</b>	<b>Files Created Using UNIFIT .....</b>	<b>230</b>
4.1	Exported Files .....	230
4.1.1	Call: [File – Export] (*.DAT) .....	230
4.1.1.1	Standard Windows .....	230
4.1.1.2	3D-Waterfall 0° .....	230
4.1.1.3	3D-Waterfall 0° Plus .....	230
4.1.1.4	3D-Waterfall 45°, 3D-Waterfall -45°, 3D-Colour Profile .....	231
4.1.1.5	Parameter Plot .....	231
4.1.1.6	Wagner Plot .....	232
4.1.1.7	XY Plot 45°, XY Plot -45°, XY Colour Profile .....	232
4.1.2	Call: [Batch Processing – Export Spectra all Windows] (*.DAT) .....	232
4.1.3	Call: [Batch Processing – Export Fit Parameters] (*.DAT) .....	233
4.1.4	Call: [Concentration - Concentration] and <span style="border: 1px solid black; padding: 2px;">Save 1</span> (*.KON) .....	233
4.1.5	Call: [Concentration - Concentration] and <span style="border: 1px solid black; padding: 2px;">Save 2</span> (*.DAT) .....	234
4.2	Project File (*.UFP) .....	234
4.3	Fit-Parameter File (*.PAR) .....	285
4.4	Annotation/Design File (*.DSG) .....	287
4.5	Inelastic Electron Scattering Cross-Section File (*.CRO) .....	338
4.6	Calculation Transmission Function Synchrotron Radiation (*.DAT) .....	338
4.7	Project Processing Steps/Design (*.PPD) .....	339
<b>5</b>	<b>Data Banks Integrated in UNIFIT .....</b>	<b>352</b>
5.1	Auger Parameter (*.AUP) .....	352
5.2	Peaks Positions of Photoelectron Lines (*.POS) .....	352
5.3	Sensitivity Factors (*.SEN) .....	352
5.4	Satellite File (satellit.set) .....	353

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5.5	Doublet File (doublet.dda) .....	354
5.6	Energies of AES Target Atom Subshells (*.apo).....	355
5.7	Coverion of PHI Peak Names .....	357
5.7.1	Data Set 1: XPS and AES.....	357
5.7.2	Data Set 2: AES.....	364
<b>6</b>	<b>References.....</b>	<b>371</b>

## 1 Line positions

All photoelectron lines are in BE, all Auger lines are in KE! [1, 2, 3] The main lines are marked by a star. The values are saved in the directories Unifit\_2024\_User\_Files\lines. The second part gives the chemical shifts of some compounds.

### line positions.pos

1 Pd 4d	16 I 5s
1 Zr (M45N1N45)	17 K 3p
1 Mo (M45N23N23)	18 Cl 3s
1 In (M45N1N45)	18 Pb 5d5
1 Sn (M45N1N45)	19* Ga 3d
2 V 3d	19 Xe 5s
2 Cr 3d	20 Sr 4p
2 Mo 4d	20 Sm 5p
2 Tc 4d	20 Ho 5p
2 Ru 4d	21 Gd 5p
3 Zr 4d	21 Pb 5d3
3 Co 3d	22 Kr 4s
3 Y 4d	22 Ba 5s
3 Cu 3d	22 Pm 5p
3 Rh 4d	22* Ta 4f7
3 Ag 4d	23* O 2s
4 Mn 3d	23* Na (L23VV)
4 Ni 3d	24 Ar 3s
4 Nb 4d	24 Cs 5s
5 Ca 3d	24* Ta 4f5
5 Ti 3d	24 Eu 5p
5 Br 4p	25 Ca 3p
6 Fe 3d	25 Er 5p
6 Se 4p	25* Sn 4d
7 Cl 3p	26 Y 4p
7 Sc 3d	26 Dy 5p
7* Lu 4f7	26 Tm 5p3
9* Lu 4f5	26 Yb 5p3
9 Cd 4d	26 Bi 5d5
10 Zn 3d	27 Br 4s
11 Kr 4p	27 Lu 5p3
12 Ar 3p	29 Rb 4s
13 Tl 5d5	29 Zr 4p
14 P 3s	29 Tb 5p
14 S 3s	29 Bi 5d3
14 Rb 4p	29* Ge 3d
14 Te 5s	30 Hf 5p3
14* Hf 4f7	30* F 2s
15 Tl 5d3	31 Na 2p
16* Hf 4f5	31 Sc 3p
16 In 4d	31* W 4f7
	32 Cr (MVV)
	32 Sb 4d

32 Tm 5p1	48* Mn 3p
33 K 3s	49 Rh 4p
33 Ti 3p	49* I 4d5
33 Yb 5p1	50* Mg 2p
33 Ta 5p3	50* Cs (M45O23O23)
33 Re 5p3	51 Ho 5s
33* W 4f5	51 Po 5d
34 Nb 4p	51 Zr 4s
34 Eu 5s	51* I 4d3
34 Lu 5p1	51* Os 4f7
35 La 5s	52 Pt 5p3
36 Mo 4p3	53* Co (M23VV)
36 Ce 5s	53* Co (MVV)
36 Gd 5s	53 Pd 4p
37 Mo 4p1	53 Ir 5p3
37 Sr 4s	53* Fe 3p
37 Hf 5p1	53* Li (KVV)
37 W 5p3	54* Se 3d
37* V 3p	54 Tm 5s
38 Pr 5s	54* Os 4f5
38 Pm 5s	55 Ge (M3M45M45)
39 Tc 4p	55 Ge (MMM)
39 Nd 5s	55* Se 3d5
40 At 5d	55 Yb 5s
40 V 3p	54 Br (M4N23N23)
40 Te 4d	54 Br (MNN)
40 Ta 5p1	56 Ag 4p3
40* Re 4f7	56* Li 1s
41 Sm 5s	56* Ba (N45O23O23)
41* As 3d	58* Ba (NOO)
41* Ne 2s	56* Se 3d
42 Cr 3p3	56* Ga (M23VV)
42* Re 4f5	58 Zn (LVV)
42* As 3d	58 Au 5p3
43* Cr 3p	58 Lu 5s
43* Mg (L23VV)	58 Fr 5d
43* Mg (LVV)	59 Ti 3s
44 Ca 3s	59 Ni (M3VV)
45 Ru 4p	60 Os 5p1
45 Mn (M23M45M45)	60* Co 3p
46 Y 4s	61 Ni (M23M45M45)
46 Tb 5s	61 Ni (MMM)
46* Cs (N5O23O23)	61 Nb 4s
47* Se (M45N23N23)	61 Er 5s
47* Se (MNN)	61* Xe 4d5
47* Fe (M23VV)	61* Ir 4f7
47* Fe (MVV)	61 Pt (N67O45O45)
47 W 5p1	61 Pt (NOO)
48 Os 5p3	61* Cu (M23VV)
48 Rn 5d	61* Cu (MVV)

62* Cs (N45O23V)	83 Rh 4s
62 Ag 4p1	83 Pb 5p3
63 Co 3p1	84 Hg 5p1
63* Xe 4d3	84* Au 4f7
63 Dy 5s	86 Os 5s
64 Mo 4s	86* Tl (N7O45O45)
64* Ir 4f5	87* Ce (N45N67O23)
64* Na 2s	87* Ce (NNO)
64 Hf 5s	87 Zn 3p3
64* La (N45O23O23)	87* Kr 3d
64* La (NOO)	87 Th 5d5
64* La (NOO)	88* Au 4f5
65 Hg 5p3	88* Tl (N6O45O45)
66 V 3s	88* Tl (NOO)
67* Ni 3p	88 Si (LVV)
67* Al (L23VV)	88 Si (L23M23M23)
67* Al (LMM)	88 Si (LMM)
68 Tc 4s	88 Pd 4s
68 Cd 4p	89* Mg 2s
68 Ra 5d	89* Zn 3p3
69* Br 3d	90* Ba 4d5
69 Ta 5s	91 Sn 4p
69 Th (N6O3O5)	91* Zn 3p1
69 Th (NOO)	91 Pr (N45N67O23)
70* Au (N7VV)	91 Pr (NNO)
70* Au (NVV)	92 Fe 3s
71 U (OPV)	93* Ba 4d3
71* Ba (N45O23V)	93 Pb (N7O45O45)
71* Au (N67VV)	94 Bi 5p3
71* Pt 4f7	94 Th 5d3
73* Al 2p	94 Zr (M45N1N23)
74 Cr 3s	96* Pb (N6O45O45)
74* Pt 4f5	96* Pb (NOO)
75* Cu 3p3	96 Nd (N45N67O23)
75* Hg (N7O45O45)	96 Nd (NNO)
75 Cs 4d5	97 As (M23M45V)
76 Tl 5p3	97 As (MMV)
76 W 5s	98 Ag 4s
77* Cs 4d5	98 Ir 5s
77* Cu 3p1	99* Si 2p
77 Ru 4s	100 Tl 5p1
78 Rb (M5N23N23)	100* Bi (N7O45O45)
78 Rb (MNN)	101* Hg 4f7
79 In 4p	102 Br (M2N45N23)
80* Cs 4d3	103* La 4d5
80 Ac 5d	103 Co 3s
81 Hg (N6O45O45)	103 Sm (N45N67O23)
81 Hg (NOO)	103 Sm (NNO)
81 Re 5s	104* Bi (N6O45O45)
83 Mn 3s	104* Bi (NOO)

104 Pt 5s	129 Pm 4d
104 Po 5p3	131* P 2p
104* Ga 3p3	131* P 2p3
104 Se (M1N45N45)	132 Po 5p1
105 Sb 4p	133 Tl 5s
105* Hg 4f5	134* Sr 3d5
106* La 4d3	136* Sr 3d3
107* Ga 3p1	136 Nb (M45N23N23)
107 Eu (NNO)	137* Pb 4f7
107 Pb 5p1	135 Sm (N45N67N67)
107 Rb (M3M45N23)	137 Sn 4s
108 Be (KL1L1)	139 Xe 4p
108 Be (KLL)	140 Fr 5p3
109 Cd 4s	140* Gd 4d
109* Ce 4d5	140 Zn 3s
111 Au 5s	140 Eu (NNN)
111 Ni 3s	141* As 3p3
111* Rb 3d5	142* Pb 4f5
112* Ce 4d3	143 Gd (M45N67N67)
112* Rb 3d	143 Gd (MNN)
112* Be 1s	145 Nb (M45N1N45)
112 Gd (M45N67O23)	146* Tb 4d
112 Gd (MNO)	146* As 3p1
114 Te 4p	148* Zr (M45N23V)
114 Nb (M45N1N23)	148* Zr (MNV)
114 Sr (M3M45N23)	148 At 5p1
115 At 5p3	150 Pb 5s
115* Pr 4d	150 Tb (N45O67O67)
116 Tb (N45N67O23)	151* S (L23M23M23)
116 Tb (NNO)	151* S (LMM)
118* Tl 4f7	151* Si 2s
118* Al 2s	152* Dy 4d
119 Zr (M45N23N23)	152* Th (N67O45O45)
120 Bi 5p1	152 Ru (M45N1N23)
121* Nd 4d	153 Sb 4s
122* Tl 4f5	153 Ra 5p3
122* Ge 3p3	154 Dy (N45N67N67)
122 Mo (M45N1N23)	154 Dy (NNN)
123 Cu 3s	156* Y 3d5
123 In 4s	157* Bi 4f7
123 I 4p	158* Y 3d3
123 P (L3M23M23)	160* Ho 4d
123 P (LMM)	160 Ga 3s
124* Y (M45N23V)	161 Bi 5s
124* Y (MNV)	161 Cs 4p3
126* Ge 3p1	162* Bi 4f5
127 Rn 5p3	162 Ho (M45N67N67)
127 Hg 5s	163* Se 3p3
128* Eu 4d	163 Mo (M45N1N45)
129* Sm 4d	164* S 2p

164 Rn 5p1	195 At 5s
167* Er 4d	196* Lu 4d5
167 Ac 5p3	197 La 4p3
168* Nb (M45N23V)	199* Cl 2p3
168* Nb (MNV)	200 Nb (M45N45N45)
168 Er (N4N67N67)	200 Nb (MNN)
168 Er (NNN)	200 Ra 5p1
169* Se 3p1	201* Cl 2p1
170 Tm (N45N67N67)	201 Ru (M45N1N45)
170 Tm (NNN)	202* Nb 3d5
171 Te 4s	205 As 3s
172* Ir (N4N67N67)	205* Nb 3d3
172* Ir (NNN)	206* Lu 4d3
173 Cs 4p1	207 Ce 4p3
173 Pt (N4N67N67)	207 Tc (M45N23V)
174 Yb (N5N67N67)	207 Xe 4s
174 Yb (NNN)	208* Kr 3p3
175* Tm 4d	210 At 4f
177 Th 5p3	210 W (N45O23O45)
177 Po 5s	211* Ar (L3M23M23)
179* Zr 3d5	211* Hf 4d5
179 Ba 4p3	213* Ar (L3M23M23)
179 Re (N4N7N7)	213 La 4p1
179 Re (NNN)	214 Rn 5s
180 Os (N4N7N7)	215 Ac 5p1
181* Zr 3d3	216* Kr 3p1
181 Ge 3s	218 Pr 4p3
182 Fr 5p1	218 K (L3M1M23)
182* B (KL23L23)	218 Re (N5O23O45)
182 W (N4N7N7)	218 Re (NOO)
182 W (NNN)	222* Hf 4d3
182* B (KLL)	223 Mo (M45N45N45)
182* Yb 4d5	223 Mo (MNN)
182* Br 3p3	223 Ce 4p1
182 Lu (N4N67N67)	223 Rh (M45N1N45)
182 Lu (NNN)	226 K (L3M1M23)
183* Cl (LVV)	226 Th 5p1
183 Ta (N4N67N67)	226 Os (N5N7O45)
183 Ta (NNN)	226* Ta 4d5
184 Po 4f	228 Nd 4p3
184 Hf (NNO)	228* Mo 3d5
187 I 4s	228* S 2s
188* P 2s	231 Ru (M4N23V)
188* Mo (M45N23V)	231 Ru (MNV)
188* Mo (MNV)	231* Mo 3d3
189* B 1s	232 Se 3s
189* Br 3p1	233 Ir (N5N7O45)
190* U (N67O45N45)	234 Fr 5s
191* Yb 4d3	234 Pr 4p1
193 Ba 4p1	234 Cs 4s

238 Rn 4f	280 Cd (M45N1N45)
238* Ta 4d3	281* Sr 3p1
240* Rb 3p3	283 Sm 4p1
241 Pt (N5N67O45)	283* U (N67O45V)
242 Pm 4p3	283* U (NOV)
242* Ar 2p3	284* Ru 3d3
243* W 4d5	285* C 1s
243 Pd (M45N1N45)	285* Tb 4p3
143 Au (N5N67O45)	287 Kr 3s
244* Ar 2p1	289 Eu 4p1
245 Nd 4p1	290 Ce 4s
246 Hg (N5N7O45)	293* Os 4d3
246 Tc (M5N45N45)	294 Th 5s
248* Th (N67O45V)	294* K 2p3
248* Th (NOV)	296 Ag (M45N23V)
248* K (L3M23M23)	297* Dy 4p3
248* K (LMM)	297* K 2p1
249* Rb 3p1	297* Ir 4d5
250 Sm 4p3	297* Ca (L2M23M23)
250* K (L3M23M23)	297* Ca (LMM)
250 Tl (N5N7O5)	298 Cs (L3M23M23)
251 Pb (M5N7O5)	299* Y 3p3
253 Tc 3d5	299 Ra 4f
253 Rh (M45N23V)	301 Gd 4p1
253 Rh (MNV)	302* Rh (M5N45N45)
253 Bi (M5N67O45)	302* Rh (MNN)
254 Ra 5s	305 Pr 4s
254 Ba 4s	307* Rh 3d5
256* W 4d3	307 Sc (L3M1M23)
256 Br 3s	309* Ho 4p3
257 Tc 3d3	311* Y 3p1
260* Re 4d5	312* Rh 3d3
261 Eu 4p3	312* Ir 4d3
262 Ag (M45N1N45)	315 Sc (L3M1M23)
264* C (KVV)	315* Pt 4d5
264 Pm 4p1	316 Cd (M45N23V)
268 Fr 4f	319 Ac 4f
270 Gd 4p3	320* Ar 2s
270* Sr 3p3	320 Nd 4s
271* Cl 2s	321* Er 4p3
272 Ac 5s	322* Tb 4p1
274* Re 4d3	325 Rb 3s
275 La 4s	328* Pd (M4N45N45)
275* C (KL23L23)	328* Pd (MNN)
275* C (KLL)	330* Zr 3p3
275* Ru (M45N45N45)	332* Pt 4d3
275* Ru (MNN)	333* Tm 4p3
276* Pd (M45N23V)	333* Th 4f7
279* Os 4d5	335* Pd 3d5
280* Ru 3d5	335* Au 4d5

337* Dy 4p1	403* In (M4N45N45)
337 Pm 4s	403* In (MNN)
338* Sc (L3M23M23)	404* Sc 2p1
338* Sc (LMM)	405* Cd 3d5
340* Pd 3d3	405 In (M5N45N45)
341* Yb 4p3	406* Tl 4d3
342* Th 4f5	411* In (M4N45N45)
344* Zr 3p1	411* Mo 3p1
346 Ti (L3M1M23)	411 V (L3M1M23)
347* Ca 2p3	412* Cd 3d3
349 Sm 4s	412* Pb 4d5
350* Ca 2p1	413* Lu 4p1
352* Ag (M5N45N45)	417 Dy 4s
352* Ag (MNN)	419* Ti (L3M23M45)
353* Au 4d3	419* Ti (LMM)
353* Ho 4p1	424 W 4p3
355 Ti (L3M1M23)	425 Tc 3p3
358* Ag (M4N45N45)	430 Zr 3s
360 Sr 3s	431* Sn (M5N45N45)
360* Lu 4p3	431* Sn (MNN)
361* Hg 4d5	432 Cr (L3M23M23)
361* Nb 3p3	434* Pb 4d3
366 Eu 4s	435 Ho 4s
368* Ag 3d5	437 Hf 4p1
368* Er 4p1	438 Sn (M4N45N45)
369 Sc (L3M23M45)	439* V (L3M23M23)
374* Ag 3d3	440* Ca 2s
376* Nb 3p1	441* Bi 4d5
377* U 4f7	444* In 3d5
377* Cd (M5N45N45)	445 Tc 3p1
377* Cd (MNN)	446 Re 4p3
378 Gd 4s	448 Cr (L3M1M23)
380 Hf 4p3	451 Er 4s
380* K 2s	451 Ti (L3M45M45)
380* N (KVV)	452* In 3d3
381* Hg 4d3	454* Ti 2p3
383 Ti (L3M23M23)	455* Sb (M4N45N45)
384* Tm 4p1	455* Sb (MNN)
384* Cd (M4N45N45)	460* Ti 2p1
385* Tl 4d5	460 Cr (L3M1M23)
388* U 4f5	462* Ru 3p3
389 Ti (L3M23M23)	463 Ta 4p1
389* Yb 4p1	465* Bi 4d3
394 Y 3s	467 Nb 3s
394* Mo 3p3	470 Tm 4s
396 Tb 4s	471 Os 4p3
399* Sc 2p3	473 Po 4d5
400* N 1s	473* V (L3M23M45)
400 V (L3M1M23)	475* V (LMM)
401 Ta 4p3	474* O (KL1L1)

482 Yb 4s	562 I (M5N45O23)
482* Te (M5N45N45)	563 Ta 4s
482* Te (MNN)	564 Fe (L3M1M23)
484* Ru 3p1	567 Rn 4d3
485* Sn 3d5	569* Cs (M4N45N45)
488 O (KL1L23)	569* Cs (MNN)
490 Cr (L3M23M23)	570 Cr (L3M45M45)
491 W 4p1	573* Ag 3p3
492* Te (M4N45N45)	573* Te 3d5
493* Sn 3d3	574* Cr 2p3
495 Ir 4p3	577 Fr 4d5
497* Rh 3p3	578 Ir 4p1
499* Sc 2s	579 Hg 4p3
500 Po 4d3	583* Cr 2p1
500 Mn (L3M1M23)	583* Te 3d3
505* I (M5N45N45)	586 Ru 3s
505* I (MNN)	587* Mn (L3M23M45)
506 Mo 3s	587* Mn (LMM)
507 At 4d5	587* Ba (M5N45N45)
509 Lu 4s	594 W 4s
509* O (KL23L23)	599 Fe (L3M23M23)
509* O (KLL)	601* Ba (M4N45N45)
510* V (L3M45M45)	601* Ba (MNN)
512* V 2p3	603 Ra 4d5
514 Mn (L3M1M23)	603 Fr 4d3
516* I (M4N45N45)	604* Ag 3p1
518 Re 4p1	607 Co (L3M1M23)
520 Pt 4p3	609 Pt 4p1
520* V 2p1	609* F (KL1L1)
521* Rh 3p1	610 Tl 4p3
527* Cr (L3M23M45)	619* I 3d5
527* Cr (LMM)	619* Cd 3p3
528* Sb 3d5	620* La (M5N45N45)
531* O 1s	620 Co (L3M1M23)
532* Xe (M5N45N45)	625 Re 4s
533 At 4d3	626 V 2s
533* Pd 3p3	628* F (KL1L23)
534 Hf 4s	629 Rh 3s
536 Xe (M5N45N45)	630 Cs (M5N45N67)
537* Sb 3d3	631* I 3d3
541 Rn 4d5	633* La (M4N45N45)
543 Mn (L3M23M23)	633* La (MNN)
544 Tc 3s	635 Mn (L3M45M45)
545* Xe (M4N45N45)	636 Ra 4d3
547 Au 4p3	638 F (KL1L23)
548 Os 4p1	639 Ac 4d5
549 Fe (L3M1M23)	639* Mn 2p3
555* Cs (M5N45N45)	643 Au 4p1
560* Pd 3p1	643 Cs (M4N45N67)
561* Ti 2s	644 Pb 4p3

648 Fe (L3M23M45)	733* Nd (M5N45N45)
649 Co (L3M23M23)	733* Nd (MNN)
650* Mn 2p1	736* U 4d5
651 Fe (L3M23M45)	740* Cs 3d3
653* Cd 3p1	740 At 4p3
653* F (KL23L23)	755* Ce (M5N45N67)
653* F (KLL)	757* Sn 3p1
654* Ce (M45N45N45)	762 Pb 4p1
655* F (KL23L23)	762 Ne (KL1L1)
656 Co (L3M23M23)	763 Au 4s
658 Os 4s	767* Sb 3p3
662 Ni (L3M1M23)	768 Rn 4p3
665* In 3p3	768 Cu (L3M23M23)
669 Ba (M5N45N67)	769 Zn (L3M1M23)
670* Xe 3d5	769 Mn 2s
671 Pd 3s	770* Pm (M5N45N45)
675 Ac 4d3	771* Ce (M4N45N67)
675 Ni (L3M1M23)	771* Ce (MNN)
676* Th 4d5	772 Cd 3s
679 Bi 4p3	774* Co (L3M45M45)
682 Hg 4p1	774* Co (LMM)
683* Xe 3d3	775 Ni (L3M23M45)
683 Ba (M4N45N67)	775 Cu (L2M23M23)
685* F 1s	778* Co 2p3
692 Ir 4s	779* U 4d3
695* Pr (M5N45N45)	781* Ba 3d5
695* Pr (MNN)	781 Ni (L3M23M45)
696* Cr 2s	784 Zn (L3M1M23)
703* In 3p1	785 Ne (KL1L23)
703* Fe (L3M45M45)	789 Co (L2M45M45)
703* Fe (LMM)	793* Co 2p1
705 Po 4p3	795* Pr (M45N45N67)
707* Fe 2p3	796* Ba 3d3
709 Ni (L3M23M23)	798 Ne (KL1L23)
710 Co (L3M23M45)	805* Sm (M5N45N45)
711* La (M5N45N67)	805* Sm (MNN)
713* Th 4d3	805 Hg 4s
715 Ni (L2M23M23)	806 Bi 4p1
715* Sn 3p3	810 Fr 4p3
715 Fe (L2M45M45)	813* Sb 3p1
716 Co (L3M23M45)	814 Ne (KL23L23)
718 Cu (L3M1M23)	818* Ne (KL23L23)
719 Ag 3s	818* Ne (KL23L23)
720 Tl 4p1	820* Te 3p3
720* Fe 2p1	827 Zn (L3M23M23)
723 Co (L2M23M45)	828 In 3s
725 Pt 4s	831 Ga (L3M1M23)
726* Cs 3d5	835 Zn (L2M23M23)
728* La (M4N45N67)	836* La 3d5
731 Cu (L3M1M23)	839* Cu (L3M23M45)

840* Nd (M45N45N67)	950* Sm (M45N45N67)
845 Fe 2s	951 Na (KL1L23)
845 Ga (L3M1M23)	952* Pr 3d3
846* Ni (L3M45M45)	953 Ge (L3M23M23)
846* Ni (LMM)	953* Cu 2p1
846* Eu (M5N45N45)	962 Ge (L3M23M23)
847 Tl 4s	965 Th 4p3
850* Eu (M45N45N45)	966 As (L3M1M23)
851 Po 4p1	967 Na (KL1L23)
853* La 3d3	973* Ga (L3M23M45)
853* Ni 2p3	978* Dy (M5N45N45)
859 Cu (L2M23M45)	980 Fr 4p1
861 Nd (M4N45O23)	980* Eu (M45N45N67)
863* Ni (L2VV)	980* Eu (MNN)
863* Ne 1s	981* Nd 3d5
870* Ni 2p1	983 Ga (L3M23M45)
871* Te 3p1	989 Na (KL23L23)
875 I 3p3	989 Na (KLL)
879 Ra 4p3	992* Zn (L3M45M45)
884* Ce 3d5	992* Zn (LMM)
884* Gd (M5N45N45)	994* Na (KL23L23)
885 Sn 3s	994* Na (KLL)
885* Pm (M45N45N67)	995 Po 4s
886 At 4p1	996 Xe 3p1
888 Ga (L3M23M23)	998* Ho (M5N45N45)
890 Ge (L3M1M23)	1000 Ga (L2M23M45)
893 Pb 4s	1002* Nd 3d3
895 Ge (L3M1M23)	1002 Cs 3p3
898 Ga (L2M23M23)	1009 Te 3s
900 Ac 4p3	1009 Ni 2s
902* Ce 3d3	1013 Se (L3M1M23)
905 Zn (L3M23M45)	1015 Zn (L2M45M45)
914 Zn (L3M23M45)	1020 As (L3M23M23)
919* Cu (L3M45M45)	1020* Gd (M45N45N67)
919* Cu (LMM)	1022* Zn 2p3
920* Tb (M5N45N45)	1030 As (L2M23M23)
921* Cu (L3VV)	1033 Se (L3M1M23)
925 Co 2s	1034* Pm 3d5
926 Na (KL1L1)	1043 Ge (L3M23M45)
928 Zn (L2M23M45)	1045* Zn 2p1
929 Rn 4p1	1045 At 4s
930 I 3p1	1047* Er (M5N45N45)
932* Pr 3d5	1058 Ra 4p1
933* Cu 2p3	1060* Pm 3d3
934 Xe 3p3	1064 Ba 3p3
938* Cu (L2VV)	1068* Sm (M5N67N67)
939* Cu (L2M45M45)	1068* Tb (M45N45N67)
940 Bi 4s	1068* Tb (MNN)
944 Sb 3s	1069* Ga (L3M45M45)
950 As (L3M1M23)	1069* Ga (LMM)

1069 Cs 3p1	1188 Se (L3M2M45)
1071 I 3s	1195 Zn 2s
1072* Na 1s	1200 Se (L3M3M45)
1075 Ge (L2M23M45)	1202* Gd (M4N67N67)
1080 Ac 4p1	1208 La 3p1
1080* Tm (M5N45N45)	1208 Ra 4s
1081* Sm 3d5	1210 Kr (L3M23M23)
1086 Se (L3M23M23)	1212 Mg (KL23M)
1091 Ga (L2M45M45)	1216 Cs 3s
1094* Sm (M4N67N67)	1217* Ge 2p3
1096 Se (L3M23M23)	1218* Er (M45N45N67)
1097 Rn 4s	1218* Er (MNN)
1097 Cu 2s	1218* Gd 3d3
1106 Mg (KL1L1)	1223 Kr (L3M23M23)
1108* Sm 3d3	1225* As (L3M45M45)
1116 As (L3M23M45)	1225* As (LMM)
1117* Ga 2p3	1227* Tb (M5N67N67)
1118* As (L3M23M45)	1230 Se (L2M23M45)
1119* Dy (M45N45N67)	1231 Hf (MNO)
1119* Dy (MNN)	1241* Tb 3d5
1120* Eu (M5N67N67)	1242 Pr 3p
1126* Eu 3d5	1248* Ge 2p1
1127 As (L3M23M45)	1253 Br (L3M23M45)
1127 Se (L3M1M45)	1256* Tb (M4N67N67)
1128 La 3p3	1261* As (L2M45M45)
1138 Ba 3p1	1264* As (L2M45M45)
1140 Mg (KL1L23)	1267 Br (L3M1M23)
1141 Xe 3s	1269 Ac 4s
1141 Yb (M5N5N5)	1270* Tm (M45N45N67)
1143 Br (L3M23M23)	1270* Tm (MNN)
1144* Ga 2p1	1271 Ta (M5N5N5)
1145* Ge (L3M45M45)	1272 Ce 3p1
1150* Ge (LMM)	1276* Tb 3d3
1150* Eu (M4N67N67)	1280* Dy (M5N67N67)
1151 As (L2M23M45)	1292 Ba 3s
1153 Fr 4s	1296* Dy 3d5
1155 Mg (KL2L23)	1300 Br (L2M23M45)
1155 Br (L3M23M23)	1301 Ga 2s
1156* Eu 3d3	1301 Nd 3p3
1165* Ho (M45N45N67)	1302 Al (KL1L1)
1165* Ho (MNN)	1303* Mg 1s
1170 Th 4p1	1306* Se (L3M45M45)
1170* Gd (M5N67N67)	1306* Se (LMM)
1177 Ge (L2M45M45)	1312 W (M5N5N5)
1181* Mg (KL23L23)	1318* Dy (M4N67N67)
1181* Mg (KLL)	1320* Yb (M45N45N67)
1184 Ce 3p3	1324* As 2p3
1186* Mg (KL23L23)	1327 Kr (L3M23M45)
1186* Gd 3d5	1330 Th 4s
1188 Lu (M5N5N5)	1332* Ho (M5N67N67)

1333* Dy 3d3	1615* Hf (MNN)
1339 Pr 3p1	1615* Lu (M4N67N67)
1341 Al (KL1L23)	1617* Si (KL23L23)
1345 Kr (L3M23M45)	1617* Si (KLL)
1347 Se (L2M45M45)	1620 Rb (L2M45M45)
1354 Re (M5N5N5)	1622 Os (M5N5N7)
1357 Al (KL1L23)	1639 Lu 3d3
1359* As 2p1	1640* Sr (L3M45M45)
1370* Ho (M4VV)	1640* Sr (LMM)
1370* Lu (M5N45N67)	1641 Pb (M5N5N5)
1372* Ho (M4N67N67)	1662 Hf 3d5
1380 Kr (L2M23M45)	1669* Hf (M4N67N67)
1387* Al (KL23L23)	1675* Ta (M5N67N67)
1387* Al (KLL)	1675* Ta (MNN)
1388* Br (L3M45M45)	1695 Zn (L3M3M45)
1388 Br (LMM)	1716 Hf 3d3
1389* Er (M5N67N67)	1718 Sr (L2M45M45)
1393* Al (KL23L23)	1725* W (M5N67N67)
1396 Os (M5N5N5)	1725* W (MNN)
1420* Hf (M45N45N67)	1725 Pt (M5N45N67)
1424 Br (L2M45M45)	1733 Ta (M4N67N67)
1428* Er (M4N67N67)	1735 Ta 3d5
1433 Rb (L3M3M3)	1737 Y (L3M45M45)
1439 Br (LMM)	1737 Y (LMM)
1439 Ir (M5N5N5)	1771 Au (M5N5N7)
1440* Tm (M5N67N67)	1787 Nb (L3M3M45)
1460 Kr (L3M45M45)	1790 Re (M5N67N67)
1462 Ta (M45N45N67)	1790 Re (MNN)
1484 Pt (M5N5N5)	1791 W (M4N6N6)
1487* Tm (M4N67N67)	1792 P (KL1L2)
1500* Yb (M5N67N67)	1793 Ta 3d3
1500* Yb (MNN)	1809 W 3d5
1513 Kr (L2M45M45)	1818 Hg (M5N5N7)
1514 Si (KL1L1)	1823 Y (L2M45M45)
1516 Sr (L3M3M5)	1831 Zr (L3M45M45)
1522 Au (M5N5N5)	1831 Zr (LMM)
1524 W (M5N5N7)	1837 Os (M5N7N7)
1549* Yb (M4N67N67)	1839 Si 1s
1559 Si (KL1L23)	1850* P (KL23L23)
1560 Al 1s	1850* P (KLL)
1560* Lu (M5N67N67)	1856 Re (M4N67N67)
1560* Lu (MNN)	1862 P (K1L3L3)
1561 Rb (L3M5M5)	1865 Tl (M5N5N67)
1561 Rb (LMM)	1872 W 3d3
1572 Re (M5N5N7)	1881 Mo (L3M3M5)
1576 Si (KL1L23)	1883 Re 3d5
1589 Lu 3d5	1901* Ir (M5N67N67)
1615* Hf (M5N67N67)	1901* Ir (MNN)
1601 Tl (M5N5N5)	1907* Os (M4N67N67)
1606 Y (L3M23M45)	1907* Os (MNN)

1914 Pb (M5M5N7)	2281 W 3p3
1920* Nb (L3M45M45)	2282 Pb (M4N67N67)
1920* Nb (LMM)	2282 Pd (L3M3M45)
1929 Zr (L2M45M5)	2291 Au 3d3
1938 P (KL1M1)	2295 Hg 3d5
1949 Re 3d3	2296 Th M5N5N7)
1949 P (KL1M23)	2343 Bi (M4N67N67)
1960 Os 3d5	2343 Bi (MNN)
1960 Bi (M5N5N67)	2365 Hf 3p1
1961* Pt (M5N67N67)	2366 Rh (L3M45M45)
1961* Pt (MNN)	2366 Rh (LMM)
1978* Ir (M4N67N67)	2367 Re 3p3
1996 P (KL23M1)	2370* Cl (KL23L23)
2001 P (KL23M23)	2370* Cl (KLL)
2016* Au (M5N67N67)	2381 Ag (L3M3M45)
2016* Au (MNN)	2385 Hg 3d3
2024 Lu 3p3	2385 Ru (L2M45M45)
2026* S (KL1L23)	2389 Tl 3d5
2031 Os 3d3	2414 U (M5N5N7)
2039* Mo (L3M45M45)	2457 Os 3p3
2039* Mo (LMM)	2469 Ta 3p1
2039 Nb (L2M45M45)	2472 S 1s
2040 Ir 3d5	2476 Pd (L3M45M45)
2040* Pt (M4N67N67)	2484 Pb 3d5
2070 Hg (M5N67N67)	2485 Tl 3d3
2078 Ru (L3M3M45)	2491 Lu 3s
2102* Au (M4N67N67)	2507 Rh (L2M5M5)
2108 Hf 3p3	2508 Ar (KL1L1)
2116 Ir 3d3	2551 Ir 3p3
2116* S (KL23L23)	2575 W 3p1
2116* S (KLL)	2576 Ar (KL1L23)
2122 Pt 3d5	2580 Bi 3d5
2128 Tl (M5N67N67)	1583 Ag (L3M45M45)
2128 Tl (MNN)	2586 Pb 3d3
2144* Mo (L2M45M45)	2600 Ar (KL1L23)
2145 P 1s	2601 Hf 3s
2160* Hg (M4N67N67)	2633 Pd (L3M3M45)
2160* Hg (MNN)	2634 Th (M5N7N7)
2180 Pb (M5N67N67)	2645 Pt 3p3
2180 Rh (L3M3M45)	2651 Ar (KL23L23)
2180 Pb (MNN)	2661 Ar (KL23L23)
2194 Ta 3p3	2682 Re 3p1
2202 Pt 3d3	2683 Po 3d5
2206 Au 3d5	2688 Bi 3d3
2223 Tl (M4N67N67)	2694 Cd (L3M5M5)
2235 Bi (M5N67N67)	2694 Cd (LMM)
2235 Bi (MNN)	2708 Ta 3s
2256 Ru (L3M45M45)	2743 Au 3p3
2256 Ru (LMM)	2755 Ag (L3M3N45)
2264 Lu 3p1	2764 U (M5N7N7)

2787 At 3d5	3604 Pd 1s
2789 Th (M4N7N7)	3608 K 1s
2792 Os 3p1	3611 Pa 3d3
2798 Po 3d3	3663 Fr 3p3
2806 In (L3M5M5)	3696 Bi 3p1
2820 W 3s	3704 Tl 3s
2822 Cl 1s	3728 U 3d3
2847 Hg 3p3	3792 Ra 3p3
2892 Rn 3d5	3806 Ag 1s
2909 Ir 3p1	3851 Pb 3s
2909 At 3d3	3854 Po 3p1
2919 Sn (L3M5M5)	3909 Ac 3p3
2932 Re 3s	3999 Bi 3s
2940 U (M4N6N7)	4002* Ti (KL23L23)
2957 Tl 3p3	4008 At 3p1
3000 Fr 3d5	4132 2p3
3004 Rh 2p3	4038 Ca 1s
3022 Rn 3d3	4046 Th 3p3
3027 Pt 3p1	4149 Po 3s
3035 Sb (M5N45N45)	4159 Rn 3p1
3049 Os 3s	4174 Pa 3p3
3066 Pb 3p3	4303 U 3p3
3105 Fr 3d5	4317 At 3s
3136 Fr 3d3	4327 Fr 3p1
3146 Rh 2p1	4380 Sb 2p1
3148 Au 3p1	4482 Rn 3s
3173 Pd 2p3	4490 Ra 3p1
3174 Ir 3s	4492 Sc 1s
3177 Bi 3p3	4652 Fr 3s
3206 Ar 1s	4656 Ac 3p1
3219 Ac 3d5	4698 Sb 2s
3248 Ra 3d3	4822 Ra 3s
3279 Hg 3p1	4830 Th 3p1
3296 Pt 3s	4966 Ti 1s
3302 Po 3p3	5001 Pa 3p1
3330 Pd 2p1	5002 Ac 3s
3332 Th 3d5	5182 Th 3s
3351 Ag 2p3	5182 U 3p1
3370 Ac 3d3	5367 Pa 3s
3412 Rh 1s	5465 V 1s
3416 Tl 3p1	5548 U 3s
3425 Au 3s	5989 Cr 1s
3426 At 3p3	6539 Mn 1s
3442 Pa 3d5	7112 Fe 1s
3491 Th 3d3	7709 Co 1s
3524 Ag 2p1	8333 Ni 1s
3538 Rn 3p3	8979 Cu 1s
3552 U 3d5	9244 Lu 2p3
3554 Pb 3p1	9561 Hf 2p3
3562 Hg 3s	9659 Zn 1s

9881 Ta 2p3	16388 Bi 2s
10207 W 2p3	16733 Pa 2p3
10349 Lu 2p1	16785 At 2p1
10367 Ga 1s	16939 Po 2s
10535 Re 2p3	17038 Y 1s
10739 Hf 2p1	17166 U 2p3
10870 Lu 2s	17337 Rn 2p1
10871 Os 2p3	17493 At 2s
11103 Ge 1s	17907 Fr 2p1
11136 Ta 2p1	17998 Zr 1s
11215 Ir 2p3	18049 Rn 2s
11271 Hf 2s	18484 Ra 2p1
11544 W 2p1	18639 Fr 2s
11564 Pt 2p3	18986 Nb 1s
11682 Ta 2s	19083 Ac 2p1
11867 As 1s	19237 Ra 2s
11919 Au 2p3	19693 Th 2p1
11959 Re 2p1	19840 Ac 2s
12100 W 2s	20000 Mo 1s
12284 Hg 2p3	20314 Pa 2p1
12385 Os 2p1	20472 Th 2s
12658 Se 1s	20948 U 2p1
12658 Tl 2p3	21044 Te 1s
12824 Ir 2p1	21105 Pa 2s
12968 Os 2s	21757 U 2s
13035 Pb 2p3	22117 Ru 1s
13273 Pt 2p1	23220 Rh 1s
13419 Ir 2s	24350 Pd 1s
13419 Bi 2p3	25514 Ag 1s
13474 Br 1s	26711 Cd 1s
13734 Au 2p1	27940 In 1s
13814 Po 2p3	29200 Sn 1s
13880 Pt 2s	30491 Sb 1s
14209 Hg 2p1	31814 Te 1s
14214 At 2p3	33169 I 1s
14326 Kr 1s	34561 Xe 1s
14353 Au 2s	35985 Cs 1s
14619 Rn 2p3	37441 Ba 1s
14698 Tl 2p1	38925 La 1s
15031 Fr 2p3	40443 Ce 1s
15200 Rb 1s	41991 Pr 1s
15200 Pb 2p1	43569 Nd 1s
15347 Tl 2s	45184 Pm 1s
15444 Ra 2p3	46834 Sm 1s
15711 Bi 2p1	48519 Eu 1s
15861 Pb 2s	50239 Gd 1s
15871 Ac 2p3	51996 Tb 1s
16105 Sr 1s	53789 Dy 1s
16244 Po 2p1	55618 Ho 1s
16300 Th 2p3	57486 Er 1s

59390 Tm 1s  
 61332 Yb 1s  
 63314 Lu 1s  
 65351 Hf 1s  
 67416 Ta 1s  
 69525 W 1s  
 71676 Re 1s  
 73871 Os 1s  
 76111 Ir 1s  
 78395 Pt 1s  
 80725 Au 1s  
 83102 Hg 1s  
 85530 Tl 1s  
 88005 Pb 1s  
 90524 Bi 1s  
 93105 Po 1s  
 95730 At 1s  
 98404 Rn 1s  
 101137 Fr 1s  
 103922 Ra 1s  
 106755 Ac 1s  
 109651 Th 1s  
 112601 Pa 1s  
 115606 U 1s

**Ag (M4N45N45).pos**

357.8 Ag  
 356.7 Ag<sub>2</sub>O  
 356.6 AgO  
 354.2 Ag<sub>2</sub>SO<sub>4</sub>

**Ag (M5N45N45).pos, Ag (MNN).pos**

352.2 Mg<sub>97</sub>Ag<sub>3</sub>  
 351.8 Ag  
 351.4 Ag<sub>2</sub>Se  
 351.2 Ag<sub>2</sub>S  
 350.7 Ag<sub>2</sub>O  
 350.6 AgO  
 350.1 AgI  
 349.6 AgF<sub>2</sub>  
 349.3 AgF

**Ag 3d5.pos**

367.3 AgF<sub>2</sub>  
 367.4 AgO  
 367.5 Ag<sub>2</sub>CO<sub>3</sub>  
 367.7 AgF

367.8 Ag<sub>2</sub>O  
 367.8 CuAgSe  
 367.8 Ag<sub>2</sub>Se  
 367.8 Ag<sub>2</sub>SO<sub>4</sub>  
 368.0 AgI  
 368.1 Ag<sub>2</sub>S  
 368.2 Ag  
 368.4 Ag(OAc)  
 368.8 Ag<sub>2</sub>Yb  
 368.8 AgOCCF<sub>3</sub>  
 368.8 Mg<sub>97</sub>Ag<sub>3</sub>

**Al (KL23L23;1D).pos, Al (KLL).pos**

1393.1 Al  
 1391.2 AlAs  
 1389.4 Al<sub>2</sub>O<sub>3</sub>/Al  
 1389.0 AlN  
 1388.4 Al<sub>2</sub>O<sub>3</sub>  
 1388.2 Al<sub>2</sub>O<sub>3</sub>/alpha  
 1388.1 Al<sub>2</sub>FeO<sub>4</sub>  
 1387.9 Al<sub>2</sub>O<sub>3</sub>/sapphire  
 1387.8 Al<sub>2</sub>O<sub>3</sub>/gamma  
 1387.7 Al<sub>2</sub>O<sub>3</sub>/anhydride  
 1387.7 Al(OH)<sub>3</sub>/bayerite  
 1387.6 AlO(OH)/boehmite  
 1387.1 KAl<sub>2</sub>(AlSi<sub>3</sub>O<sub>10</sub>)<sub>2</sub>(OH)<sub>2</sub>/muscovite  
 1387.1 LiAlSi<sub>2</sub>O<sub>6</sub>/spodumene  
 1386.9 Mol Sieve A  
 1386.9 Al<sub>2</sub>SiO<sub>5</sub>/sillimannite  
 1386.9 Al<sub>6</sub>Si<sub>2</sub>O<sub>13</sub>/mullite  
 1386.8 Al<sub>2</sub>SiO<sub>5</sub>  
 1386.8 Al<sub>2</sub>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>/pyrophyllite  
 1386.7 Al<sub>4</sub>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>8</sub>/kaolinite  
 1386.5 Na[AlSi<sub>3</sub>O<sub>8</sub>]/albite  
 1386.5 Na<sub>2</sub>Al<sub>2</sub>Si<sub>3</sub>O<sub>10</sub>.2H<sub>2</sub>O/natrolite  
 1386.3 Mol Sieve X  
 1385.9 Mol Sieve Y  
 1385.5 H Zeolon

**Al (L23VV).pos, Al (LMM).pos**

67.2 Al  
 53.4 Al<sub>2</sub>O<sub>3</sub>/Al  
 66.4 Al<sub>2</sub>O<sub>3</sub>/Al

**Al 2p.pos**

71.0 AlB<sub>2</sub>  
 72.9 Al

73.4 Fe <sub>3</sub> Al	1221.1 Ph <sub>3</sub> As
73.6 AlAs	1219.5 Ph <sub>3</sub> AsO
73.6 AlGaAs	1218.8 As <sub>2</sub> O <sub>3</sub>
73.6 CoAl <sub>2</sub> O <sub>4</sub>	1217.5 As <sub>2</sub> O <sub>5</sub>
73.7 Mol Sieve A	1213.8 KAsF <sub>6</sub>
73.7 Al <sub>2</sub> O <sub>3</sub> /gamma	1218.1 AsBr <sub>3</sub>
73.9 Al <sub>2</sub> O <sub>3</sub> /alpha	1222.9 AsI <sub>3</sub>
74.0 AlN	
74.1 Al <sub>2</sub> O <sub>3</sub> /sapphire	<b>As 3d.pos</b>
74.2 AlO <sub>2</sub> H/boehmite	
74.2 Al <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	40.6 InAs
74.2 NiAl <sub>2</sub> O <sub>4</sub>	41.0 AlGaAs
74.2 AlO <sub>2</sub> H	41.0 AlAs
74.2 Al(OH) <sub>3</sub> /bayerite	41.2 GaAs
74.3 Al <sub>2</sub> (WO <sub>4</sub> ) <sub>3</sub>	41.5 As
74.3 Mica/muskovite	42.8 Ph <sub>3</sub> As
74.6 Al <sub>2</sub> S <sub>3</sub>	43.4 As <sub>2</sub> S <sub>3</sub>
74.6 AlI <sub>3</sub>	43.4 AsI <sub>3</sub>
74.6 Al <sub>2</sub> SiO <sub>5</sub> /sillimanite	44.3 Ph <sub>3</sub> AsO
74.7 AlCl <sub>3</sub>	44.9 As <sub>2</sub> O <sub>3</sub>
74.7 MgAl <sub>2</sub> O <sub>4</sub>	45.3 AsBr <sub>3</sub>
74.8 Al <sub>2</sub> SiO <sub>5</sub> /mullite	46.2As <sub>2</sub> O <sub>5</sub>
74.8 H Zeolon	47.8 KAsF <sub>6</sub>
75.2 AlBr <sub>3</sub>	
75.6 LiAlH <sub>4</sub>	<b>As 2p3.pos</b>
76.3 AlF	

**Ar (L3M23M23).pos**

211.0 Ar

**Ar (L3M23M23;3P).pos**

212.8 Ar

**Ar 2p.pos**

241.5 Ar in graphite

**As (L2M45M45).pos**

1254.9 As<sub>2</sub>O<sub>3</sub>  
 1254.6 NaAsO<sub>2</sub>  
 1252.9 Na<sub>2</sub>HAsO<sub>4</sub>

**As (L3M45M45).pos, As (LMM).pos**

1225.1 GaAs  
 1224.8 As  
 1222.1 As<sub>2</sub>S<sub>3</sub>

1323.1 GaAs  
 1324.3 As  
 1325.7 AsO  
 1326.4 As<sub>2</sub>O<sub>3</sub>  
 1327.4 As<sub>2</sub>O<sub>5</sub>

**Au (M4N67N67).pos**

2101.5 Au

**Au (M5N67N67).pos, Au (MNN).pos**

2015.7 Au

**Au (N7VV).pos**

69.8 Au

**Au (N67VV).pos, Au (NVV).pos**

71.2 Au

**Au 4f7.pos**

84.0 Au  
84.5 AuSn  
85.1 AuSn<sub>4</sub>  
85.3 ClAuPh<sub>3</sub>P

**B 1s.pos**

186.5 B<sub>4</sub>C  
187.2 NaBH<sub>4</sub>  
187.3 B  
187.5 TiB  
187.8 B<sub>10</sub>H<sub>14</sub>  
188.5 AlB<sub>2</sub>  
190.5 BN  
193.0 H<sub>3</sub>BO<sub>3</sub>  
192.6 Na<sub>2</sub>B<sub>4</sub>O<sub>7</sub>·10H<sub>2</sub>O  
193.1 B<sub>2</sub>O<sub>3</sub>  
194.9 NaBF<sub>4</sub>

**Ba (M4N45N45).pos, Ba (MNN).pos**

601.6 Ba  
598.0 BaO  
596.3 Ba(ClO<sub>3</sub>)·H<sub>2</sub>O  
596.1 BaSO<sub>4</sub>  
596.1 Ba(NO<sub>3</sub>)<sub>2</sub>  
595.3 Ba(ClO<sub>4</sub>)<sub>2</sub>  
595.2 Ba/Ca/Cd/Sr/in\_montmorillonite  
594.9 BaF<sub>2</sub>  
594.9 BaCl<sub>2</sub>·2H<sub>2</sub>O

**Ba (N45O23O23).pos, Ba (NOO).pos**

59.5 BaF<sub>2</sub>/Au  
56.0 BaCl<sub>2</sub>  
57.8 BaBr<sub>2</sub>  
55.4 BaBr<sub>2</sub>  
55.3 BaTiO<sub>3</sub>

**Ba (N45O23V).pos**

71.4 BaBr<sub>2</sub>  
71.2 BaCl<sub>2</sub>  
68.6 BaTiO<sub>3</sub>

**Ba 3d5.pos**

778.9 BaCrO<sub>4</sub>  
779.1 BaMoO<sub>4</sub>  
779.8 BaS

779.9 BaO  
779.9 BaCO<sub>3</sub>  
780.6 Ba  
780.7 Ba(NO<sub>3</sub>)<sub>2</sub>  
780.8 BaSO<sub>4</sub>  
781.7 BaF<sub>2</sub>

**Be 1s.pos**

111.8 Be  
113.7 BeO  
115.3 BeF<sub>2</sub>  
115.3 NaBeF<sub>3</sub>

**Bi (N6O45O45).pos, Bi (NOO)**

103.7 Bi

**Bi (N7O45O45).pos**

100.1 Bi

**Bi 4f7.pos**

156.8 Bi  
158.3 Bi<sub>2</sub>MoO<sub>6</sub>  
158.9 Bi<sub>2</sub>S<sub>3</sub>  
159.3 BiI<sub>3</sub>  
159.8 Bi<sub>2</sub>O<sub>3</sub>  
159.9 BiOCl  
160.8 BiF<sub>3</sub>  
161.2 Bi<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>·H<sub>2</sub>O

**Br (L3M45M45).pos, Br (LMM).pos**

1390.1 [N(C<sub>16</sub>H<sub>33</sub>)(CH<sub>3</sub>)<sub>3</sub>]Br  
1389.2 LiBr  
1388.3 NaBr  
1388.0 KBr  
1384.4 KBrO<sub>3</sub>

**Br 3d.pos**

66.7 Ph<sub>4</sub>AsBr  
68.3 CsBr  
68.4 RbBr  
68.7 KBr  
68.8 NaBr  
68.9 LiBr  
68.9 CuBr<sub>2</sub>

69.2 K<sub>2</sub>PtBr<sub>6</sub>  
 69.3 K<sub>2</sub>PtBr<sub>4</sub>  
 70.1 Bromanil  
 74.8 KBrO<sub>3</sub>

### C (KLL).pos, C (KLL).pos

262.0 Graphite

### C 1s.pos

281.6 TiC  
 282.8 WC  
 283.9 Fe<sub>3</sub>C  
 283.9 K<sub>3</sub>Fe(CN)<sub>6</sub>  
 284.5 Graphite  
 284.6 PhNH<sub>2</sub>  
 284.7 Benzene  
 285.0 -CH<sub>2</sub>-  
 285.5 C<sub>5</sub>H<sub>5</sub>N  
 285.6 C<sub>6</sub>H<sub>5</sub>F(C\*H)  
 285.6 EtNH<sub>2</sub>  
 285.7 C<sub>6</sub>H<sub>5</sub>Cl(C\*H)  
 285.7 ( -C\*H<sub>2</sub>CFH-)n  
 285.9 PVC(-C\*H<sub>2</sub>CHCl-)  
 286.1 KCN  
 286.3 CH<sub>3</sub>C\*H<sub>2</sub>OH  
 286.3 C\*H<sub>3</sub>CN  
 286.4 (-C\*H<sub>2</sub>CF<sub>2</sub>-)  
 286.5 ( CH<sub>3</sub>C\*H<sub>2</sub>)<sub>2</sub>O  
 286.5 PVA(-CH<sub>2</sub>C\*HOH-)n  
 286.9 CH<sub>3</sub>COOC\*H<sub>2</sub>CH<sub>3</sub>  
 287.0 CS<sub>2</sub>  
 287.0 PVC(-CH<sub>2</sub>C\*HCl-)  
 287.1 C<sub>6</sub>H<sub>5</sub>Cl(C\*Cl)  
 287.2 CH<sub>3</sub>C\*N  
 287.8 C<sub>6</sub>H<sub>5</sub>F(C\*F)  
 287.9 (-CH<sub>2</sub>C\*FH-)n  
 287.9 CH<sub>3</sub>C\*OCH<sub>3</sub>  
 288.0 Fe(CO)<sub>5</sub>  
 288.0 H<sub>2</sub>NCSNH<sub>2</sub>  
 288.2 CH<sub>3</sub>C\*OONa  
 288.4 CH<sub>3</sub>C\*ONH<sub>2</sub>  
 288.7 H<sub>2</sub>NCONH<sub>2</sub>  
 289.3 CH<sub>3</sub>C\*OOH  
 289.4 Na<sub>2</sub>CO<sub>3</sub>  
 289.5 Cl<sub>3</sub>C\*COONa  
 289.6 CaCO<sub>3</sub>  
 289.6 HCCl<sub>3</sub>  
 290.0 NaHCO<sub>3</sub>

290.9 (-CH<sub>2</sub>C\*F<sub>2</sub>-)n  
 291.9 CO<sub>2</sub>  
 292.2 Teflon(-CF<sub>2</sub>CF<sub>2</sub>-)n  
 292.4 CCl<sub>4</sub>  
 292.9 C\*F<sub>3</sub>COOEt  
 294.7 HCF<sub>3</sub>  
 296.7 CF<sub>4</sub>

### Ca (L2M23M23).pos, Ca (LMM).pos

298.2 Ca  
 292.5 CaO  
 291.9 CaCO<sub>3</sub>  
 291.9 CaCl<sub>2</sub>  
 288.9 CaF<sub>2</sub>

### Ca 2p3.pos

345.9 Ca  
 346.3 CaCrO<sub>4</sub>  
 346.5 CaS  
 347.0 CaCO<sub>3</sub>  
 347.0 Ca<sub>3</sub>Si<sub>3</sub>O<sub>9</sub>  
 347.3 CaO  
 347.9 CaF<sub>2</sub>  
 348.0 CaSO<sub>4</sub>  
 348.3 CaCl<sub>2</sub>

### Cd (M4N45N45).pos, Cd (MNN).pos

383.6 Cd  
 382.5 CdO  
 382.4 CdTe  
 382.2 CdSe<sub>0.65</sub>Te<sub>0.35</sub>  
 381.4 Zn<sub>0.30</sub>Cd<sub>0.70</sub>Se  
 381.5 Zn<sub>0.50</sub>Cd<sub>0.50</sub>Se  
 381.2 Zn<sub>0.70</sub>Cd<sub>0.30</sub>Se  
 381.0 Zn<sub>0.90</sub>Cd<sub>0.10</sub>Se  
 381.3 CdS  
 381.0 CdSe  
 380.5 CdI<sub>2</sub>  
 380.0 Cd(OH)<sub>2</sub>  
 380.0 CdBr<sub>2</sub>·4H<sub>2</sub>O  
 379.8 (CdCl<sub>2</sub>)<sub>2</sub>·5H<sub>2</sub>O  
 378.5 CdF<sub>2</sub>  
 378.3 Ba/Ca/Cd/Sr/in\_montmorillonite

### Cd (M5N45N45).pos

377.0 Cd

370.5 Cd  
 374.4 CdI<sub>2</sub>  
 375.8 CdTe  
 369.5 CdTe  
 368.5 CdTe  
 375.6 CdO  
 374.8 CdSe  
 374.5 CdS  
 372.2 CdF<sub>2</sub>

**Cd 3d5.pos**

404.2 CdO  
 404.6 Hg<sub>0.8</sub>Cd<sub>0.2</sub>Te  
 405.0 CdSe  
 405.1 Cd  
 405.1 Cd(OH)<sub>2</sub>  
 405.1 CdCO<sub>3</sub>  
 405.2 CdTe  
 405.3 CdS  
 405.4 CdI<sub>2</sub>  
 405.9 CdF<sub>2</sub>  
 406.0 CdBr<sub>2</sub>  
 406.1 CdCl<sub>2</sub>

**Ce (M4N45N67).pos, Ce (MNN).pos**

771.0 CeO<sub>2</sub>

**Ce (M5N45N67).pos**

755.0 CeO<sub>2</sub>

**Ce 3d5.pos**

881.9 CeO<sub>2</sub>  
 883.5 CeAl<sub>2</sub>  
 883.6 CeCu<sub>2</sub>Si<sub>2</sub>  
 883.9 Ce  
 884.3 CePd<sub>3</sub>  
 884.3 CeSe  
 886.0 CeH<sub>3</sub>

**Cl (Kl23L23).pos, Cl (KLL).pos**

2392.2 CsCl  
 2391.3 KCl  
 2391.0 RbCl  
 2391.4 LiCl  
 2390.9 NaCl

**Cl (LVV).pos**

182.5 GdCl<sub>3</sub>.H<sub>2</sub>O  
 181.0 KCl  
 181.0 KClO<sub>3</sub>  
 180.7 KClO<sub>4</sub>

**Cl 2p3.pos**

196.3 CsCl  
 198.3 UOCl<sub>2</sub>  
 198.4 KCl  
 198.5 LiCl  
 198.5 ZnCl<sub>2</sub>  
 198.6 NaCl  
 198.6 RhCl<sub>3</sub>  
 198.8 K<sub>2</sub>PdCl<sub>4</sub>  
 198.8 K<sub>2</sub>PtCl<sub>4</sub>  
 198.9 PdCl<sub>2</sub>  
 199.4 NiCl<sub>2</sub>  
 199.6 CuCl<sub>2</sub>  
 199.7 ZnCl<sub>2</sub>  
 200.5 Poly(-chlorostyren)  
 200.6 PVC  
 206.2 KClO<sub>3</sub>  
 208.7 KClO<sub>4</sub>

**Co (L3M45M45).pos**

773.6 Co<sub>3</sub>O<sub>4</sub>  
 773.2 Co  
 769.4 CoO  
 766.8 K<sub>3</sub>Co(CN)<sub>6</sub>  
 768.6 Co(NH<sub>3</sub>)<sub>6</sub>Cl<sub>3</sub>  
 768.3 CoSiF<sub>6</sub>

**Co (LMM).pos**

770.7 Co((C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>PO)<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>

**Co (M23VV).pos**

53.6 Co

**Co 2p3.pos**

778.1 CoS<sub>2</sub>  
 778.3 Co  
 779.9 Co<sub>3</sub>O<sub>4</sub>

780.3 CoOOH	
780.4 CoO	61.6 CsBr
781.3 Co(OH) <sub>2</sub>	61.4 CsCl
781.3 CoAl <sub>2</sub> O <sub>4</sub>	
781.7 Co(NH <sub>3</sub> ) <sub>6</sub> Cl <sub>3</sub>	<b>Cs 3d5.pos</b>
781.9 K <sub>3</sub> Co(CN) <sub>6</sub>	
782.4 CoF <sub>3</sub>	723.6 CsF
783.0 CoF <sub>2</sub>	723.9 CsI
783.6 CoSiF <sub>6</sub>	723.9 Cs <sub>2</sub> SO <sub>4</sub>
784.0 CoSO <sub>4</sub>	724.0 CsBr
	724.0 CsCl
<b>Cr (L3M23M45).pos, Cr (LMM).pos</b>	724.0 CsF
	724.2 CsOH
528.8 Cr <sub>2</sub> O <sub>3</sub>	726.4 Cs
527.2 Cr	
525.5 CrF <sub>3</sub>	<b>Cu (L2M45M45).pos</b>
<b>Cr 2p3.pos</b>	939.0 Cu
	937.80 CuO
574.3 Cr	934.10 (GeO <sub>2</sub> ) <sub>0.5</sub> (Na <sub>2</sub> O) <sub>0.3</sub> (CuO) <sub>0.2</sub> /glass
576.3 K <sub>3</sub> Cr(CN) <sub>6</sub>	934.00 (GeO <sub>2</sub> ) <sub>0.6</sub> (Na <sub>2</sub> O) <sub>0.3</sub> (CuO) <sub>0.1</sub> /glass
576.6 Cr <sub>2</sub> O <sub>3</sub>	933.50
576.6 Cr(CO) <sub>6</sub>	(GeO <sub>2</sub> ) <sub>0.65</sub> (Na <sub>2</sub> O) <sub>0.3</sub> (CuO) <sub>0.05</sub> /glass
576.9 Cr(acac) <sub>3</sub>	
577.0 CrOOH	<b>Cu (L2VV).pos</b>
577.3 Cr(OH) <sub>3</sub>	
577.4 CrCl <sub>3</sub>	938.3 Cu
579.4 Na <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	934.7 Cu
579.9 K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub>	
580.1 CrO <sub>3</sub>	<b>Cu (L3M45M45).pos, Cu (LMM).pos</b>
580.5 Na <sub>2</sub> CrO <sub>4</sub>	
<b>Cs (M4N45N45).pos, Cs (MNN).pos</b>	918.6 Cu
	918.6 Cu <sub>64</sub> Zn <sub>36</sub>
568.7 CsOH	918.5 Ag <sub>28.6</sub> Au <sub>17.1</sub> Cu <sub>54.3</sub>
568.4 Cs <sub>2</sub> SO <sub>4</sub>	918.4 CuSe
	918.1 CuS
<b>Cs (N5O23O23).pos</b>	918.0 CuCr <sub>2</sub> O <sub>4</sub>
	917.9 CuO
46.3 Cs	917.8 CuFeS <sub>2</sub>
	917.7 Cu <sub>2</sub> Se
<b>Cs (N45O23O23).pos</b>	917.7 AgCuSe
	917.6 CuInSe <sub>2</sub>
50.8 CsF/Au	917.1 Cu <sub>2</sub> S
49.0 CsCl	917.0 Cu <sub>2</sub> CO <sub>3</sub> (OH) <sub>2</sub>
51.2 CsCl	917.0 CuIn <sub>3</sub> Se <sub>5</sub>
49.2 CsBr	917.0 CuGa <sub>5</sub> Se <sub>8</sub>
51.4 CsBr	916.8 Cu(OH) <sub>2</sub>
	916.8 Al <sub>2</sub> CuO <sub>4</sub>
<b>Cs (N45O23V).pos</b>	916.7 Cu <sub>2</sub> O
	916.7 CuInS <sub>2</sub>

916.6 CuMoO4	<b>Dy (M5N45N45).pos</b>
916.6 Cu3Mo2O9	
916.3 CuCO3	960.0 Dy
916.3 CuBr2	
916.1 CuI	<b>Dy (M5N67N67).pos</b>
916.1 CuSO4	
915.3 CuCl	1280.0 Dy
915.5 CuCl2	
915.3 Cu(NO3)2	<b>Dy (M45N45N67).pos, Dy (MNN).pos</b>
915.2 CuSiO3	
915.1 CuF2	1115.0 Dy
914.6 CuCN	
914.5 [CuC(CN)3]	<b>Dy 3d5.pos</b>
914.4 Cu2S	
	1295.5 Dy
<b>Cu (L3VV).pos</b>	1298.9 Dy2O3
921.2 Cu	<b>Dy 4d.pos</b>
918.4 Cu	
916.0 Cu	152.4 Dy
914.1 Cu	167.7 Dy2O3
911.0 Cu	
<b>Cu (M23VV).pos, Cu (MVV).pos</b>	
62.4 Cu	
63.7 6-8A Fe/Cu	
60.8 6-8A Fe/Cu	
<b>Cu 2p3.pos</b>	
931.9 CuInSe2	1035.0 Er
932.3 CuS	1037.0 Er2O3
932.5 Cu2O	
932.5 Cu2S	
932.5 CuCl	
932.6 Cu64Zn36	
932.7 Cu	<b>Er (M5N67N67).pos</b>
933.1 CuCN	
933.8 CuO	1387.0 Er
935.2 CuCl2	1386.0 Er2O3
934.5 Cu(acac)2	
934.9 CuSO4	
935.1 Cu(OH)2	<b>Er (M45N45N67).pos, Er (MNN).pos</b>
936.1 CuF2	
<b>Dy (M4N67N67).pos</b>	
1318.0 Dy	
	<b>Er 4d.pos</b>
	167.3 Er
	168.7 Er2O3
	<b>Eu (M4N67N67).pos</b>
	1150.0 Eu

<b>Eu (M5N45N45).pos</b>	655.5 MnF <sub>2</sub>
846.0 Eu	655.5 NiF <sub>2</sub>
<b>Eu (M5N67N67).pos</b>	655.4 CaF <sub>2</sub>
1120.0 Eu	655.3 HfF <sub>4</sub>
<b>Eu (M45N45N67).pos, Eu (MNN).pos</b>	655.2 K <sub>2</sub> NbF <sub>7</sub>
980.0 Eu	655.1 Na <sub>2</sub> TiF <sub>6</sub>
<b>Eu 3d5.pos</b>	655.1 Na <sub>2</sub> ZrF <sub>6</sub>
1125.6 Eu	655.0 NaF
<b>Eu 4d.pos</b>	655.0 K <sub>2</sub> TaF <sub>7</sub>
128.2 Eu	654.7 LiF
135.9 Eu <sub>2</sub> O <sub>3</sub>	654.4 MgF <sub>2</sub>
<b>F (KL1L1).pos</b>	654.4 NaSnF <sub>3</sub>
608.0 LiF	654.1 Na <sub>3</sub> AlF <sub>6</sub>
<b>F (KL1L23).pos</b>	654.0 Na <sub>2</sub> GeF <sub>6</sub>
627.4 LiF	653.9 KSbF <sub>6</sub>
<b>F (KL23L23).pos, F (KLL).pos</b>	653.8 CsF
659.3 AgF	653.5 SiF <sub>6</sub> monolayer/Ni
658.5 PbF <sub>2</sub>	653.0 Na <sub>2</sub> SiF <sub>6</sub>
658.0 LaF <sub>3</sub>	653.0 SiF <sub>6</sub> monolayer/O <sub>2</sub> /Ni
657.2 PrF <sub>3</sub>	652.9 [Ni(CF <sub>3</sub> COO) <sub>2</sub> ]
657.0 SmF <sub>3</sub>	652.8 NaBF <sub>4</sub>
657.0 NdF <sub>3</sub>	652.6 Al <sub>2</sub> .3(OH)0.3.H <sub>2</sub> O
657.0 ThF <sub>4</sub>	652.4 (-CF <sub>2</sub> -CF <sub>2</sub> -) <sub>n</sub>
656.6 CuF <sub>2</sub>	651.7 AlF <sub>3</sub>
656.4 InF <sub>3</sub>	<b>F 1s.pos</b>
656.3 SrF <sub>2</sub>	683.9 KF
656.2 BaF <sub>2</sub>	684.5 CuF <sub>2</sub>
656.1 GdF <sub>3</sub>	684.5 NaF
656.0 CdF <sub>2</sub>	684.6 CdF <sub>2</sub>
656.0 K <sub>3</sub> FeF <sub>6</sub>	684.8 CaF <sub>2</sub>
655.8 YF <sub>3</sub>	684.8 UF <sub>2</sub>
655.7 K <sub>2</sub> TiF <sub>6</sub>	685.0 LiF
655.6 ZnF <sub>2</sub>	685.5 MgF <sub>2</sub>
655.6 CrF <sub>3</sub>	685.5 Na <sub>3</sub> AlF <sub>6</sub>
	685.9 CsF
	686.2 Na <sub>2</sub> SiF <sub>6</sub>
	686.9 (-CHF-CH <sub>2</sub> -) <sub>n</sub>
	687.0 NaBF <sub>4</sub>
	688.2 (-CF <sub>2</sub> -CH <sub>2</sub> -) <sub>n</sub>
	689.7 (-CF <sub>2</sub> -CF <sub>2</sub> -) <sub>n</sub>
	694.2 NF <sub>4</sub> BF <sub>4</sub>
	<b>Fe (L3M45M45).pos, Fe (LMM).pos</b>
	703.0 FeS <sub>2</sub>
	702.9 FeB
	702.9 Fe <sub>2</sub> B
	702.7 Fe

702.6 CuFeS <sub>2</sub>	20.5 Ga <sub>2</sub> O <sub>3</sub>
<b>Fe (M23VV).pos, Fe (MVV).pos</b>	<b>Gd (M4N67N67).pos</b>
48.6 8-9A Fe/Cu	1202.0 Gd
<b>Fe 2p3.pos</b>	<b>Gd (M5N45N45).pos</b>
706.7 Fe	884.0 Gd
707.1 K <sub>4</sub> Fe(CN) <sub>6</sub>	<b>Gd (M5N6N67).pos</b>
707.2 FeS <sub>2</sub>	1170.0 Gd
707.4 FeB	
708.1 Fe <sub>3</sub> C	<b>Gd (M45N45N67).pos, Gc (MNN).pos</b>
709.6 FeO	1020.0 Gd
709.6 K <sub>3</sub> Fe(CN) <sub>6</sub>	
710.6 Fe <sub>3</sub> O <sub>4</sub>	<b>Gd 3d5.pos</b>
710.9 Fe <sub>2</sub> O <sub>3</sub>	1187.0 Gd
712.1 FeSO <sub>4</sub>	1189.0 Gd <sub>2</sub> O <sub>3</sub>
<b>Ga (L2M4M4).pos</b>	1190.0 Gd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>
1091.5 GaN	<b>Gd 4d.pso</b>
<b>Ga (L3M45M45).pos, Ga (LMM).pos</b>	140.4 Gd
1068.0 Ga	143.8 Gd <sub>2</sub> O <sub>3</sub>
1066.3 GaAs	143.8 Gd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>
1065.6 GaP	<b>Ge (L3M45M45).pos, Ge (LMM).pos</b>
1065.3 Ga <sub>2</sub> Se <sub>3</sub>	1145.2 Ge
1065.3 CuGa <sub>5</sub> Se <sub>8</sub>	1144.8 GeTe
1064.3 GaN	1143.7 GeS
1062.3 Ga <sub>2</sub> O <sub>3</sub>	1143.5 GeSe
<b>Ga (M23VV).pos, Ga (MVV).pos</b>	1142.8 Ge <sub>2</sub> Se <sub>3</sub>
56.1 Ga	1141.8 GeSe <sub>2</sub>
<b>Ga 2p3.pos</b>	1141.7 GeSe <sub>3</sub>
1116.7 Ga	1137.8 GeO <sub>2</sub>
1116.8 GaP	1136.6 Si <sub>0.4</sub> Ge <sub>0.9</sub> O <sub>0.6</sub>
1116.9 Ga <sub>2</sub> O <sub>3</sub>	1135.7 Na <sub>2</sub> GeF <sub>6</sub> 1135.7 Na <sub>2</sub> GeF <sub>6</sub>
<b>Ga 3d.pos</b>	<b>Ge 2p3.pos</b>
18.7 Ga	1217.2 Ge
19.0 AlGaAs	1219.8 GeS <sub>2</sub>
19.3 GaAs	1220.4 GeO <sub>2</sub>
19.3 GaP	1221.3 Na <sub>2</sub> GeF <sub>6</sub>
19.5 GaN	

**Ge 3d.pos**

29.3 Ge  
 30.5 GeS  
 30.7 GeSe  
 32.7 GeO<sub>2</sub>  
 33.3 Na<sub>2</sub>GeF<sub>6</sub>

**Hf (M4N67N67).pos**

1669.0 Hf

**Hf (M5N67N67).pos, Hf (MNN).pos**

1615.0 Hf

**Hf (M45N45N67).pos**

1420.0 Hf

**Hf 4f7.pos**

14.2 Hf  
 16.7 HfO<sub>2</sub>

**Hg (M4N67N67).pos, Hg (MNN).pos**

2159.8 Hg

**Hg 4f7.pos**

99.9 Hg  
 100.2 Hg<sub>0.8</sub>Cd<sub>0.2</sub>Te  
 100.8 Hg<sub>2</sub>Cl<sub>2</sub>  
 100.8 HgO  
 101.0 HgS/cinnabar  
 101.4 HgCl<sub>2</sub>

**Ho (M4N67N67).pos**

1372.0 Ho

**Ho (M5N45N45).pos**

998.0 Ho

**Ho (M5N67N67).pos**

1332.0 Ho

**Ho (M45N45N67).pos, Ho (MNN).pos**

1165.0 Ho

**Ho 4d.pos**

159.6 Ho

**I (M4N45N45).pos**

519.0 I<sub>2</sub>  
 518.3 AgI  
 517.7 CdI  
 517.3 UI<sub>3</sub>  
 517.0 KI  
 517.0 LiI  
 516.4 SrI<sub>2</sub>  
 513.8 KNiIO<sub>6</sub>

**I (M5N45N45).pos, I (MNN).pos**

507.3 NiI<sub>2</sub>  
 507.1 CuI  
 507.0 CdI<sub>2</sub>  
 506.8 AgI  
 506.0 ZnI<sub>2</sub>  
 503.6 KNiIO<sub>6</sub>

**I 3d5.pos**

618.4 NaI  
 618.8 KI  
 619.2 CdI  
 619.4 AgI  
 619.7 LiI  
 619.9 I<sub>2</sub>  
 620.3 UI<sub>3</sub>  
 621.5 ICl  
 622.5 ICl<sub>3</sub>  
 623.3 I<sub>2</sub>O<sub>5</sub>  
 623.5 NaIO<sub>3</sub>  
 624.0 NaIO<sub>3</sub>

**In (M4N45N45).pos, In (MNN).pos**

410.2 In  
 409.3 InP  
 408.9 In<sub>2</sub>Te<sub>3</sub>  
 408.5 CuInSe<sub>2</sub>  
 408.0 InP

408.1 In <sub>2</sub> Se <sub>3</sub>	<b>Ir (M5N67N67).pos, Ir (MNN).pos</b>
407.4 CuIn <sub>3</sub> Se <sub>5</sub>	
407.3 In <sub>2</sub> S <sub>3</sub>	1900.8 Ir
407.3 CuInS <sub>2</sub>	
406.5 In <sub>2</sub> O <sub>3</sub>	<b>Ir (N4N67N67).pos, Ir (NNN).pos</b>
405.8 InI <sub>3</sub>	
405.7 In(OH) <sub>3</sub> .nH <sub>2</sub> O	172.2 Ir
405.3 In(OH) <sub>3</sub>	
404.8 InBr <sub>3</sub>	<b>Ir 4f7.pos</b>
404.7 InPO <sub>4</sub>	
404.6 InCl <sub>3</sub>	60.8 Ir
404.6 In(PO <sub>3</sub> ) <sub>3</sub>	62.0 IrO <sub>2</sub>
404.4 In(PO <sub>3</sub> ) <sub>4</sub>	62.7 IrCl <sub>3</sub>
404.1 (NH <sub>4</sub> ) <sub>3</sub> [InF <sub>6</sub> ]	63.5 K <sub>2</sub> IrCl <sub>6</sub>
403.7 InF <sub>3</sub>	
401.6 InSb	<b>K (L2M23M23;1D).pos</b>
<b>In (M5N45N45).pos</b>	250.7 KBr
	250.1 KF
397.5 In	249.3 KSbF <sub>6</sub>
393.0 In	
397.5 InP	<b>K (L3M23M23).pos, K (LMM).pos</b>
396.0 InP	
<b>In (M5N45N45;1G).pos</b>	250.1 KF
	249.3 KSbF <sub>6</sub>
402.6 In	248.3 KBr
<b>In 3d5.pos</b>	<b>K 2p3.pos</b>
	292.2 K <sub>4</sub> P <sub>2</sub> O <sub>7</sub>
443.8 In	292.8 KCl
444.1 CuInSe <sub>2</sub>	292.8 KI
444.3 InSb	292.5 KF
444.5 InP	293.1 KBr
444.5 In <sub>2</sub> Te <sub>3</sub>	293.5 K <sub>3</sub> PO <sub>4</sub>
444.8 In <sub>2</sub> Se <sub>3</sub>	293.7 KSbF <sub>6</sub>
444.8 In <sub>2</sub> O <sub>3</sub>	294.6 K
444.9 In <sub>2</sub> S <sub>3</sub>	294.7 KCN
444.9 InCl	
445.0 In(OH) <sub>3</sub>	<b>Kr (L3M45M45).pos</b>
445.4 In(acac) <sub>3</sub>	
445.8 InI <sub>3</sub>	1460.4 Kr(gas)(vac)
446.0 InBr <sub>3</sub>	
446.0 InCl <sub>3</sub>	<b>Kr 3d.pos</b>
446.2 InF <sub>3</sub>	
<b>Ir (M4N67N67).pos</b>	87.0 Kr in graphite
	<b>La (M4N45N67).pos</b>
1977.8 Ir	
	728.0 La <sub>2</sub> O <sub>3</sub>

**La (M5N45N67).pos**711.0 La<sub>2</sub>O<sub>3</sub>**La (N45O23O23).pos, La (NOO).pos**64.0 LaF<sub>3</sub>/Au**La 3d5.pos**834.8 La<sub>2</sub>O<sub>3</sub>

835.8 La

838.8 LaH<sub>3</sub>**La 4d5.pos**101.3 La<sub>2</sub>O<sub>3</sub>

103.9 La

**Li (KVV).pos**

52.9 Li

48.4 Li-O/1L O<sub>2</sub>43.6 Li-O/1L O<sub>2</sub>37.6 Li-O/1L O<sub>2</sub>42.3 Li-O/5L O<sub>2</sub>36.0 Li-O/5L O<sub>2</sub>**Li 1s.pos**

54.8 Li

54.9 LiOH

55.2 Li<sub>2</sub>CO<sub>3</sub>55.6 Li<sub>2</sub>O

55.7 LiF

56.1 LiCl

56.8 LiBr

**Lu (M4N67N67).pos**

1615.0 Lu

**Lu (M5N45N67).pos**

1370.0 Lu

**Lu (M5N67N67).pos, Lu (MNN).pos**

1560.0 Lu

**Lu 4d5.pos**196.5 Lu<sub>2</sub>O<sub>3</sub>

196.6 Lu

198.5 Lu<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>**Lu 4f7.pos**

6.3 Lu

**Mg (KL23L23).pos, Mg (KLL).pos**

1185.6 Mg

1180.7 MgBr<sub>2</sub>·6H<sub>2</sub>O1180.6 (Mg/Fe)<sub>2</sub>SiO<sub>4</sub>1180.5 KMg<sub>3</sub>Si<sub>3</sub>AlO<sub>10</sub>(OH/F)<sub>2</sub>1180.5 Mg<sub>3</sub>H<sub>2</sub>(SiO<sub>3</sub>)<sub>4</sub>1180.5 (Mg/Fe)SiO<sub>3</sub>

1180.4 MgO

1179.0 (Na/Al/Mg)Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>·nH<sub>2</sub>O1178.8 MgSO<sub>4</sub>·7H<sub>2</sub>O1178.5 MgCl<sub>2</sub>/Au1178.2 MgF<sub>2</sub>**Mg (L23VV).pos**

43.0 Mg/Ru

31.0 O<sub>2</sub>/Mg/Ru**Mg 1s.pos**1302.7 Mg(OH)<sub>2</sub>

1303.2 Mg

1304.0 MgAl<sub>2</sub>O<sub>3</sub>1305.0 MgF<sub>2</sub>**Mg 2p.pos**49.5 Mg(OH)<sub>2</sub>

49.6 Mg

50.4 MgAl<sub>2</sub>O<sub>4</sub>

50.4 MgO

51.0 MgF<sub>2</sub>51.6 MgSO<sub>4</sub>·7H<sub>2</sub>O**Mn (L3M23M45).pos, Mn (LMM).pos**

586.4 Mn

585.7 MnO<sub>2</sub>

585.0 Mn2O3  
 584.8 MnS  
 583.7 Mn3O4  
 581.0 MnSO4

**Mn 2p3.pos**

638.3 Na4Mn(CN)6  
 638.5 Mn(C5H5)2  
 638.8 Mn  
 640.9 MnO  
 640.9 MnS  
 641.4 Mn3O4  
 641.6 Mn2O3  
 641.7 MnOOH  
 642.0 MnCl2  
 642.1 MnBr2  
 642.6 MnO2  
 642.6 MnF2  
 644.9 MnSO4  
 647.0 KMnO4

**Mo (L2M45M45).pos, Mo (LMM).pos**

2137.4 MoOx  
 2143.6 Mo

**Mo (L3M45M45).pos**

2039.0 MoSi2  
 2038.8 Mo  
 2032.2 MoOx

**Mo 3d5.pos**

227.7 MoSi2  
 227.9 Mo  
 227.9 MoB2  
 229.0 MoS2  
 229.6 MoO2  
 230.0 MoCl3  
 230.6 MoCl4  
 231.0 MoCl5  
 232.1 (NH4)2MoO4  
 232.7 MoOx  
 232.8 MoO3

**N (KVV).pos**

396.6 Gd(NO3)3.5H2O

385.0 GaN  
 383.0 Fe2N  
 379.2 BN  
 376.6 NH3

**N 1s.pos**

397.0 GaN  
 397.7 Si3N4  
 398.0 K4Fe(CN)6  
 398.1 BN  
 398.5 Na(N\*NN\*)  
 398.7 NH3  
 398.8 C5H5N/Pyridine  
 398.9 EtNH2  
 399.2 PhCN  
 399.5 H2NCONH2  
 399.4 C6H12N4/Urotropin  
 399.8 KCN  
 400.2 C4H5N/Pyrrrole  
 401.3 (NH4)2SO4  
 401.4 Et4NCl  
 401.7 NH4Cl  
 402.2 Bu4NH5O4  
 402.9 Na(NN\*N)  
 403.1 Pyridine N-oxide  
 403.8 NaNO2  
 404.7 K2Pt(NO2)6  
 405.5 R-NO2  
 407.3 NaNO3  
 408.2 R-ONO2

**Na (KL23L23).pos, Na (KLL).pos**

994.3 Na  
 991.2 NaI  
 990.6 NaBr  
 990.5 Na2C2O4  
 990.3 NaCl  
 990.1 Na3PO4  
 989.9 NaOAc  
 989.8 Na2CO3  
 989.8 Na2SO4  
 989.8 Na2O  
 989.7 Na2HPO4  
 989.4 NaNO3  
 989.4 NaPO3  
 989.1 NaH2PO4  
 988.6 NaF  
 987.7 Na2SiF6

987.1 NaBF <sub>4</sub>	733.0 Nd
<b>Na (L23VV).pos</b>	<b>Nd (M45N45N67).pos</b>
23.8 NaI	840.0 Nd
23.1 NaBr	<b>Nd 3d5.pos</b>
21.6 NaCl	980.8 Nd
20.2 NaF	982.0 Nd <sub>2</sub> O <sub>3</sub>
<b>Na 1s.pos</b>	984.9 Nd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>
1070.8 NaN <sub>3</sub>	<b>Nd 4d.pos</b>
1070.8 Na <sub>2</sub> C <sub>2</sub> O <sub>4</sub>	120.8 Nd <sub>2</sub> O <sub>3</sub>
1071.1 Na <sub>3</sub> PO <sub>4</sub>	122.5 Nd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>
1071.1 NaOAc	<b>Ne (KL23L23).pos</b>
1071.2 NaF	818.0 Ne in Fe
1071.2 Na <sub>2</sub> SO <sub>4</sub>	<b>Ne 1s.pos</b>
1071.4 NaNO <sub>3</sub>	861.6 Ne in Au
1071.5 Na <sub>2</sub> CO <sub>3</sub>	863.1 Ne in graphite
1071.5 Na <sub>2</sub> HPO <sub>4</sub>	863.4 Ne in Fe
1071.6 NaI	<b>Ni (L2VV).pos</b>
1071.6 NaPO <sub>3</sub>	866.6 NiO
1071.6 NaCl	863.7 Ni(OH) <sub>2</sub>
1071.7 Na <sub>2</sub> SiF <sub>6</sub>	863.3 (Ni(OH) <sub>2</sub> ) <sub>0.75</sub> (H <sub>2</sub> O) <sub>0.16</sub> (NiCO <sub>3</sub> ) <sub>0.09</sub>
1071.7 NaBr	863.3 (Ni(OH) <sub>2</sub> ) <sub>3.2</sub> H <sub>2</sub> O
1071.8 Na	862.9 NiOOH
1072.0 NaH <sub>2</sub> PO <sub>4</sub>	862.7 KNiIO <sub>6</sub>
1072.5 Na <sub>2</sub> O	<b>Ni (L3M45M45).pos, Ni (LMM).pos</b>
1072.7 NaBF <sub>4</sub>	856.0 ((P <sub>2</sub> O <sub>5</sub> ) <sub>0.40</sub> (V <sub>2</sub> O <sub>5</sub> ) <sub>0.60</sub> ) <sub>0.95</sub> (NiO) <sub>0.05</sub>
<b>Nb (M45N23V).pos, Nb (MNV).pos</b>	855.7 ((P <sub>2</sub> O <sub>5</sub> ) <sub>0.40</sub> (V <sub>2</sub> O <sub>5</sub> ) <sub>0.60</sub> ) <sub>0.98</sub> (NiO) <sub>0.02</sub>
167.8 Nb	855.7 ((P <sub>2</sub> O <sub>5</sub> ) <sub>0.40</sub> (V <sub>2</sub> O <sub>5</sub> ) <sub>0.60</sub> ) <sub>0.90</sub> (NiO) <sub>0.10</sub>
165.6 NbH <sub>x</sub>	855.3 ((P <sub>2</sub> O <sub>5</sub> ) <sub>0.40</sub> (V <sub>2</sub> O <sub>5</sub> ) <sub>0.60</sub> ) <sub>0.85</sub> (NiO) <sub>0.15</sub>
161.6 Nb <sub>2</sub> O <sub>5</sub>	849.8 NiO
<b>Nb 3d5.pos</b>	848.1 Ni(OH) <sub>2</sub>
202.4 Nb	848.1 NiOOH
203.2 NbH <sub>x</sub>	847.3 (Ni(OH) <sub>2</sub> ) <sub>0.75</sub> (H <sub>2</sub> O) <sub>0.16</sub> (NiCO <sub>3</sub> ) <sub>0.09</sub>
203.7 NbO	846.2 Ni
203.8 NbN	846.0 Ni/Ca <sub>0.166</sub> Ni <sub>0.833</sub>
206.5 KNbO <sub>3</sub>	845.2 Al <sub>70</sub> Co <sub>15</sub> Ni <sub>15</sub>
207.1 NbBr <sub>5</sub>	844.9 AlNi
207.6 Nb <sub>2</sub> O <sub>5</sub>	
207.7 NbS <sub>2</sub>	
208.0 NbCl <sub>5</sub>	
<b>Nd (M5N45N45).pos, Nd (MNN).pos</b>	

843.2 ((P2O5)0.40(V2O5)0.60)0.90(NiO)0.10  
 842.9 NiO/Ca0.166Ni0.833  
 842.9 NiO  
 842.9 (Ni(OH)2)3.2H2O  
 842.4 NiF2  
 842.4 Ni(acac)2  
 841.7 Ni(OH)2/Ca0.166Ni0.833

**Ni 2p3.pos**

852.7 Ni  
 852.8 NiS  
 854.4 NiO  
 855.7 Ni(acac)2  
 855.9 Ni(OH)2  
 856.0 Ni2O3  
 856.7 NiCl2  
 856.8 NiSO4  
 857.1 Ni(NO3)2  
 857.5 NiF2.4H2O  
 861.0 K2NiF6

**O (KL23L23).pos, O (KLL).pos**

515.1 PbO2  
 513.1 PbO  
 513.2 Ag2O  
 511.8 H2MoO4  
 511.6 H2WO4  
 511.3 PbCO3  
 510.8 ZrO2  
 510.6 (CH3)2CH(CH2)CH(NH2)COOH  
 510.2 C6H5C(O)C(O)C6H5  
 510.0 NaC2H3O2  
 510.0 ZnO  
 509.9 CuCo3  
 509.7 CaCO3  
 509.5 COOH(CH2)4COOH  
 509.3 CaO  
 509.3 Mg(OH)2  
 509.3 [Mg(CH3C(O)CHC(O)CH3)2]  
 509.7 Na2Co3  
 509.4 HOCH2(CH2)8CH2OH  
 509.1 Na8(AlSiO4)6Cl2(OH)n  
 509.0 [Mg(C6H10OC(O)C3H7)]  
 508.8 CaSiO3  
 508.7 CaSO4  
 508.6 Al(OH)3  
 508.6 LiOH  
 508.5 Al2O3

508.5 Mol-Sieve-A  
 508.3 NaOH  
 508.1 KAl2(AlSi3O10)2(OH)2  
 507.9 NaPO3  
 507.7 H2O  
 507.7 NaAlSi3O8  
 507.6 -C6H5Si2O3C6H5-  
 507.4 Al2Si4O10(OH)2  
 507.0 H zeolon  
 506.8 SiO2

**O 1s.pos**

529.3 CrO2  
 529.5 NiO  
 529.6 Fe2O3  
 529.8 FeO  
 529.9 Co2O3  
 530.0 Fe3O4  
 530.1 K4P2O7  
 530.2 Co3O4  
 530.2 CrO3  
 530.2 CoO  
 530.4 K3PO4  
 530.6 Na2SiO3.3H2O  
 531.0 Al2O3/sapphire  
 531.2 Ni(OH)2  
 531.4 Al(OH)3  
 531.4 CaCO3  
 531.5 Cr2O3  
 531.6 Na2CO3  
 531.7 BeO  
 531.7 R-O-CO\*-Ph  
 531.8 Ni2O3  
 532.1 NiSO4  
 532.2 KClO4  
 532.2 p-Benzoquinone  
 532.2 PhCONH2  
 532.2 R-O-CO\*-(CH2)n-  
 532.3 KClO3  
 532.5 Na2SiO3.H2O\*  
 532.9 -(CH2)n-OH  
 533.0 B2O3  
 533.0 Ba(NO3)2  
 533.0 SiO2  
 533.1 R-O\*-CO-Ph  
 533.1 H2O  
 533.5 Hydroquinone  
 533.6 R-O\*-CO-(CH2)n-

**Os 4f7.pos**

50.7 Os  
 51.9 K<sub>2</sub>OsI<sub>6</sub>  
 52.0 OsO<sub>2</sub>  
 52.2 Os(HSO<sub>3</sub>)<sub>2</sub>  
 52.9 K<sub>2</sub>OsBr<sub>6</sub>  
 53.1 OsCl<sub>3</sub>  
 53.2 K<sub>2</sub>OsCl<sub>6</sub>  
 53.4 K<sub>2</sub>Os(NO)Cl<sub>5</sub>  
 55.2 K<sub>2</sub>OsO<sub>2</sub>(OH)<sub>4</sub>

**Os (M4N67N67).pos, Os (MNN).pos**

1907.7 K<sub>2</sub>OsCl<sub>6</sub>  
 1909.8 K<sub>4</sub>Os(CN)<sub>6</sub>

**P (KL23L23).pos, P (KLL).pos**

1858.6 Cd<sub>3</sub>P<sub>2</sub>  
 1858.4 InP  
 1858.2 Zn<sub>3</sub>P<sub>2</sub>  
 1858.0 Cd(3-x)Zn(x)P<sub>2</sub>  
 1858.0 CdP<sub>2</sub>  
 1858.0 Fe<sub>40</sub>Ni<sub>40</sub>P<sub>14</sub>B<sub>8</sub>  
 1858.0 ZnSiP<sub>2</sub>  
 1857.5 CdGeP<sub>2</sub>  
 1857.3 ZnP<sub>2</sub>  
 1857.3 GaP  
 1856.3 P  
 1856.1 P/red  
 1853.2 P<sub>4</sub>S<sub>10</sub>  
 1851.6 Na<sub>3</sub>SPO<sub>3</sub>  
 1850.9 Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>  
 1850.9 Ni<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>  
 1850.8 Mn<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>  
 1850.8 Na<sub>2</sub>HPO<sub>4</sub>  
 1850.6 FePO<sub>4</sub>  
 1850.5 Na<sub>3</sub>PO<sub>4</sub>  
 1849.9 Na<sub>4</sub>P<sub>2</sub>O<sub>7</sub>  
 1849.8 PON  
 1849.8 InPO<sub>4</sub>  
 1849.6 GaPO<sub>4</sub>  
 1849.0 BPO<sub>4</sub>  
 1848.6 NaPO<sub>3</sub>  
 1848.4 Na<sub>2</sub>PFO<sub>3</sub>  
 1848.0 P<sub>4</sub>O<sub>10</sub>  
 1845.4 [NH<sub>4</sub>]PF<sub>6</sub>  
 1845.4 [(CH<sub>3</sub>)P(N(CH<sub>3</sub>)<sub>2</sub>)<sub>2</sub>]  
 1845.2 NH<sub>4</sub>PF<sub>6</sub>  
 1843.8 [PCl<sub>2</sub>(C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>]

1843.4 [PCl<sub>2</sub>(N(CH<sub>3</sub>)<sub>2</sub>)<sub>2</sub>]  
 1842.8 [PCl(CH<sub>3</sub>)<sub>2</sub>]  
 1842.1 [PCl<sub>2</sub>(CH<sub>3</sub>O)]  
 1842.1 [P(O)(CH<sub>3</sub>O)(CH<sub>3</sub>)<sub>2</sub>]  
 1841.3 [PSF<sub>2</sub>(N(CH<sub>3</sub>)<sub>2</sub>)<sub>2</sub>]  
 1841.2 [PF(N(CH<sub>3</sub>)<sub>2</sub>)<sub>2</sub>]  
 1841.0 [P(O)Cl<sub>2</sub>(CH<sub>3</sub>O)]  
 1840.4 [PF<sub>2</sub>N]<sub>5</sub>

**P 2p3.pos**

128.3 Zn<sub>3</sub>P<sub>2</sub>  
 128.9 InP  
 129.4 GaP  
 129.8 ZnP<sub>2</sub>  
 130.7 P/red  
 130.9 Ph<sub>3</sub>P  
 132.5 Ph<sub>3</sub>PS  
 132.5 Ph<sub>3</sub>PO  
 132.8 Na<sub>3</sub>PO<sub>4</sub>  
 132.9 AlPO<sub>4</sub>  
 133.1 Na<sub>2</sub>HPO<sub>4</sub>  
 134.2 NaH<sub>2</sub>PO<sub>4</sub>  
 134.7 NaPO<sub>3</sub>  
 134.7 (PhO)<sub>3</sub>P  
 135.2 P<sub>4</sub>O<sub>10</sub>  
 137.7 NH<sub>4</sub>PF<sub>6</sub>  
 133.6 Na<sub>4</sub>P<sub>2</sub>O<sub>7</sub>

**Pb (N6O45O45).pos, Pb (NOO).pos**

96.3 Pb  
 95.5 PbTe  
 94.8 PbSe  
 94.6 PbS  
 93.4 PbI<sub>2</sub>  
 93.1 PbO<sub>2</sub>  
 92.9 PbO  
 92.8 PbCrO<sub>4</sub>  
 92.8 Pb<sub>3</sub>O<sub>4</sub>  
 92.6 PbBr<sub>2</sub>  
 92.6 PbTiO<sub>3</sub>  
 92.1 PbCl<sub>2</sub>  
 92.1 PbCO<sub>3</sub>  
 92.0 Pb(OH)<sub>2</sub>  
 91.7 Pb(NO<sub>3</sub>)<sub>2</sub>  
 91.7 Pb<sub>3</sub>(OH)<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>  
 91.7 PbZrO<sub>3</sub>  
 91.5 Pb(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>  
 91.1 PbSiO<sub>3</sub>

90.6 PbF2  
90.1 PbSO4

**Pb 4f7.pos**

136.8 Pb  
137.3 PbTe  
137.3 PbO  
137.4 PbO2  
137.5 PbS  
137.6 PbSe  
138.0 Pb(OH)2  
138.2 Ph4Pb  
138.5 PbI2  
138.6 PbSO3  
138.8 PbBr2  
138.8 PbF2  
138.9 PbCl2  
139.3 Pb(NO3)2  
140.0 PbSO4

**Pd (M4N45N45).pos, Pd (MNN).pos**

329.4 PdCl2  
327.8 Pd  
325.7 PdO  
323.1 K2PdCl4

**Pd (M45N23V).pos**

276.9 Pd  
274.7 PdO  
274.0 PdCl2

**Pd (M45N45N45).pos**

337.9 K2PdCl4  
327.8 Pd

**Pd 3d5.pos**

335.1 Pd  
336.3 PdO  
336.4 PdI2  
336.6 Pd2(Ph3P)2  
337.1 PdBr2  
337.7 K2PdBr4  
337.8 PdCl2  
337.9 PdO2  
337.9 K2PdCl4

338.6 Pd(OAc)2  
338.8 K2Pd(NO2)4  
340.3 K2PdCl6

**Pm (M5N45N45).pos**

770.0 Pm

**Pm (M45N45N67).pos**

885.0 Pm

**Pm 3d5.pos**

1033..5 PmCl3

**Pr (M5N45N45).pos, Pr (MNN).pos**

695.0 Pr

**Pr (M45N45N67).pos**

795.0 Pr

**Pr 3d5.pos**

931.8 Pr  
933.6 Pr2O3  
935.3 PrO2

**Pr 4d.pos**

116.1 Pr2O3  
116.2 PrO2

**Pt (M4N67N67).pos**

2040.5 Pt  
2035.2 K2PtCl4

**Pt (M5N67N67).pos, Pt (MNN).pos**

1960.7 Pt

**Pt 4f7.pos**

71.2 Pt  
71.4 Pt(Ph3P)3  
71.4 Pt(Ph3P)4  
72.5 Pt2Si

72.6 I2Pt(Me3P)2/cis  
 72.6 K2PtBr4  
 72.6 Pt(OH)2  
 72.7 I2Pt(Me3P)2/trans  
 73.0 PtSi  
 73.0 Cl2Pt(Ph3P)2/cis  
 73.4 K2PtCl4  
 73.4 K2PtI6  
 73.4 Pt(NH3)4Cl2  
 73.6 PtCl2  
 74.2 PtO  
 74.6 K2PtBr6  
 75.0 PtO2  
 75.4 K2PtCl6  
 75.5 PtCl4  
 75.9 Cl4Pt(Et3P)2  
 76.3 Pt(NH3)6Cl4  
 77.6 K2PtF6

**Rb 3d5.pos**

109.8 RbF  
 109.9 RbCl  
 110.0 Rb3PO4  
 110.0 RbBr  
 110.4 RbI  
 111.5 Rb

**Re 4f7.pos**

40.5 Re  
 43.2 ReO2  
 43.9 Cl3ReO(Ph3P)2  
 44.0 K2ReCl6  
 46.8 ReO3

**Rh 3d5.pos**

307.2 Rh  
 307.4 ClRh(Ph3P)3  
 308.5 KRhO2  
 308.6 RhI3  
 308.7 Rh2O3  
 308.8 CaRh2O4  
 309.4 Rh2WO6  
 309.8 K3RhCl6  
 310.0 RhCl3.3H2O  
 310.1 RhCl3  
 310.5 K3Rh(NO2)6

312.2 K3RhF6

**Ru 3d5.pos**

280.2 Ru  
 280.9 RuO2  
 281.8 RuCl3  
 282.5 RuO3  
 283.3 RuO4  
 284.2 BaRuO4

**S (KL23L23).pos, S (KLL).pos**

2119.9 FeS  
 2119.9 NiS  
 2119.9 PbS  
 2119.1 Ag2S  
 2119.1 FeAsS  
 2118.9 Sb2S3  
 2118.4 MoS2  
 2118.2 HgS  
 2118.1 Cu2S  
 2117.6 CdS  
 2117.1 ZnS  
 2116.7 K2S  
 2116.1 S  
 2116.1 S8  
 2116.1 Na2S.9H2O  
 2116.0 FeS2  
 2115.9 Na((C2H5)2NCS2).3H2O  
 2115.9 NiWS2  
 2115.2 Na2S2O3.5H2O  
 2115.1 H2CH2CH(NH2)C(O)OH  
 2114.8 (CH3)S  
 2114.8 WS2  
 2114.6 NH4SCN  
 2114.3 (C10H12AuClN2S)n  
 2114.0 ZnSO4  
 2114.0 K(CH(CH3)2OCS2)  
 2113.9 C4H3S(CH)5C(CN)2  
 2113.9 CH3SCH2CH2CH(NH2)C(O)OH  
 2111.6 CS2  
 2111.2 NaSCN  
 2110.7 (C10H12AuClN2S)n  
 2110.6 Na2S2O3.5H2O  
 2110.5 CoSO4  
 2110.5 Na2SO3  
 2110.4 CuSO4  
 2110.4 NaHSO3  
 2110.3 FeSO4.7H2O

2110.3	NiSO <sub>4</sub>	160.8	PbS
2110.2	Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .nH <sub>2</sub> O	161.6	FeS
2110.2	MnSO <sub>4</sub>	161.7	CdS
2109.9	BaSO <sub>4</sub>	162.1	NH <sub>2</sub> CSNH <sub>2</sub>
2109.7	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> .FeSO <sub>4</sub> .6H <sub>2</sub> O	162.3	ZnS
2109.7	CaSO <sub>4</sub> .2H <sub>2</sub> O	162.8	NiS
2109.6	HgSO <sub>4</sub>	162.8	Na <sub>2</sub> S*SO <sub>3</sub>
2109.5	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	162.8	WS <sub>2</sub>
2109.3	(NH <sub>4</sub> ) <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub>	163.0	FeS <sub>2</sub> /Pyrite
2109.3	SrSO <sub>4</sub>	163.2	Ph <sub>2</sub> S
2109.3	Al(NH <sub>4</sub> )(SO <sub>4</sub> ) <sub>2</sub> .12H <sub>2</sub> O	163.2	Cysteine
2109.2	KAl(SO <sub>4</sub> ) <sub>2</sub> .12H <sub>2</sub> O	163.7	CS <sub>2</sub>
2109.2	MgSO <sub>4</sub> .7H <sub>2</sub> O	163.8	S
2109.1	K <sub>2</sub> S <sub>2</sub> O <sub>7</sub>	164.3	Thiophene
2109.1	BeSO <sub>4</sub>	164.4	PhSSPh
2109.1	Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> .18H <sub>2</sub> O	166.3	PhSO <sub>2</sub> Na
2109.0	SnSO <sub>4</sub>	166.5	Me <sub>2</sub> SO
2108.9	K <sub>2</sub> (SO <sub>4</sub> ) <sub>2</sub>	167.4	SO <sub>2</sub>
2108.8	Li <sub>2</sub> SO <sub>4</sub>	167.6	Na <sub>2</sub> SO <sub>3</sub>
2108.5	Na <sub>2</sub> SO <sub>4</sub>	168.1	p-NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> SO <sub>3</sub> Na
2108.2	K <sub>2</sub> SO <sub>4</sub>	168.6	Na <sub>2</sub> SS*O <sub>3</sub>
2107.8	Na <sub>2</sub> S <sub>2</sub> O <sub>3</sub>	169.0	Me <sub>2</sub> SO <sub>2</sub>
2105.9	CaSO <sub>4</sub>	169.1	CuSO <sub>4</sub>
2103.9	(CH <sub>3</sub> ) <sub>2</sub> S	169.4	Na <sub>2</sub> SO <sub>4</sub>
2103.7	[PS(CH <sub>3</sub> O) <sub>3</sub> ]	169.7	CaSO <sub>4</sub>
2103.3	[PSCI <sub>2</sub> (CH <sub>3</sub> O)]	174.4	SF <sub>6</sub>
2103.2	[PSCI <sub>2</sub> (CH <sub>3</sub> )]		
2102.9	[PSCI <sub>3</sub> ]		
2102.5	(CH <sub>3</sub> S) <sub>2</sub>		
2102.5	(CH <sub>3</sub> S) <sub>2</sub>		
2100.9	(CF <sub>3</sub> S) <sub>2</sub>		
2100.7	[PSF <sub>3</sub> ]		
2100.5	CH <sub>3</sub> SH		
2100.4	SF <sub>6</sub>		
2099.9	(CH <sub>3</sub> ) <sub>2</sub> SO		
2098.7	SO(CH <sub>3</sub> O) <sub>2</sub>		
2098.6	H <sub>2</sub> S		
2098.1	SOCl <sub>2</sub>		
2097.6	(CH <sub>3</sub> O) <sub>2</sub> SO <sub>2</sub>		
2097.0	SO <sub>2</sub> Cl <sub>2</sub>		
2095.5	SO <sub>2</sub> ClF		
2095.5	SO <sub>2</sub>		
2094.5	SOF <sub>2</sub>		
2094.3	SClF <sub>5</sub>		
2093.9	SF <sub>4</sub>		
2093.8	SO <sub>2</sub> F <sub>2</sub>		
2092.6	SF <sub>6</sub>		

**S 2p.pos****Sb (M4N45N45).pos, Sb (MNN).pos**

464.5	Sb
462.2	Sb <sub>2</sub> S <sub>5</sub>
462.1	Sb <sub>2</sub> S <sub>3</sub>
459.7	Sb <sub>2</sub> O <sub>3</sub>
454.4	KSbF <sub>6</sub>

**Sb 3d5.pos**

528.1	Bu <sub>3</sub> Sb
528.2	Sb
528.6	AlSb
528.9	Ph <sub>3</sub> Sb
529.3	Sb <sub>2</sub> S <sub>5</sub>
529.5	Sb <sub>2</sub> S <sub>3</sub>
530.0	Sb <sub>2</sub> O <sub>3</sub>
530.8	Sb <sub>2</sub> O <sub>5</sub>
532.9	KSbF <sub>6</sub>

**Sc 2p3.pos**

398.6	Sc
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400.7 ScN	<b>Si (KL23L23).pos, Si (KLL).pos</b>
401.4 ClSc(C5H5)2	
401.8 Sc2O3	1617.2 MoSi2
401.9 Sc2O3	1616.6 Si
	1613.8 SiC
<b>Sc (L3M23M23).pos, Sc (LMM).pos</b>	1611.5 Si3N4
334.9 Sc2O3	1610.1 Mol Sieve A
333.5 Sc oxalate	1610.0 Penthylsilicone
333.4 Sc acetylacetonate	1609.6 Mica/Muscovite
329.8 ScF3	1609.5 AlSiO5/Sillimanite
	1609.4 Mol Sieve X
	1609.0 Kaolinite
<b>Se (L3M45M45).pos</b>	1608.8 SiO2
1307.3 Zn0.30Cd0.70Se	1608.8 Methylsilicone
1307.2 Zn0.42Cd0.58Se	1608.6 Mol Sieve Y
1307.0 Se	1608.6 SiO2/Quartz
1306.8 CdSe	1606.4 Na2SiF6
1306.7 Zn0.50Cd0.50Se	
1306.5 Zn0.70Cd0.30Se	<b>Si 2p.pos</b>
1305.9 Zn0.90Cd0.10Se	98.8 NiSi
1305.8 ZnSe	99.5 Si
1304.3 Ph2Se2	99.5 Fe3Si
1304.0 Ph2Se	99.6 MoSi2
1302.9 Cl2SePh2	99.8 PdSi
1302.1 I2SePh2	100.5 PtSi
1301.9 Ph2SeO	100.6 SiC
1301.6 SeO2	100.9 Me3SiOSiMe3
1301.0 H2SeO3	101.0 Ph4Si
1298.1 H2SeO4	101.1 Et3SiOH
	101.3 Ph3SiOSiPh3
<b>Se 3d5.pos</b>	101.4 Mol Sieve A
53.4 PbSe	102.0 Si3N4
53.8 CuInSe2	102.2 Mol Sieve X
54.5 GeSe2	102.4 Mica/Muscovite
54.6 Ga2Se3	102.6 Al2SiO5/Sillimanite
54.8 In2Se3	102.7 Phenylsilicone
54.9 As2Se3	102.8 Mol Sieve Y
55.1 Se	102.9 EtSiCl3
55.8 Ph2Se	102.9 Methylsilicone
55.8 Ph2Se2	103.0 Al2SiO5/Mullite
57.6 Ph2SeO	103.0 Kaolinite
57.7 Cl2SePh2	103.3 SiO2
58.1 I2SePh2	103.7 SiO2/Quartz
58.8 SeO2	104.3 Na2SiF6
58.8 PhSeO(OH)	
59.0 H2SeO3	<b>Sm (M4N67N67).pos</b>
61.0 H2SeO4	1094.0 Sm2O3

<b>Sm (M5N45N45).pos</b>	133.8 SrF2
	134.3 SrSO4
808.0 Sm2O3	134.4 Sr
	134.7 Sr(NO3)2
<b>Sm (M5N67N67).pos</b>	135.3 SrO
1068.0 Sm2O3	<b>Ta (M5N67N67).pos, Ta (MNN).pos</b>
<b>Sm (M45N45N67).pos</b>	1674.7 Ta
950.0 Sm2O3	<b>Ta 4f7.pos</b>
<b>Sm 3d5.pos</b>	21.9 Ta
	25.9 KTaO4
1081.1 Sm	26.5 Ta2O5
1083.2 Sm2O3	26.6 TaS
1083.4 Sm2(SO4)3	26.7 TaS2
	26.9 TaBr5
<b>Sn (M4N45N45).pos, Sn (MNN).pos</b>	27.3 TaCl5
	27.8 TaF5
437.3 Sn	29.4 K2TaF7
435.7 SnS	
434.1 SnO	<b>Tb (M4N67N67).pos</b>
432.6 SnO2	
431.7 Na2SnO3	1256.0 Tb
430.8 NaSnF	
<b>Sn 3d5.pos</b>	<b>Tb (M5N45N45).pos</b>
	920.0 Tb
484.9 Sn	
485.6 SnS	<b>Tb (M5N67N67).pos</b>
485.6 Ph3SnOH	
485.7 SnSe	1223.0 Tb
486.6 Ph4Sn	
486.6 SnO2	<b>Tb (M45N45N67).pos, Tb (MNN).pos</b>
486.7 SmCl2	
486.7 (NH4)2SnCl6	1068.0 Tb
486.7 KSnF3	
486.7 Na2SnO3	<b>Tb 3d5.pos</b>
486.9 SnBr2	
486.9 SnO	1241.4 TbO2
487.0 Ph3SnCl	1241.5 Tb2O3
487.4 SnF2	1242.0 Tb
487.4 NaSnF3	
487.6 K2SnF6	<b>Tb 4d.pos</b>
488.2 SnF4	
<b>Sr 3d5.pos</b>	146.0 Tb
	148.7 Tb2O3
133.2 SrCO3	149.2 TbO2

**Te (M4N45N45).pos, Te (MNN).pos**

492.1 Te  
 491.1 CdSe<sub>0.65</sub>Te<sub>0.35</sub>  
 490.8 CdTe  
 488.5 Ph<sub>2</sub>Te<sub>2</sub>  
 487.6 TeI<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>  
 487.3 TeBr<sub>4</sub>  
 487.1 TeO<sub>2</sub>  
 486.7 [TeBr<sub>2</sub>(C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>]  
 486.6 [TeI<sub>2</sub>(CH<sub>3</sub>)<sub>2</sub>]  
 486.6 [TeBr<sub>2</sub>(C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub>)]  
 486.4 (NH<sub>4</sub>)<sub>2</sub>TeCl<sub>6</sub>  
 486.3 Cl<sub>2</sub>TePh<sub>2</sub>  
 486.3 TeCl<sub>2</sub>(C<sub>6</sub>H<sub>5</sub>)<sub>2</sub>  
 486.1 TeCl<sub>4</sub>  
 485.5 Na<sub>2</sub>TeO<sub>4</sub>  
 485.5 TeO<sub>3</sub>  
 485.1 Te(OH)<sub>6</sub>

**Te 3d5.pos**

572.3 Hg<sub>0.8</sub>Cd<sub>0.2</sub>Te  
 572.7 CdTe  
 572.7 GeTe  
 572.9 Te  
 573.9 Ph<sub>2</sub>Te<sub>2</sub>  
 575.5 K<sub>2</sub>TeO<sub>3</sub>  
 575.8 TeI<sub>4</sub>  
 576.1 TeO<sub>2</sub>  
 576.2 Cl<sub>2</sub>TePh<sub>2</sub>  
 576.7 TeBr<sub>4</sub>  
 576.8 Na<sub>2</sub>TeO<sub>4</sub>  
 576.9 TeCl<sub>4</sub>  
 576.9 (NH<sub>4</sub>)<sub>2</sub>TeCl<sub>6</sub>  
 577.1 Te(OH)<sub>6</sub>  
 577.3 TeO<sub>3</sub>

**Th (N67O45O45).pos**

154.0 Th

**Th (N67O45V).pos, Th (NOV).pos**

249.0 Th

**Th 4d5.pos**

675.2 Th  
 675.5 ThO<sub>2</sub>

**Th 4f7.pos**

333.1 Th  
 334.4 ThO<sub>2</sub>  
 336.5 ThF<sub>4</sub>

**Ti (KL23L23).pos**

4002.0 TiO<sub>2</sub>

**Ti (L3M23M45).pos, Ti (LMM).pos**

419.0 Ti  
 418.2 TiC  
 409.8 Na<sub>2</sub>TiF<sub>6</sub>

**Ti 2p3.pos**

454.0 Ti  
 454.4 TiB<sub>2</sub>  
 454.6 TiC  
 455.1 TiO  
 455.8 TiN  
 457.1 Cl<sub>2</sub>Ti(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>  
 458.5 TiCl<sub>4</sub>  
 458.5 BaTiO<sub>3</sub> (cubic/tetra)  
 458.7 TiO<sub>2</sub>  
 459.2 TiO<sub>2</sub> (anatase/rutile)  
 462.6 Na<sub>2</sub>TiF<sub>6</sub>

**Tl 4f7.pos**

117.5 Tl<sub>2</sub>O<sub>3</sub>  
 117.7 Tl  
 118.5 TlI  
 118.7 Tl<sub>2</sub>S  
 118.7 Tl<sub>4</sub>S<sub>3</sub>  
 119.0 TlCl  
 119.2 TlBr  
 119.2 TlF

**Tm (M4N67N67).pos**

1487.0 Tm

**Tl (N6O45O45).pos, Tl (NOO).pos**

85.1 Tl

	381.3 UO3
<b>Tm (M5N45N45).pos</b>	381.6 UO2Cl2
1080.0 Tm	381.6 U(SO4)2
	381.9 UCl5
<b>Tm (M5N67N67).pos</b>	382.2 UF4
1440.0 Tm	382.4 K2UF6
	383.0 UO2F2
	384.9 UF6
<b>Tm (M45N45N67).pos, Tm (MNN).pos</b>	<b>V (L3M23M45).pos, V (LMM).pos</b>
1270.0 Tm	472.0 V
<b>Tm 4d.pos</b>	468.0 V2O5
175.4 Tm	468.6 VO2
176.6 Tm2O3	<b>V 2p3.pos</b>
178.3 Tm2(SO4)3	512.2 V
<b>U (N67O45N45).pos</b>	512.9 V(C5H5)2
190.0 U	513.3 K4V(CN)6
<b>U (N67O45V).pos</b>	514.2 V(acac)3
284.0 U	514.4 VN
	515.1 VO(acac)2
<b>U 4f7.pos</b>	516.3 VO2
377.4 U	516.4 VOCl2
378.3 UCl3	517.3 Na3VO4
378.4 UBr3	517.6 V2O5
379.1 USe3	<b>W (M5N67N67).pos, W (MNN).pos</b>
379.4 US3	1727.8 WS2
379.9 UBr4	1723.9 H2WO4
380.0 UOCl	1723.8 WO3
380.1 US	1722.0 Na2WO4
380.1 UF3	<b>W 4f7.pos</b>
380.1 UOBr	31.3 W
380.2 UCl4	31.5 WC
380.2 UO2	32.7 WO2
380.3 UOCl2	33.2 WS2
380.3 USe	35.1 CaWO4
380.4 UOBr2	35.7 WO3
380.5 UO2Br	35.9 WBr6
380.5 U2Te3	36.2 H2WO4
380.7 U3O8	36.3 Na2WO4
380.7 CaUO4	36.3 WBr5
381.1 UO2Br2	36.3 Al2(WO4)3
381.3 UTe3	36.9 WCl6
	37.2 WOCl4

<b>Xe (M4N45N45).pos</b>	<b>Zn (L3M45M45).pos, Zn (LMM).pos</b>
545.2 Xe in graphite	992.7 Cu <sub>64</sub> Zn <sub>36</sub>
544.8 Xe in Fe	992.2 Zn
545.2 Xe in graphite	991.3 ZnTe
545.2 Xe	989.7 ZnS
544.8 Xe in Fe	989.5 ZnSe
543.7 Xe/Ni	989.4 ZnCl <sub>2</sub>
541.4 Na <sub>4</sub> XeO <sub>6</sub>	989.3 ZnFe <sub>2</sub> O <sub>4</sub>
	988.7 ZnI <sub>2</sub>
<b>Xe 3d5.pos</b>	988.6 ZnO/SiO <sub>2</sub>
668.9 Xe in Au	988.2 ZnO/Si
669.6 Xe in Cu	988.0 Zn <sub>5</sub> (CO <sub>3</sub> ) <sub>2</sub> (OH) <sub>6</sub>
669.7 Xe in graphite	987.8 Al <sub>2</sub> ZnO <sub>4</sub>
670.2 Xe in Fe	987.7 [Zn(CH <sub>3</sub> C(O)CHC(O)CH <sub>3</sub> ) <sub>2</sub> ]
674.1 Na <sub>4</sub> XeO <sub>6</sub>	987.7 Zn(acac) <sub>2</sub>
	987.7 ZnAl <sub>2</sub> O <sub>4</sub>
<b>Y (M45N23V).pos, Y (MNV).pos</b>	987.7 ZnO
124.3 Y	987.4 ZnCO <sub>3</sub>
123.3 YH <sub>x</sub>	987.3 Zn <sub>4</sub> Si <sub>2</sub> O <sub>7</sub> (OH) <sub>2</sub> ·2H <sub>2</sub> O
117.8 Y <sub>2</sub> O <sub>3</sub>	987.3 ZnBr <sub>2</sub>
	987.0 Zn <sub>2</sub> SiO <sub>4</sub>
<b>Y 3d5.pos</b>	986.5 Zn(OH) <sub>2</sub>
155.8 Y	986.2 ZnF <sub>2</sub>
156.2 YH <sub>x</sub>	986.2 ZnSO <sub>4</sub>
157.0 Y <sub>2</sub> O <sub>3</sub>	
160.0 Y <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	<b>Zn 2p3.pos</b>
<b>Yb (M4N67N67).pos</b>	1020.9 ZnP <sub>2</sub>
1549.0 Yb	1021.4 Zn(acac) <sub>2</sub>
	1021.6 ZnS
<b>Yb (M5N67N67).pos</b>	1021.7 Zn
1500.0 Yb	1021.8 ZnF <sub>2</sub>
	1021.9 ZnCl <sub>2</sub>
<b>Yb (M45N45N67).pos</b>	1022.1 ZnO
1320.0 Yb	1022.5 ZnI <sub>2</sub>
	1023.1 ZnSO <sub>4</sub>
<b>Yb 4d5.pos</b>	1023.4 ZnBr <sub>2</sub>
182.4 Yb	
185.4 Yb <sub>2</sub> O <sub>3</sub>	<b>Zr (M45N23V).pos, Zr (MNV).pos</b>
187.3 Yb <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	148.6 Zr
	145.3 ZrH <sub>x</sub>
	141.9 ZrO <sub>2</sub>
	<b>Zr 3d5.pos</b>
	179.0 Zr
	179.6 ZrH <sub>x</sub>
	183.3 ZrO <sub>2</sub>

184.2  $\text{K}_2\text{ZrF}_6$

185.3  $\text{ZrF}_4$

## 2 Auger Parameters

All photoelectron lines are in BE, all Auger lines are in KE [1, 2, 3]! The Auger parameters are the sum of the energy of the photoelectron line (BE) and Auger line (KE). The values are saved in the directory Unifit\_2024\_User\_Files\auger parameters\\*.aup.

### Ag 3d5 + Ag (M4N45N45).aup

2099.7=84.0+2015.7 Au

727.0=368.8+358.2 Mg97Ag3

726.0=368.2+357.8 Ag

725.3=368.1+357.2 Ag2S

725.2=367.8+357.4 Ag2Se

724.5=367.8+356.7 Ag2O

724.1=368.0+356.1 AgI

724.0=367.4+356.6 AgO

723.0=367.7+355.3 AgF

722.9=367.3+355.6 AgF2

722.0=367.8+354.2 Ag2SO4

### Al 2p + Al (KL23L23).aup

1466.2=72.9+1393.3 Al

1464.8=73.6+1391.2 AlAs

1463.0=74.0+1389.0 AlN

1462.1=73.9+1388.2 Al2O3/alpha

1461.5=73.7+1387.8 Al2O3/gamma

1462.0=74.1+1387.9 Al2O3/sapphire

1461.8=74.2+1387.6 AlOOH/boehmite

1461.5=74.6+1386.9 Al2SiO5/sillimannite

1461.4=74.3+1387.1 Mica/muscovite

1462.0=74.3+1387.7 Al(OH)3/bayerite

1460.3=74.8+1385.5 H Zeolon

1460.6=73.7+1386.9 Mol Sieve A

### As 3d + As (L3M45M45).aup

1266.5=41.5+1225.0 As

1266.4=43.5+1222.9 AsI3

1266.2=41.2+1225.0 GaAs

1265.4=43.4+1222.0 As2S3

1263.9=42.8+1221.1 Ph3As

1263.8=44.3+1219.5 Ph3AsO

1263.6=44.9+1218.7 As2O3

1263.5=46.1+1217.4 As2O5

1263.4=45.3+1218.1 AsBr3

1261.6=47.8+1213.8 KAsF6

### Au 4f7 + Au (M5N67N67).aup

### Ba 3d5 + Ba (M4N45N45).aup

1381.6=780.6+601.0 Ba

1377.9=779.9+598.0 BaO

1376.9=780.8+596.1 BaSO4

1376.6=781.7+594.9 BaF2

### Br 3d + Br (L3M45M45).aup

1458.0=68.9+1389.1 LiBr

1459.2=74.8+1384.4 KBrO3

1456.7=68.7+1388.0 KBr

### Ca 2p3 + Ca (L23M23M23).aup

644.1=345.9+298.2 Ca

639.8=347.3+292.5 CaO

640.2=348.3+291.9 CaCl2

636.8=347.9+288.9 CaF2

638.8=347.0+291.8 CaCO3

### Cd 3d5 + Cd (M4N45N45).aup

789.0=405.0+384.0 Cd

787.6=405.2+382.4 CdTe

786.7=405.0+381.7 CdSe

786.6=405.3+381.3 CdS

786.6=404.2+382.4 CdO

786.6=405.4+381.2 CdI2

784.9=405.9+379.0 CdF2

### Co 2p3 + Cu (L3M45M45).aup

1551.8=783.6+768.3 CoSiF6

1551.2=778.2+773.0 Co

1550.3=781.7+768.6 Co(NH3)6Cl3

1548.7=781.9+766.8 K3Co(CN)6

### Cr 2p3 + Cr (L3M23M45).aup

1101.5=574.3+527.2 Cr

**Cs 3d5 + Cs (M4N45N45).aup**

1292.9=724.2+568.7 CsOH  
 1292.3=723.9+568.4 Cs2SO4

**Cu 2p3 + Cu (L3M45M45).aup**

1852.1=936.1+916.0 CuF2  
 1851.7=933.8+917.9 CuO  
 1851.3=932.7+918.6 Cu  
 1850.5=935.2+915.3 CuCl2  
 1849.4=931.8+917.6 CuInSe2  
 1849.1=932.5+916.6 Cu2O  
 1848.0=932.5+915.5 CuCl

**F 1s + F (KL23L23).aup**

1341.4=689.0+652.4 (-CF2-CF2-)n  
 1340.7=684.5+656.2 CuF2  
 1340.5=684.5+656.0 CdF2  
 1340.2=684.8+655.4 CaF2  
 1340.2=685.8+654.4 MgF2  
 1339.8=685.1+654.7 LiF  
 1339.8=687.0+652.8 NaBF4  
 1339.7=685.9+653.8 CsF  
 1339.6=685.5+654.1 Na3AlF6  
 1339.5=684.5+655.0 NaF  
 1339.0=686.0+653.0 Na2SiF6

**Fe 2p3 + Fe (L3M45M45).aup**

1410.3=707.4+702.9 FeB  
 1409.3=706.9+702.4 Fe

**Ga 3d + Ga (L3M45M45).aup**

1086.8=18.7+1068.1 Ga  
 1085.6=19.3+1066.3 GaAs  
 1084.9=19.3+1065.6 GaP  
 1084.0=19.5+1064.5 GaN  
 1082.9=20.5+1062.4 Ga2O3

**Ge 3d + Ge (L3M45M45).aup**

1174.5=29.3+1145.2 Ge  
 1174.2=30.5+1143.7 GeS  
 1173.6=30.7+1142.9 GeSe  
 1170.4=32.7+1137.7 GeO2  
 1169.0=33.3+1135.7 Na2GeF6

**I 3d5 + I (M4N45N45).aup**

1137.7=619.4+518.3 AgI  
 1137.6=620.3+517.3 UI3  
 1136.7=619.7+517.0 LiI  
 1135.7=618.7+517.0 KI

**In 3d5 + In (M4N45N45).aup**

854.2=443.8+410.4 In  
 853.4=444.5+408.9 In2Te3  
 852.7=444.1+408.6 CuInSe2  
 852.6=444.6+408.0 InP  
 852.5=444.5+408.0 In2Se3  
 852.0=444.7+407.3 In2S3  
 851.6=445.8+405.8 InI3  
 850.8=444.4+406.4 In2O3  
 850.8=446.0+404.8 InBr3  
 850.6=446.0+404.6 InCl3  
 849.9=446.2+403.7 InF3

**K 2p3 + K (L2M23M23).aup**

543.8=293.1+250.7 KBr  
 543.0=293.7+249.3 KSbF6  
 542.6=292.5+250.1 KF

**Mg 2p + Mg (KL23L23).aup**

1235.2=49.6+1185.6 Mg  
 1230.8=50.4+1180.4 MgO  
 1230.4=51.6+1178.8 MgSO4.7H2O  
 1229.1=51.0+1178.1 MgF2

**Mn 2p3 + Mn (L2M23M45).aup**

1227.3=641.6+585.7 MnO2  
 1225.7=640.9+584.8 MnS  
 1225.4=639.0+586.4 Mn  
 1223.7=642.7+581.0 MnSO4

**Mo 3d5 + Mo (L3M45M45).aup**

2266.8=228.0+2038.8 Mo  
 2266.7=227.7+2039.0 MoSi2  
 2264.9=232.7+2032.2 MoOx

**N 1s + N (KVV).aup**

803.9=407.3+396.6 Gd(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O  
 782.1=397.1+385.0 GaN  
 777.3=398.1+379.2 BN  
 775.4=398.8+376.6 NH<sub>3</sub>

### Na 1s + Na (KL23L23).aup

2066.1=1071.8+994.3 Na  
 2062.8=1071.6+991.2 NaI  
 2062.3=1072.5+989.8 Na<sub>2</sub>O  
 2062.3=1071.7+990.6 NaBr  
 2061.9=1071.6+990.3 NaCl  
 2061.3=1071.5+989.8 Na<sub>2</sub>CO<sub>3</sub>  
 2061.3=1070.8+990.5 Na<sub>2</sub>C<sub>2</sub>O<sub>4</sub>  
 2061.3=1071.1+990.2 Na<sub>3</sub>PO<sub>4</sub>  
 2061.2=1071.5+989.7 Na<sub>2</sub>HPO<sub>4</sub>  
 2061.1=1071.6+989.4 NaPO<sub>3</sub>  
 2061.1=1072.0+989.1 NaH<sub>2</sub>PO<sub>4</sub>  
 2061.0=1071.2+989.8 Na<sub>2</sub>SO<sub>4</sub>  
 2061.0=1071.1+989.9 NaOAc  
 2060.8=1071.4+989.4 NaNO<sub>3</sub>  
 2059.8=1072.7+987.1 NaBF<sub>4</sub>  
 2059.8=1071.2+988.6 NaF  
 2059.4=1071.7+987.7 Na<sub>2</sub>SiF<sub>6</sub>

### Nb 3d<sub>5</sub> + Nb (M45N23V).aup

370.2=202.4+167.8 Nb  
 369.7=208.1+161.6 Nb<sub>2</sub>O<sub>5</sub>  
 368.6=203.2+165.6 NbH<sub>x</sub>

### Ne 1s + Ne (KL23L23).aup

1681.4=863.4+818.0 Ne in Fe

### Ni 2p<sub>3</sub> + Ni (L3M45M45).aup

1699.8=857.4+842.4 NiF<sub>2</sub>  
 1698.9=852.7+846.2 Ni  
 1698.1=855.7+842.4 Ni(acac)<sub>2</sub>

### O 1s + O (KL23L23).aup

1043.8=528.7+515.1 PbO<sub>2</sub>  
 1042.1=529.0+513.1 PbO  
 1041.7=530.9+510.8 ZrO<sub>2</sub>  
 1041.0=531.3+509.7 CaCO<sub>3</sub>  
 1040.8=533.1+507.7 H<sub>2</sub>O  
 1040.7=532.0+508.7 CaSO<sub>4</sub>

1040.6=531.3+509.3 CaO  
 1040.2=531.4+508.8 CaSiO<sub>3</sub>  
 1040.1=531.5+508.6 Al(OH)<sub>3</sub>  
 1039.9=532.0+507.9 NaPO<sub>3</sub>  
 1039.6=532.8+506.8 SiO<sub>2</sub>  
 1039.6=531.9+507.7 NaAlSi<sub>3</sub>O<sub>8</sub>  
 1039.1=530.6+508.5 Al<sub>2</sub>O<sub>3</sub>

### P 2p + P (KL23L23).aup

1987.3=128.9+1858.4 InP  
 1986.8=130.7+1856.1 P/red  
 1986.7=129.4+1857.3 GaP  
 1986.5=133.3+1853.2 P<sub>4</sub>S<sub>10</sub>  
 1983.8=135.8+1848.0 P<sub>4</sub>O<sub>10</sub>  
 1983.5=133.6+1849.9 Na<sub>4</sub>P<sub>2</sub>O<sub>7</sub>  
 1983.3=132.8+1850.5 Na<sub>3</sub>PO<sub>4</sub>  
 1983.3=134.7+1848.6 NaPO<sub>3</sub>  
 1982.9=137.7+1845.2 NH<sub>4</sub>PF<sub>6</sub>

### Pb 4f<sub>7</sub> + Pb (N6O45O45).aup

233.1=136.8+96.3 Pb  
 232.7=137.3+95.4 PbTe  
 232.4=137.6+94.8 PbSe  
 232.1=137.5+94.6 PbS  
 231.7=138.4+93.3 PbI<sub>2</sub>  
 231.4=138.8+92.6 PbBr<sub>2</sub>  
 231.0=138.9+92.1 PbCl<sub>2</sub>  
 230.5=137.4+93.1 PbO<sub>2</sub>  
 230.2=138.5+91.7 Pb(NO<sub>3</sub>)<sub>2</sub>  
 230.1=137.3+92.8 PbO  
 230.1=140.0+90.1 PbSO<sub>4</sub>  
 229.9=138.0+91.9 Pb(OH)<sub>2</sub>  
 229.1=138.5+90.6 PbF<sub>2</sub>

### Pd 3d<sub>5</sub> + Pd (M4N45N45).aup

662.9=335.1+327.8 Pd  
 661.0=337.9+323.1 K<sub>2</sub>PdCl<sub>4</sub>

### Pt 4f<sub>7</sub> + Pt (M4N67N67).aup

2111.7=71.2+2040.5 Pt  
 2108.6=73.4+2035.2 K<sub>2</sub>PtCl<sub>4</sub>

### S 2p + S (KL23L23).aup

2278.9=162.8+2116.1 NiS  
 2278.8=163.0+2115.8 FeS<sub>2</sub>/Pyrite

2278.4=162.8+2115.6 WS2  
 2277.2=163.8+2113.4 S  
 2277.1=169.1+2108.0 CuSO4  
 2276.2=168.6+2107.6 Na2SS\*O3  
 2275.8=162.3+2113.5 ZnS  
 2275.3=169.4+2105.9 Na2SO4  
 2274.9=167.6+2107.3 Na2SO3  
 2274.9=174.4+2100.5 SF6  
 2274.6=162.8+2111.8 Na2S\*SO3  
 2273.6=167.4+2106.1 SO2

**Sb 3d5 + Sb (M4N45N45).aup**

992.7=528.2+464.5 Sb  
 991.6=529.5+462.1 Sb2S3  
 991.5=529.3+462.2 Sb2S5  
 989.7=530.0+459.7 Sb2O3  
 987.3=532.9+454.4 KSbF6

**Se 3d5 + Se (L3M45M45).aup**

1362.1=55.1+1307.0 Se  
 1360.4=58.8+1301.6 SeO2  
 1360.1=55.8+1304.3 Ph2Se2  
 1360.0=59.0+1301.0 H2SeO3  
 1359.8=55.8+1304.0 Ph2Se  
 1359.5=57.6+1301.9 Ph2SeO  
 1359.1=61.0+1298.1 H2SeO4

**Si 2p + Si (KL23L23).aup**

1716.8=99.6+1617.2 MoSi2  
 1716.1=99.5+1616.6 Si  
 1714.4=100.6+1613.8 SiC  
 1713.5=102.0+1611.5 Si3N4  
 1712.3=103.7+1608.6 SiO2/Quartz  
 1712.0=102.4+1609.6 Mica/Muscovite  
 1712.0=103.0+1609.0 Kaolinite  
 1711.5=101.4+1610.1 Mol Sieve A  
 1711.1=102.6+1609.5 Al2SiO5/Sillimanite  
 1710.7=104.3+1606.4 NaSiF6

**Sn 3d5 + Sn (M4N45N45).aup**

922.2=484.9+437.3 Sn  
 921.3=485.6+435.7 SnS  
 919.2=486.6+432.6 SnO2  
 918.2=487.4+430.8 NaSnF3

**Ta 4f7 + Ta (M5N67N67).aup**

1696.6=21.9+1674.7 Ta

**Te 3d5 + Te (M4N45N45).aup**

1065.0=572.9+492.1 Te  
 1064.0=576.7+487.3 TeBr4  
 1063.5=572.7+490.8 CdTe  
 1063.3=576.9+486.4 (NH4)2TeCl6  
 1063.2=576.1+487.1 TeO2  
 1063.0=576.9+486.1 TeCl4  
 1062.8=577.3+485.5 TeO3  
 1062.5=576.2+486.3 Cl2TePh2  
 1062.4=573.9+488.5 Ph2Te2  
 1062.3=576.8+485.5 Na2TeO4  
 1062.2=577.1+485.1 Te(OH)6

**Ti 2p3 + Ti (L3M23M45).aup**

873.0=454.0+419.0 Ti  
 872.8=454.6+418.2 TiC  
 872.4=462.6+409.8 Na2TiF6

**V 2p3 + V (L3M23M45).aup**

984.2=512.2+472.0 V

**W 4f7 + W (M5N67N67).aup**

1761.0=33.2+1727.8 WS2  
 1760.0=36.1+1723.9 H2WO4  
 1759.9=36.1+1723.8 WO3  
 1758.3=36.3+1722.0 Na2WO4

**Xe 3d5 + Xe (M4N45N45).aup**

1215.5=674.1+541.4 Na4XeO6  
 1215.0=670.2+544.8 Xe in Fe  
 1214.9=669.7+545.2 Xe in graphite

**Y 3d5 + Y (M45N23V).aup**

280.2=155.9+124.3 Y  
 279.5=156.2+123.3 YHx  
 276.4=158.6+117.8 Y2O3

**Zn 2p3 + Zn (L3M45M45).aup**

2013.8=1021.7+992.1 Zn  
 2012.9=1021.6+991.3 ZnTe

2011.5=1022.0+989.5 ZnSe

2011.3=1021.6+989.7 ZnS

2011.3=1021.9+989.4 ZnCl<sub>2</sub>

2011.2=1022.5+988.7 ZnI<sub>2</sub>

2010.7=1023.4+987.3 ZnBr<sub>2</sub>

2009.8=1022.1+987.7 ZnO

2009.2=1023.0+986.2 ZnSO<sub>4</sub>

2009.1=1021.4+987.7 Zn(acac)<sub>2</sub>

2008.0=1021.8+986.2 ZnF<sub>2</sub>

**Zr 3d5 + Zr (M45N23V).aup**

327.6=179.0+148.6 Zr

325.2=183.3+141.9 ZrO<sub>2</sub>

324.9=179.6+145.3 ZrHx

## 3 Experimental Files

### 3.1 XPS Data

#### 3.1.1 ESCALAB Eclipse (\*.TAP;\*.TXT)

Comment:

- All necessary acquisition parameters are available
- Example: multiregion measurement with 8 spectra
- Folder: Install-Memory Card: \XPS\_Measurement\_Reference\_Data\01-ESCALAB Eclips(.TAP)\ESCALAB-MultiReg-Ver1-with-lense-name.TAP

Eclipse Standard Data Transfer Format v2.0  
File: 'C:\DAT\NEU' contains 8 spectra.

Spectrum: 1

Name (Spectrum): Al 2p  
Label: St EK neu  
Data Version: 1  
Technique: XPS  
Acquired at 14:56:33 on Monday 8-12-1997  
ANALYSER:  
Mode: CAE  
Value: 10  
Magnification: 1  
Work function: 4.55  
Width x: 0  
Width y: 0  
Source azimuth: 0  
Polar angle: 0  
Target bias: 0  
Lens mode ID: 8  
Lens name: Large Area XL  
SOURCE:  
Type: AL KALPHA  
Non-Monochromated  
Energy: 1486.6  
Voltage: 0  
Current: 0  
Width x: 0  
Width y: 0  
Polar angle: 0  
Azimuth: 0  
Atomic number: 0  
Atoms: 0  
Charge: 0  
Name: Al K-alpha  
SIGNAL:  
Time: 0.1 seconds  
Scans: 15  
Correction: 0  
SAMPLE:  
Charging: 0  
Polar angle: 0  
Azimuth: 0  
Rotation: 0  
PROFILE INFO:  
None

## INSTRUMENT INFO:

Model: EscaLab 220-IXL

Transmission function coefficients:

1: 4.06581

2: -0.151464

3: 0.0432657

4: -0.0691272

Abscissa label: Kinetic Energy

Abscissa units: eV

Abscissa start: 1401.6

Abscissa end: 1419.6

Abscissa increment: 0.04

Ordinate label:

Ordinate units: Counts

Ordinate data: 451 values

Ordinate minimum, maximum: 1173.25 2435.98

1480.8

1463.72

1483.72

...

1249.83

1238.93

Spectrum: 2

Name (Spectrum): C 1s

Label: St EK neu

Data Version: 1

Technique: XPS

Acquired at 14:56:33 on Monday 8-12-1997

ANALYSER:

Mode: CAE

Value: 10

Magnification: 1

Work function: 4.55

Width x: 0

Width y: 0

Source azimuth: 0

Polar angle: 0

Target bias: 0

Lens mode ID: 8

Lens name: Large Area XL

SOURCE:

Type: AL KALPHA

Non-Monochromated

Energy: 1486.6

Voltage: 0

Current: 0

Width x: 0

Width y: 0

Polar angle: 0

Azimuth: 0

Atomic number: 0

Atoms: 0

Charge: 0

Name: Al K-alpha

SIGNAL:

Time: 0.1 seconds

Scans: 12

Correction: 0

SAMPLE:

Charging: 0

Polar angle: 0

Azimuth: 0

Rotation: 0

PROFILE INFO:

None

INSTRUMENT INFO:  
Model: EscaLab 220-IXL  
Transmission function coefficients:  
  1: 4.06581  
  2: -0.151464  
  3: 0.0432657  
  4: -0.0691272  
Abscissa label: Kinetic Energy  
Abscissa units: eV  
Abscissa start: 1181.6  
Abscissa end: 1206.6  
Abscissa increment: 0.04  
Ordinate label:  
Ordinate units: Counts  
Ordinate data: 626 values  
Ordinate minimum, maximum: 1659.28 4300.5  
1910.85  
1975.97  
...  
1704.28  
1690.68  
  
Spectrum: 3  
  
Name (Spectrum): Fe 2p  
Label: St EK  
Data Version: 1  
Technique: XPS  
Acquired at 14:56:33 on Monday 8-12-1997  
ANALYSER:  
Mode: CAE  
Value: 10  
Magnification: 1  
Work function: 4.55  
Width x: 0  
Width y: 0  
Source azimuth: 0  
Polar angle: 0  
Target bias: 0  
Lens mode ID: 8  
Lens name: Large Area XL  
SOURCE:  
Type: AL KALPHA  
Non-Monochromated  
Energy: 1486.6  
Voltage: 0  
Current: 0  
Width x: 0  
Width y: 0  
Polar angle: 0  
Azimuth: 0  
Atomic number: 0  
Atoms: 0  
Charge: 0  
Name: Al K-alpha  
SIGNAL:  
Time: 0.1 seconds  
Scans: 12  
Correction: 0  
SAMPLE:  
Charging: 0  
Polar angle: 0  
Azimuth: 0  
Rotation: 0  
PROFILE INFO:  
None  
INSTRUMENT INFO:

Model: EscaLab 220-IXL  
Transmission function coefficients:  
1: 4.06581  
2: -0.151464  
3: 0.0432657  
4: -0.0691272  
Abscissa label: Kinetic Energy  
Abscissa units: eV  
Abscissa start: 748.6  
Abscissa end: 783.6  
Abscissa increment: 0.04  
Ordinate label:  
Ordinate units: Counts  
Ordinate data: 876 values  
Ordinate minimum, maximum: 3318.28 10694.6  
9387.9  
9342.67  
9209.9  
...  
3343.3  
3409.8

Spectrum: 4

Name (Spectrum): Na 1s  
Label: St EK neu  
Data Version: 1  
Technique: XPS  
Acquired at 14:56:34 on Monday 8-12-1997  
ANALYSER:  
Mode: CAE  
Value: 10  
Magnification: 1  
Work function: 4.55  
Width x: 0  
Width y: 0  
Source azimuth: 0  
Polar angle: 0  
Target bias: 0  
Lens mode ID: 8  
Lens name: Large Area XL  
SOURCE:  
Type: AL KALPHA  
Non-Monochromated  
Energy: 1486.6  
Voltage: 0  
Current: 0  
Width x: 0  
Width y: 0  
Polar angle: 0  
Azimuth: 0  
Atomic number: 0  
Atoms: 0  
Charge: 0  
Name: Al K-alpha  
SIGNAL:  
Time: 0.1 seconds  
Scans: 8  
Correction: 0  
SAMPLE:  
Charging: 0  
Polar angle: 0  
Azimuth: 0  
Rotation: 0  
PROFILE INFO:  
None  
INSTRUMENT INFO:

Model: EscaLab 220-IXL  
Transmission function coefficients:  
1: 4.06581  
2: -0.151464  
3: 0.0432657  
4: -0.0691272  
Abscissa label: Kinetic Energy  
Abscissa units: eV  
Abscissa start: 403.6  
Abscissa end: 419.6  
Abscissa increment: 0.04  
Ordinate label:  
Ordinate units: Counts  
Ordinate data: 401 values  
Ordinate minimum, maximum: 13493.5 19037.6  
13689  
13877.8  
13782.6  
...  
13847.3  
13846.7  
13683.1  
  
Spectrum: 5  
  
Name (Spectrum): O 1s  
Label: St EK neu  
Data Version: 1  
Technique: XPS  
Acquired at 14:56:33 on Monday 8-12-1997  
ANALYSER:  
Mode: CAE  
Value: 10  
Magnification: 1  
Work function: 4.55  
Width x: 0  
Width y: 0  
Source azimuth: 0  
Polar angle: 0  
Target bias: 0  
Lens mode ID: 8  
Lens name: Large Area XL  
SOURCE:  
Type: AL KALPHA  
Non-Monochromated  
Energy: 1486.6  
Voltage: 0  
Current: 0  
Width x: 0  
Width y: 0  
Polar angle: 0  
Azimuth: 0  
Atomic number: 0  
Atoms: 0  
Charge: 0  
Name: Al K-alpha  
SIGNAL:  
Time: 0.1 seconds  
Scans: 7  
Correction: 0  
SAMPLE:  
Charging: 0  
Polar angle: 0  
Azimuth: 0  
Rotation: 0  
PROFILE INFO:  
None

## INSTRUMENT INFO:

Model: EscaLab 220-IXL

Transmission function coefficients:

1: 4.06581

2: -0.151464

3: 0.0432657

4: -0.0691272

Abscissa label: Kinetic Energy

Abscissa units: eV

Abscissa start: 942.6

Abscissa end: 960.6

Abscissa increment: 0.04

Ordinate label:

Ordinate units: Counts

Ordinate data: 451 values

Ordinate minimum, maximum: 1226.07 10376.7

2004.45

1971.05

1981.03

...

1281.15

1294.15

Spectrum: 6

Name (Spectrum): Si 2p

Label: St EK neu

Data Version: 1

Technique: XPS

Acquired at 14:56:34 on Monday 8-12-1997

ANALYSER:

Mode: CAE

Value: 10

Magnification: 1

Work function: 4.55

Width x: 0

Width y: 0

Source azimuth: 0

Polar angle: 0

Target bias: 0

Lens mode ID: 8

Lens name: Large Area XL

SOURCE:

Type: AL KALPHA

Non-Monochromated

Energy: 1486.6

Voltage: 0

Current: 0

Width x: 0

Width y: 0

Polar angle: 0

Azimuth: 0

Atomic number: 0

Atoms: 0

Charge: 0

Name: Al K-alpha

SIGNAL:

Time: 0.1 seconds

Scans: 20

Correction: 0

SAMPLE:

Charging: 0

Polar angle: 0

Azimuth: 0

Rotation: 0

PROFILE INFO:

None

INSTRUMENT INFO:  
Model: EscaLab 220-IXL  
Transmission function coefficients:  
1: 4.06581  
2: -0.151464  
3: 0.0432657  
4: -0.0691272  
Abscissa label: Kinetic Energy  
Abscissa units: eV  
Abscissa start: 1373.6  
Abscissa end: 1388.6  
Abscissa increment: 0.04  
Ordinate label:  
Ordinate units: Counts  
Ordinate data: 376 values  
Ordinate minimum, maximum: 2281.43 2833.18  
2501.45  
2450.4  
2489.18  
...  
2556.43  
2568.73

Spectrum: 7

Name (Spectrum): Si 2p  
Label: St EK neu  
Data Version: 1  
Technique: XPS  
Acquired at 16:25:43 on Monday 8-12-1997  
ANALYSER:  
Mode: CAE  
Value: 10  
Magnification: 1  
Work function: 4.55  
Width x: 0  
Width y: 0  
Source azimuth: 0  
Polar angle: 0  
Target bias: 0  
Lens mode ID: 8  
Lens name: Large Area XL  
SOURCE:  
Type: AL KALPHA  
Non-Monochromated  
Energy: 1486.6  
Voltage: 0  
Current: 0  
Width x: 0  
Width y: 0  
Polar angle: 0  
Azimuth: 0  
Atomic number: 0  
Atoms: 0  
Charge: 0  
Name: Al K-alpha  
SIGNAL:  
Time: 0.1 seconds  
Scans: 20  
Correction: 0  
SAMPLE:  
Charging: 0  
Polar angle: 0  
Azimuth: 0  
Rotation: 0  
PROFILE INFO:  
None

## INSTRUMENT INFO:

Model: EscaLab 220-IXL

Transmission function coefficients:

1: 4.06581  
2: -0.151464  
3: 0.0432657  
4: -0.0691272

Abscissa label: Kinetic Energy

Abscissa units: eV

Abscissa start: 1373.6

Abscissa end: 1394.6

Abscissa increment: 0.04

Ordinate label:

Ordinate units: Counts

Ordinate data: 526 values

Ordinate minimum, maximum: 2279 2917.02

2433.98

2443.35

2441.97

...

2815.25

2884.63

2861.65

Spectrum: 8

Name (Spectrum): Survey

Label: St EK neu

Data Version: 1

Technique: XPS

Acquired at 14:47:17 on Monday 8-12-1997

ANALYSER:

Mode: CAE

Value: 70

Magnification: 1

Work function: 4.55

Width x: 0

Width y: 0

Source azimuth: 0

Polar angle: 0

Target bias: 0

Lens mode ID: 8

Lens name: Large Area XL

SOURCE:

Type: AL KALPHA

Non-Monochromated

Energy: 1486.6

Voltage: 0

Current: 0

Width x: 0

Width y: 0

Polar angle: 0

Azimuth: 0

Atomic number: 0

Atoms: 0

Charge: 0

Name: Al K-alpha

SIGNAL:

Time: 0.1 seconds

Scans: 1

Correction: 0

SAMPLE:

Charging: 0

Polar angle: 0

Azimuth: 0

Rotation: 0

PROFILE INFO:

```

None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
    1: 4.06581
    2: -0.151464
    3: 0.0432657
    4: -0.0691272
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 136.6
Abscissa end: 1486.6
Abscissa increment: 0.5
Ordinate label:
Ordinate units: Counts
Ordinate data: 2701 values
Ordinate minimum, maximum: 300.64 29010.5
23993.9
23681.5
23669.4
...
490.024
449.588
300.486

```

### 3.1.2 ESCALB/K-ALPHA Advantage (\*.AVG)

Comment:

- All necessary acquisition parameters are available
- Single spectrum, profile of one region, line scan of one region, multipoint (area) scan of one region, multipoint scans of a SDP of one region are saved
- Example: profile measurement with 5 Zn2p<sub>3/2</sub> spectra
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\02-Avanatge(.AVG)\Avantage-Profile-Zn2p3.AVG

```

;=====
;Dump of DataSpace 'C:\Documents and
Settings\vgengineer\Desktop\DW\Twin\profile\Depth Profile\Manual Source\Manual
Point\Zn2p3.VGD'
; on 12/5/2006 at 11:29:42
;=====

```

```

;[Note that this file can be reloaded only if certain syntax rules are NOT
broken]

```

```
$FORMAT=3
```

```
;Summary Properties present:
```

```
$PROPERTIES=SUM
```

```

DS_EXT_SUPROPID_TITLE      : VT_BSTR = 'Zn2p3'
DS_EXT_SUPROPID_SUBJECT    : VT_BSTR = 'VG Scientific acquisition datafile'
DS_EXT_SUPROPID_AUTHOR     : VT_BSTR = 'vgengineer'
DS_EXT_SUPROPID_COMMENTS   : VT_BSTR = ''
DS_EXT_SUPROPID_CREATED    : VT_DATE = 11/5/2006   13:35:36
DS_EXT_SUPROPID_SAVED      : VT_DATE = 11/5/2006   14:31:53

```

```
;Standard Properties present:
```

```
$PROPERTIES=STD
```

```

DS_GEPROPID_TECHNIQUE      : VT_I4   = 17
DS_GEPROPID_INSTRUMENT     : VT_BSTR = 'ESCALab250'
DS_GEPROPID_SOURCE_TYPE    : VT_I4   = 1

```

```

DS_GEPROPID_GUID : VT_BSTR = '{823B2E65-8BB2-4D75-
8518-536FEE14F4F7}'
DS_GEPROPID_SOURCE_GUID : VT_BSTR = '{823B2E65-8BB2-4D75-
8518-536FEE14F4F7}'
DS_GEPROPID_EXPT_RUN_GUID : VT_BSTR = '{007F1444-1B99-4164-
893C-A1522841C235}'
DS_GEPROPID_VALUE_TYPE : VT_I4 = 11
DS_GEPROPID_VALUE_LABEL : VT_BSTR = 'Counts'
DS_GEPROPID_VALUE_SYMBOL : VT_BSTR = 'C'
DS_GEPROPID_VALUE_UNIT : VT_BSTR = ''
DS_DATASTOREID_DATA_STORAGE_METHOD : VT_I4 = 0
DS_SOPROPID_ENERGY : VT_R4 = 1253.599976
DS_SOPROPID_GUN : VT_I2 = -1
DS_STPROPID_POS_X : VT_I4 = 0
DS_STPROPID_POS_Y : VT_I4 = 0
DS_STPROPID_POS_Z : VT_I4 = 0
DS_STPROPID_POS_TILT : VT_I4 = 0
DS_STPROPID_POS_AZIM : VT_I4 = 0
DS_ACPROPID_START_TIME : VT_DATE = 11/5/2006 13:36:22
DS_ACPROPID_END_TIME : VT_DATE = 11/5/2006 14:31:53
DS_ACPROPID_ACQ_TIME : VT_R4 = 0.099960
DS_ACPROPID_PERIODS : VT_I4 = 6
DS_ACPROPID_CORRECTION : VT_R4 = 0.000000
DS_ACPROPID_MODE : VT_I2 = 0
DS_ACPROPID_DIRECTION : VT_I2 = 1
DS_ACPROPID_SIG_COMP : VT_BOOL = False
DS_ACPROPID_EV_SCALE : VT_I2 = 1
DS_DEPTHPROFILE_IONGUNPROPID_CURRENT : VT_R4 = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_ENERGY : VT_R4 = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_RASTER_WIDTH : VT_R4 = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_RASTER_HEIGHT : VT_R4 = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_ANGLETOSURFACE : VT_R4 = 45.000000
DS_DEPTHPROFILE_IONGUNPROPID_IONTYPE : VT_BSTR = 'Ar+'
DS_DEPTHPROFILE_IONGUNPROPID_DESCRIPTION : VT_BSTR = ''
DS_DEPTHPROFILE_PROPS_ROTATION : VT_I4 = 0
DS_ANPROPID_MODE : VT_I2 = 1
DS_ANPROPID_PASS : VT_R4 = 50.000000
DS_ANPROPID_WORK_FTN : VT_R4 = 4.444000
DS_ANPROPID_LENS_MODE_NAME : VT_BSTR = 'LargeAreaXL'
DS_ANPROPID_TXFN_COEFFS : VT_I4 = 1
; Property list for DS_ANPROPID_TXFN_COEFF (expecting 1) follows:
DS_ANPROPID_TXFN_COEFF[0] : VT_R4 = 1.000000

```

```
;Extended Properties present:
```

```
$PROPERTIES=EXT
```

```
; NONE found
```

```
;=====
```

```
;DataSpace has 2 data axes as follows:
```

```
; #= start, end, numSpaceAxes
```

```
$DATAAXES=2,#empty#
```

```
0= 0, 75, 1
1= 0, 5, 2
```

```
;=====
```

```
;DataSpace has 3 space axes as follows:
```

```
; #= start, width, numPoints, axisType, linear,
```

```
symbol, unit, label
```

```
$$SPACEAXES=3
```

```
0= 223.600000, 0.200000, 76, ENERGY, LINEAR, 'E',
'ev', 'Energy'
1= 0.000000, 600.840000, 6, ETCHTIME, NON-LINEAR,
'EtchTime', 's', 'Etch Time'
2= 0.000000, 1.000000, 6, ETCHLEVEL, LINEAR,
'EtchLevel', '', 'Etch Level'
```

```

;=====
;Values on axis 0 where axis 1 = 0;
$DATA=*,0
LIST@ 0= 19186.025000, 19079.575000, 19180.500000, 19178.750000
LIST@ 4= 18997.150000, 19176.925000, 19086.925000, 19211.875000
LIST@ 8= 19306.350000, 19227.400000, 19212.075000, 19246.350000
...
LIST@ 64= 18063.500000, 17865.725000, 17767.975000, 17861.800000
LIST@ 68= 17686.075000, 17823.650000, 17677.975000, 17630.000000
LIST@ 72= 17787.625000, 17609.825000, 17442.175000, 17448.350000
;Values on axis 0 where axis 1 = 1;
$DATA=*,1
LIST@ 0= 19433.975000, 19309.825000, 19231.775000, 19069.775000
LIST@ 4= 19257.475000, 19321.475000, 19220.950000, 19115.775000
LIST@ 8= 19145.350000, 18944.100000, 19225.050000, 19007.300000
...
LIST@ 64= 17840.950000, 17731.225000, 17549.100000, 17532.500000
LIST@ 68= 17628.275000, 17661.725000, 17514.100000, 17395.025000
LIST@ 72= 17413.875000, 17612.175000, 17520.850000, 17616.550000
;Values on axis 0 where axis 1 = 2;
$DATA=*,2
LIST@ 0= 19329.350000, 19038.225000, 19016.375000, 19156.375000
LIST@ 4= 19302.300000, 19573.500000, 19358.675000, 19300.350000
LIST@ 8= 19339.025000, 19134.900000, 19240.500000, 19314.850000
...
LIST@ 64= 17817.875000, 17714.900000, 17651.725000, 17777.975000
LIST@ 68= 17753.100000, 17617.675000, 17685.375000, 17594.900000
LIST@ 72= 17555.375000, 17561.600000, 17627.900000, 17717.550000
;Values on axis 0 where axis 1 = 3;
$DATA=*,3
LIST@ 0= 19551.675000, 19281.150000, 19552.600000, 19474.000000
LIST@ 4= 19437.075000, 19277.850000, 19320.700000, 19393.000000
LIST@ 8= 19207.675000, 19145.975000, 19272.475000, 19172.225000
...
LIST@ 64= 17479.325000, 17631.750000, 17405.000000, 17591.775000
LIST@ 68= 17445.825000, 17513.500000, 17570.800000, 17682.825000
LIST@ 72= 17733.200000, 17692.100000, 17667.150000, 17721.125000
;Values on axis 0 where axis 1 = 4;
$DATA=*,4
LIST@ 0= 19871.975000, 19996.475000, 19934.325000, 19808.125000
LIST@ 4= 19762.275000, 19920.025000, 19900.300000, 19781.275000
LIST@ 8= 19731.275000, 19586.200000, 19651.875000, 19657.850000
...
LIST@ 64= 17623.525000, 17558.325000, 17414.050000, 17548.525000
LIST@ 68= 17419.300000, 17239.225000, 17251.750000, 17210.975000
LIST@ 72= 17302.400000, 17715.925000, 17560.250000, 17798.900000
;Values on axis 0 where axis 1 = 5;
$DATA=*,5
LIST@ 0= 20492.700000, 20459.300000, 20373.050000, 20337.350000
LIST@ 4= 20319.000000, 20352.300000, 20372.175000, 20321.225000
...
LIST@ 64= 17851.300000, 17631.200000, 17534.500000, 17429.850000
LIST@ 68= 17376.850000, 17203.375000, 17426.150000, 17421.550000
LIST@ 72= 17605.375000, 17806.950000, 17963.275000, 18285.675000

```

### 3.1.3 ESCA3 (\*.TAP)

Comment:

- First row: \*\* + region name
- Second row: 8 characters number of steps, 8 characters start energy, 8 characters empty, 8 characters step width, 8 characters pass energy, 8 characters excitation energy, 8 characters number of scans, 8 characters time per step

- Third row to start of next region: 15 characters intensity ten times per row
- Example: multiregion measurement, 1 survey, 4 single regions (S 2p, C 1s, N 1s, O 1s)
- Folder: Install-Memory Card:\Measurement\_Reference\_Data\03-Esca3(.TAP)\Esca3-MultiReg2.TAP

```

**US
1200****1500*****.8*****50*****1486.6**1*****.4*****
280          207          201          243          204          206
226          221          233          218
252          277          266          247          239          258
279          284          271          279

...
9848          9888          9938          9983          9846          9817
9869          9913          10023         10003

**S2p
200****1330*****.1*****20*****1486.6**3*****1*****
2374          2334          2383          2299          2177          2179
2191          2189          2193          2105
2035          2061          1949          1985          2008          1931
1950          1970          1933          1863

...
2871          2866          2783          2885          2887          2899
2893          2823          2999          2890
2884          2949          2982          2956          2950          2971
2989          2952          2934          3068

**C1s
200****1210*****.1*****20*****1486.6**3*****1*****
8371          8274          8204          8384          8307          8060
8024          7841          7911          7799
7712          7745          7245          7029          7024          6879
6858          6749          6535          6485

...
9292          9421          9408          9170          9259          9228
9306          9257          9263          9196
9233          9129          9274          9045          9234          9198
9166          9241          9191          9562

**N1s
200****1093*****.1*****20*****1486.6**5*****1*****
18327         18075         18128         18163         18351         17911
18006         17780         18030         18093
17978         18101         17998         18011         17880         18067
18060         17946         17995         17680

...
18193         18522         18462         18410         18675         18442
18566         18438         18578         18508
18285         18592         18553         18612         18546         18356
18771         18669         18597         18595

**O1s
200****962*****.1*****20*****1486.6**3*****1*****
12530         12412         12270         12341         12263         12323
12218         12219         12046         12048
12036         12036         11769         12169         11998         12001
12059         11893         11735         11841

...
13163         13029         13096         12800         12906         13365
13075         13071         13097         13024
13222         12930         13149         13103         13047         13139
13246         13015         13219         13291

```

### 3.1.4 BESSY (\*.\*)

Comment:

- 1. – 14. row: acquisition parameters
- from row 15: column1: kinetic energy, column 2: intensity, column 3: flux

- Excitation energy not available
- Intensities are divided by flux (only flux<> 0)
- One single regions is saved
- Example: single region, Cu 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\ 04-BESSY(.TXT)\ BESSY-SingleReg-Cu2p-EP=1486.6.TXT

```

komm_row   : Cu 2p
prob_row   : xpsrew Cu Ar+5keV/5mA 5min Al12/20
date       :
time       :
source     :
MessMode   : EDC
max_energy : 561.62557
min_energy : 511.60555
pass_energy : 20
step_w     : 0.06100
anz_scans  : 3
count_time : 100
num_of_data : 821
E_kin;resCh;secCh
511.60555;8202;1.0000
511.66655;9032;1.0000
511.72755;9055;1.0000
511.78855;8922;1.0000
511.84955;9028;1.0000
...
561.50355;5248;1.0000
561.56455;5183;1.0000
561.62555;5123;1.00001

```

### 3.1.5 VSI (\*.GPH)

Comment:

- Excitation energy not available
- Example: single region, survey, excitation energy: 1253.6 eV
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\ 04-VSI(.GPH)\ VSI-SingleReg-survey-EP=1253.6.GPH

```

%%%%% 001 # General data
2.10 0.40 HSA FFFFE1F # P-Version, C-Version, Type
05.12.1997 11:00 # Date, Time
14 # Unit TYPE
%%%%% 010 # Comment

```

```

##### 002 # Modul data
KINETIC 1000.000000000 1 1 1.0000000000 0.0000000000 FFFF529
CHANNELT 2000.000000000 6 1 1.0000000000 0.0000000000 FFFF651
##### 003 # Segment
0 # Flag für Segmentauswahl
865.000000000 890.000000000 0.050000007 # min max inc
2 # Segmentanzahl
0.0099999998 860.000000000 885.000000000 0.2999999821
0.2000000030 # wait start stop inc
0.0099999998 1100.000000000 1130.000000000 0.2999999821
0.2000000030 # wait start stop inc
##### 004 # Channel data
0 # main channel
COUNTER 0.0000000000 1.0000000000 0 1 1
FFFFD5D0
Channel 2 0.0000000000 1.0000000000 0 0 0
FFFFF3D0
Channel 3 0.0000000000 1.0000000000 0 0 0
FFFFE4D0
Channel 4 0.0000000000 1.0000000000 0 0 0
FFFFD5D0
Channel 5 0.0000000000 1.0000000000 0 0 0
FFFFC6D0
##### 005 # Averagedata
\SAVEMEAS # Filename Measure Values
0063 # Flags
0003 # Anzahl
000 # Start extension
003 # Save extension
\SAVEAV # Filename Average Values
\EXPMEAS # Filename Export Measure Values
\EXPAV # Filename Export Average Values
\expmcd # Filename MCD Values
##### 006 # Options
1.0000000000 # xFactor
0.0000000000 # xOffset
1000000.0000000000 # warning level
##### 007 # Ramp Mode Parameter
1 # mode
5.000 # parameter FRR
5.000 # parameter FAT
0 # kinetic energy mode
2 # MCD
0 # adjustable magnification
0.000000 # XPS-Gain
0 # polarity
##### 008 # Timedata
0.1999999285 # Meas time
5.3999977112 # startTime
0.0099999998 # sleepTime
##### 009 # Graphicoptionen
880.000000 882.000000# X-Zoom
20000.000000 30000.000000# Y-Zoom
##### 011 # Transformation
-1 # Length of Differentiation
-1 # Length of Smoothing
##### 012 # Background Correction
0 # Active
0.000000 # LeftX
0.000000 # LeftY
0.000000 # RightX
0.000000 # RightY
##### 020 # Measure Global
12-05-1997 10:51:01 # Startzeit
12-05-1997 10:59:53 # Endzeit

```

```

 3 # Averageanzahl
000 # Scanindex
10000 # Kanäle
%%%% 021 # Measure Segment
1 # Number of Segments
501 0.0099999998 865.000000000 890.000000000 0.0500000007
0.1999999285 # Segmentsize wait start stop inc meastime
0.000000 # MCD Correction
%%%% 022 # Measure Data
COUNTER
S 0000 865.000000
M 0000 552.333313
S 0001 865.049988
M 0001 567.000000
S 0002 865.099976
M 0002 557.333374
S 0003 865.149963
M 0003 574.333313
...
S 0500 889.993896
M 0500 294.000000
%%%% ENDE # end of file

```

### 3.1.6 HHUD (\*.DAT)

Comment:

- Acquisition parameters saved in 22 rows:
  1. row: XPS2 for file identification
  2. row: date and time
  3. row: comment
  4. row: comment
  5. row: excitation source (Magnesium, Aluminium ...)
  6. row: reserved for Xfit
  7. row: region name (O 1s, ...)
  8. row: analyser mode (e.g. CAE 10)
  9. row: number of scans, dwell time in ms and acquisition time in min
  10. row: cross section, area,... (no relevance for UNIFIT!)
  11. row to 20. row no relevance for UNIFIT!
  21. row: lowest binding energy in eV, highest binding energy in eV, smallest intensity, highest intensity, number of steps, total area of the spectrum
  22. row: ',@' start of experimental data
- from row 23: binding energy, intensity
- Example: single region, survey, Au sample
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\ 04-HHUD-Uni-Düsseldorf(.DAT)\ HHUD-SingleReg-survey-Au.DAT

```

XPS 2: XE2425.DAT
Thu Mar 25 16:55:39 1999
nach wartung
au stand nach 4min 4kevar+ mg
Magnesium

```

```

Au
3,CAE 20 eV
3,300,3.9
19.51000,0.000,0.000
82.60,90.40

```

```

80.00,71623.34,93.00,413927.75,260,0
@
80.00,88337.78
80.05,82141.11
80.10,81136.66
80.15,79423.34
80.20,78223.34
80.25,76981.11
80.30,75856.66
80.35,75372.23
80.40,75014.45
80.45,74244.45
80.50,73836.66
...
81.85,86532.22
81.90,88875.55
81.95,89601.12
82.00,92637.78
...

```

### 3.1.7 CAF (\*.CAF)

Comment:

- Acquisition parameters saved in 5 rows
- 1. row: start energy, 2. row: step width, 3. row: number of steps, from row 6: intensities
- Excitation energy not saved
- Example: single region
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\05-CAF(.CAF)\CAF-SingleReg.CAF

```

xstart 34
xstep 0.025
nop 321
mmean 3206.87961931464
BEGIN
936.83042
914.93686
930.38953
...
283.63007
296.45818
282.19061
307.78396
252.03781
END

```

### 3.1.8 KRATOS (\*.CIL)

Comment:

- Acquisition parameters are not saved
- 1. column: xywe, 2. column: binding energy BE, 3. column: intensities
- Manual input of all acquisition parameters

- Excitation energy  $E_P$ , initial  $E_I$  and final energy  $E_F$  must give the BE values of the first and last saved energy value
- For the example: Name: K 2p,  $E_P = 1486.6$  eV,  $E_I = 1173.6$  eV ( $1486.6 - 1173.6 = 313$ ),  $E_F = 1198.4$  eV ( $1486.6 - 1198.4 = 288.2$ ), step width = 0.2 eV, dwell time = 1, accumulations = 1
- Example: single region K 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\05-Kratos(.CLI)\Kratos-SingleReg-K2p.CIL

```
xywe -3.130e+02  7.040e+02
xywe -3.128e+02  2.240e+02
xywe -3.126e+02  1.600e+02
xywe -3.124e+02  2.240e+02
xywe -3.122e+02  2.240e+02
...
xywe -2.888e+02  1.344e+03
xywe -2.886e+02  1.472e+03
xywe -2.884e+02  1.312e+03
xywe -2.882e+02  1.376e+03
komm
```

### 3.1.9 PHI-5400/PHI-5600 (\*.INF), (\*.ASC)

Comment:

- Acquisition parameters: inf-files, intensities: asc-files with the same name
- asc-files: 10 characters binding energy, 11 characters intensity
- Example: multiregion measurement, 5 spectra: S 2p, C 1s, O 1s, Pb 4f, S 2s
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\06-PHI5400-5600 (\*.INF.ASC)\PHI5400-MultiReg.INF

#### File (\*.INF)

IDENTIFICATION: identification information

ESCA	Technique
MULTIPLEX	Type
4	File version number
812372901	Fri Sep 29 09:08:21 1995 (Time of acquisition)
PbS, 15 min at +70 mV (= afmp)	User's comment
3 POINT	Acquisition mode
CONTINUOUS	Sputter mode
AUTO	Input mode
FIXED PASS ENERGY	SCA detector mode
EXTENDED	Input lens
2.0 INCH	Lens mode
.	Primary beam gating
TV IMAGE	Electron gun mode during SIMS acq.
SOURCE 90	X-ray source angle
NO	Rotating profile
NO	Signal-to-noise acquisition
0.000000	Sputter interval in seconds
3676	Number of pre sputter cycles
596	Save every Nth cycle
3709	Number of points per line
210.000000	Acquisition time entered
96.900009	Actual acquisition time
0.000000	SIMS time to sputter before acquisition
0.000000	Linear gating (percent)
3676	SIMS resolution
1486.599976	ESCA anode reference energy
NO	Image registration



NEGATIVE IONS	Positive or negative ions
0.000000	Percent gating
QUAD OFF	Analyzer mode
0.000000	Mass
0.000000	Resolution
TV IMAGE	Electron gun mode
0	Peak range
0.000000	Time per step in msec

ACQUISITION TIMES: acquisition times for each region (area for surveys)

5	Number of acquisition time values stored
24.133337	Acquisition times
8.416666	Acquisition times
8.066668	Acquisition times
2.683334	Acquisition times
53.600002	Acquisition times

REGION INFORMATION: acquisition control block

5	Number of acb_region structures stored
---	--

Region acquisition control block structure

S1	Element name
100	Old time per step
8	Number of sweeps
174.000000	Energy upper limit
18.000000	Energy range
174.000000	Analysis upper limit
18.000000	Analysis range
0.100000	Volts per step
181	Steps per sweep
5	Number of diff points
0.000000	Window width for test acq
1	Flag, acquire data
0	Flag, triggered acquisition
2	Resolution
1	Calculation type
0	Gate trigger
0	Ion polarity
1	Transition
0.000000	Trigger relative rise %
0.000000	Trigger relative fall %
3636	Minimum counts
7850	Maximum counts
2147483647	Peak to peak minimum
0	Peak to peak maximum
0.000000	Actual sputter time
35.750000	Pass energy
35.750000	Retard ratio
2	Number of mcd channels
0.000000	Trigger fracture beam gating
0.000000	Trigger time beam gating
0.000000	Retard energy
0.000000	Ion energy
0.000000	Focus voltage
0.000000	Acceleration voltage
500	Signal to noise limit
100.000000	Time per step

Region acquisition control block structure

C1	Element name
100	Old time per step

5	Number of sweeps
292.000000	Energy upper limit
10.000000	Energy range
292.000000	Analysis upper limit
10.000000	Analysis range
0.100000	Volts per step
101	Steps per sweep
5	Number of diff points
0.000000	Window width for test acq
1	Flag, acquire data
0	Flag, triggered acquisition
2	Resolution
1	Calculation type
0	Gate trigger
0	Ion polarity
1	Transition
0.000000	Trigger relative rise %
0.000000	Trigger relative fall %
1558	Minimum counts
2794	Maximum counts
2147483647	Peak to peak minimum
0	Peak to peak maximum
0.000000	Actual sputter time
35.750000	Pass energy
35.750000	Retard ratio
2	Number of mcd channels
0.000000	Trigger fracture beam gating
0.000000	Trigger time beam gating
0.000000	Retard energy
0.000000	Ion energy
0.000000	Focus voltage
100.000008	Acceleration voltage
500	Signal to noise limit
100.000000	Time per step

## Region acquisition control block structure

01	Element name
100	Old time per step
4	Number of sweeps
538.000000	Energy upper limit
12.000000	Energy range
538.000000	Analysis upper limit
12.000000	Analysis range
0.100000	Volts per step
121	Steps per sweep
5	Number of diff points
0.000000	Window width for test acq
1	Flag, acquire data
0	Flag, triggered acquisition
2	Resolution
1	Calculation type
0	Gate trigger
0	Ion polarity
1	Transition
0.000000	Trigger relative rise %
0.000000	Trigger relative fall %
1832	Minimum counts
2281	Maximum counts
2147483647	Peak to peak minimum
0	Peak to peak maximum
0.000000	Actual sputter time
35.750000	Pass energy
35.750000	Retard ratio
2	Number of mcd channels
0.000000	Trigger fracture beam gating
0.000000	Trigger time beam gating
0.000000	Retard energy

```

0.000000      Ion energy
0.000000      Focus voltage
0.000000      Acceleration voltage
500           Signal to noise limit
100.000000    Time per step

Region acquisition control block structure
Pb1           Element name
100          Old time per step
1            Number of sweeps
149.000000   Energy upper limit
16.000000   Energy range
149.000000   Analysis upper limit
16.000000   Analysis range
0.100000    Volts per step
161         Steps per sweep
5           Number of diff points
0.000000    Window width for test acq
1           Flag, acquire data
0           Flag, triggered acquisition
2           Resolution
1           Calculation type
1           Gate trigger
0           Ion polarity
1           Transition
0.000000    Trigger relative rise %
0.000000    Trigger relative fall %
81          Minimum counts
4646        Maximum counts
2147483647  Peak to peak minimum
0           Peak to peak maximum
0.000000    Actual sputter time
35.750000   Pass energy
35.750000   Retard ratio
2           Number of mcd channels
0.000000    Trigger fracture beam gating
0.000000    Trigger time beam gating
0.000000    Retard energy
0.000000    Ion energy
0.000000    Focus voltage
-7.625010   Acceleration voltage
50          Signal to noise limit
100.000000  Time per step

Region acquisition control block structure
S2           Element name
100          Old time per step
16           Number of sweeps
240.000000   Energy upper limit
20.000000   Energy range
240.000000   Analysis upper limit
20.000000   Analysis range
0.100000    Volts per step
201         Steps per sweep
5           Number of diff points
0.000000    Window width for test acq
1           Flag, acquire data
0           Flag, triggered acquisition
2           Resolution
1           Calculation type
0           Gate trigger
0           Ion polarity
1           Transition
0.000000    Trigger relative rise %
0.000000    Trigger relative fall %
6087        Minimum counts
8912        Maximum counts

```

2147483647	Peak to peak minimum
0	Peak to peak maximum
0.000000	Actual sputter time
35.750000	Pass energy
35.750000	Retard ratio
2	Number of mcd channels
0.000000	Trigger fracture beam gating
0.000000	Trigger time beam gating
0.000000	Retard energy
0.000000	Ion energy
0.000000	Focus voltage
0.000000	Acceleration voltage
50	Signal to noise limit
100.000000	Time per step

### File (\*.ASC)

174.000000	3647.000000
173.899994	3789.000000
173.799988	3685.000000
173.699982	3817.000000
...	
220.198792	6255.000000
220.098785	6193.000000
219.998779	6303.000000

## 3.1.10 PHI-545/590

### 3.1.10.1 Single Region (\*.TXT)

Comment:

- Acquisition parameters are saved in first row
- First column: binding energies, second column: intensities in counts
- Example: survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\07-PHI545-590 (.TXT)\PHI545-SingleReg.TXT

```
Element ; Region 1 of 1; Depth Cycle 1 of 1; Time Per Step 50; Sweeps 5; Anode
Mg; Photon Energy 1253.6; XPS;
1000 66517
999 66561
998 66742
997 66295
...
5 6557
4 4785
3 2797
2 1563
1 1058
```

### 3.1.10.2 Multiregion (\*.TXT)

Comment:

- Acquisition parameters are saved in first row of each region
- First row: number of regions, excitation energy
- First column: binding energies, second column: intensities in counts
- Example: multiregion C 1s, C KVV, O 1s

- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\ 07-PHI545-590 (.TXT)\ PHI545-MultiReg.TXT

Cycles 9; Regions 3; Anode Mg; Photon Energy 1253.6; XPS;

C 1s CKVV O 1s

86.9897 0.000192393 13.0101

Element C 1s; Region 1 of 3; Depth Cycle 1 of 1; Time Per Step 50; Sweeps 90;

Anode Mg; Photon Energy 1253.6; XPS;

340 2775

339.95 2789

339.9 2845

...

275.15 1707

275.1 1723

275.05 1630

275 1876

Element CKVV; Region 2 of 3; Depth Cycle 1 of 1; Time Per Step 50; Sweeps 108;

Anode Mg; Photon Energy 1253.6; XPS;

1037 14170

1036.9 14298

1036.8 14560

...

957.3 8263

957.2 8116

957.1 8344

957 8109

Element O 1s; Region 3 of 3; Depth Cycle 1 of 1; Time Per Step 50; Sweeps 90;

Anode Mg; Photon Energy 1253.6; XPS;

540 3435

539.9 3362

539.8 3460

...

525.3 3153

525.2 3271

525.1 3867

525 3282

### 3.1.10.3 Profile (\*.TXT)

Comment:

- Acquisition parameters are saved in first row of each region
- First row: number of depth cycles, sputter interval, number of regions, excitation energy
- Second row: number of pre-sputter cycles
- First column: binding energies, second column: intensities in counts
- Example: profile with the regions C 1s, C KVV, O 1s, 3 sputter cycles
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\ 07-PHI545-590 (.TXT)\ PHI545-Profile.TXT

Depth Cycles 3; Regions 3; SputterTime Interval 180; Photon Energy 1253.6; XPS

NumberOfPreSputterCycles 1;

Cycle C 1s CKVV O 1s

0 64.9423 14.9515 6.00912

1 64.751 13.63 8.49895

2 69.822 12.6472 6.28457

Element C 1s; Region 1 of 3; Depth Cycle 1 of 3; Time Per Step 50; Sweeps 90;

Anode Mg; Photon Energy 1253.6; XPS;

340 2775

339.95 2789

339.9 2845

...

275.15	1707
275.1	1723
275.05	1630
275	1876

Element CKVV; Region 2 of 3; Depth Cycle 1 of 3; Time Per Step 50; Sweeps 108;  
Anode Mg; Photon Energy 1253.6; XPS;

1037	14170
1036.9	14298
1036.8	14560

...  

957.3	8263
957.2	8116
957.1	8344
957	8109

Element O 1s; Region 3 of 3; Depth Cycle 1 of 3; Time Per Step 50; Sweeps 90;  
Anode Mg; Photon Energy 1253.6; XPS;

540	3435
539.9	3362
539.8	3460

...  

525.3	3153
525.2	3271
525.1	3867
525	3282

Element C 1s; Region 1 of 3; Depth Cycle 2 of 3; Time Per Step 50; Sweeps 90;  
Anode Mg; Photon Energy 1253.6; XPS;

340	2775
339.95	2789
339.9	2845

...  

275.15	1707
275.1	1723
275.05	1630
275	1876

Element CKVV; Region 2 of 3; Depth Cycle 2 of 3; Time Per Step 50; Sweeps 108;  
Anode Mg; Photon Energy 1253.6; XPS;

1037	14170
1036.9	14298
1036.8	14560

...  

957.3	8263
957.2	8116
957.1	8344
957	8109

Element O 1s; Region 3 of 3; Depth Cycle 2 of 3; Time Per Step 50; Sweeps 90;  
Anode Mg; Photon Energy 1253.6; XPS;

540	3435
539.9	3362
539.8	3460

...  

525.3	3153
525.2	3271
525.1	3867
525	3282

Element C 1s; Region 1 of 3; Depth Cycle 3 of 3; Time Per Step 50; Sweeps 90;  
Anode Mg; Photon Energy 1253.6; XPS;

340	2775
339.95	2789
339.9	2845

...  

275.15	1707
--------	------

275.1	1723
275.05	1630
275	1876

Element CKVV; Region 2 of 3; Depth Cycle 3 of 3; Time Per Step 50; Sweeps 108;  
Anode Mg; Photon Energy 1253.6; XPS;

1037	14170
1036.9	14298
1036.8	14560

...

957.3	8263
957.2	8116
957.1	8344
957	8109

Element O 1s; Region 3 of 3; Depth Cycle 3 of 3; Time Per Step 50; Sweeps 90;  
Anode Mg; Photon Energy 1253.6; XPS;

540	3435
539.9	3362
539.8	3460

...

525.2	3271
525.1	3867
525	3282

### 3.1.11 PHI-1600/1600C

#### 3.1.11.1 Standard Format, Version 1 (\*.csv)

Comment:

- Acquisition parameters saved in header
- Intensities are in counts
- Example: multiregion measurement survey, Ag 3d, Au 4f
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\08-PHI-16001600C  
(.CSV)\PHI1600-MultiReg-Ver1-SurvAgAu.CSV

```
[ID INFO]
App,PHI SCA XPS
Technique,XPS
Type,MULTIPLEX
Mode,7FAT
Version,1.00
Comment,
[VACUUM INFO]
Vacuum(Pa),0.00
[TRANSMISSION FUNCTION INFO]
A,24.500
B,0.207
[CONTROL INFO]
NumberOfRegions,3
NumberOfAreas,1
NumberOfAngles,1
NumberOfCycles,16
[INPUT LENS INFO]
LensType,Omnii2
Aperture,4
LensMode,MINIMUM
[SCA CONTROL INFO]
SCAControlType,Model_80_365_B
MinimumEnergyStep,0.025
[X RAY INFO]
Source,Conventional
```

```
Anode#, 2
WorkFunction (eV), 3.50
HighVoltage (kV), 15.0
AnodeName, Al
SourceEnergy (eV), 1486.6
Power (W), 400
[ION GUN INFO]
GasSpecies, Ar
IonCurrent (uA), 1.000
SputterRate (nm/min), 1.00
BeamVoltage (kV), 3.0
GridSupply (V), 200
Emission (mA), 25.00
Float (V), 0
Condenser (%), 80.0
Objective (%), 65.0
Bend (%), 0.0
XRaster (%), 0.0
YRaster (%), 0.0
XOffset (mm), 0.00
YOffset (mm), 0.00
SputterTime (sec), 30
[ION GUN NEUTRALIZE INFO]
GasSpecies, Ar
IonCurrent (uA), 1.000
BeamVoltage (kV), 0.5
GridSupply (V), 120
Emission (mA), 25.00
Float (V), 450
Condenser (%), 80.0
Objective (%), 65.0
Bend (%), 5.0
XRaster (%), 0.0
YRaster (%), 0.0
XOffset (mm), 0.00
YOffset (mm), 0.00
FilamentStatus, OFF
[NEUTRALIZER INFO]
EmissionCurrent (mA), 0.000
BiasVoltage (V), 0.0
Extractor (V), 0.0
XSteering (%), 0.0
YSteering (%), 0.0
FilamentStatus, OFF
[STAGE INFO]
X (mm), 0
Y (mm), 0
Z (mm), 0
Rotate (deg), 0
Tilt (deg), 45
DirectionOfRotation, CCW
[DETECTOR INFO]
MultiplierOffset (V), 80
MultiplierVoltage (V), 1830
[ENERGY SCAN INFO]
EnergyScanMode, Scanned
[IMAGE INFO]
ImageSize (mm), 2.000
FileName,
[REGION INFO]
RegionNumber, RegionName, Lower (eV), Range (eV), PassEnergy (eV), EnergyStep (eV), Time/S
tep (ms), Repeats
1, SUR, 0.000, 1400.000, 187.850, 1.000, 20, 1
2, Ag3d, 362.000, 20.000, 11.750, 0.100, 20, 8
3, Au4f, 79.000, 20.000, 11.750, 0.100, 20, 8
[POINT INFO]
PointNumber, Xposition, Yposition
```

```
1,1024,1024
[SPECTRA DATA]
PointNumber,1
RegionName,SUR
Cycle,16
Data(Counts)
1400.000,47766
1399.000,47046
1398.000,46461
1397.000,45741
1396.000,44900
...
4.000,7848
3.000,6246
2.000,4812
1.000,3701
0.000,2933
RegionName,Ag3d
Cycle,16
Data(Counts)
382.000,9121
381.900,9355
381.800,9547
381.700,9231
...
362.300,7560
362.200,7536
362.100,7557
362.000,7506
RegionName,Au4f
Cycle,16
Data(Counts)
99.000,4387
98.900,4193
98.800,4221
...
79.200,2247
79.100,2278
79.000,2251
ddd
```

### 3.1.11.2 Standard Format, Version 2 (\*.csv)

#### Comment:

- All acquisition parameters (dwell time, number of scans, pass energy, excitation energy, analyser mode) are not saved and has to be defined manually
- First column: binding energies, second column: intensities
- Example: measurement of 2 regions (Ag 3d, Au 4d3)
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\ 08-PHI-16001600C (.CSV)\ PHI1600-MultiReg-Ver2-AuAg.CSV

Area1

```
Ag3d
1
378.0000,4067.9966
377.9000,4137.0375
377.8000,4127.4420
...
362.2000,2712.6659
362.1000,2768.1670
362.0000,2801.7648
```

Area1

Au4d3

1  
 364.0000,2823.8659  
 363.9000,2844.2625  
 363.8000,2902.7648  
 ...  
 344.3000,2473.8477  
 344.2000,2479.6977  
 344.1000,2547.6761  
 344.0000,2434.0284

### 3.1.11.3 Parameter Dependent Measurement (Depth Profile) (\*.CSV)

Comment:

- All acquisition parameters saved in header
- Example: sputter depth profile, 5 regions (C 1s, O 1s, Pt 4f, Cu 2p<sub>3/2</sub>, Si 2p), 35 sputter cycles
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\08-PHI-16001600C  
 (.CSV)\PHI1600-Profile.CSV

```
[ID INFO]
App,PHI_SCA_XPS_V1.3
Technique,XPS
Type,DEPTHPROFILE
Mode,FAT
Version,1.30
Comment,SiO2_3
[VACUUM INFO]
Vacuum(Pa),0.00
[TRANSMISSION FUNCTION INFO]
A,24.500
B,0.207
[CONTROL INFO]
NumberOfRegions,5
NumberOfAreas,1
NumberOfAngles,1
NumberOfCycles,35
[INPUT LENS INFO]
LensType,Omnis3
Aperture,5
LensMode,MINIMUM
[SCA CONTROL INFO]
SCAControlType,Model_80_365
MinimumEnergyStep,0.025
[X RAY INFO]
Source,Monochromated
Anode#,1
WorkFunction(eV),3.70
HighVoltage(kV),13.0
AnodeName,Al
SourceEnergy(eV),1486.7
Power(W),300
[ION GUN INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
SputterRate(nm/min),1.00
BeamVoltage(kV),3.0
GridSupply(V),200
Emission(mA),25.00
Float(V),0
Condenser(%),80.0
Objective(%),65.0
Bend(%),0.0
```

```
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
SputterTime(sec),30
Pressure(mPa),0.000
[ION GUN NEUTRALIZE INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
BeamVoltage(kV),0.5
GridSupply(V),120
Emission(mA),25.00
Float(V),450
Condenser(%),80.0
Objective(%),65.0
Bend(%),5.0
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
FilamentStatus,OFF
[NEUTRALIZER INFO]
EmissionCurrent(mA),20.000
BiasVoltage(V),3.0
Extractor(V),0.0
XSteering(%),0.0
YSteering(%),0.0
FilamentStatus,ON
[STAGE INFO]
X(mm),0
Y(mm),0
Z(mm),0
Rotate(deg),0
Tilt(deg),0
DirectionOfRotation,CCW
[DETECTOR INFO]
MultiplierOffset(V),200
MultiplierVoltage(V),1900
[ENERGY SCAN INFO]
EnergyScanMode,Scanned
[PEAK DATA INFO]
PeakDataMode,Height
[SPUTTER INFO]
SputterType,Alternate
ZalarRotation,notused
DirectionOfRotation,CW
XrayWhileSputtering,Off
SputterTime(min),33.00
IntervalTime(min),1.00
DelayTime(sec),15
[IMAGE INFO]
ImageSize(mm),2.000
FileName,
[REGION INFO]
RegionNumber,RegionName,Lower(eV),Range(eV),PassEnergy(eV),EnergyStep(eV),Time/Step(ms),Repeats
1,C1s,278.000,20.000,11.750,0.100,20,2
2,O1s,523.000,20.000,11.750,0.100,20,5
3,Pt4f,66.000,20.000,11.750,0.100,20,2
4,Cu2p3,927.000,30.000,11.750,0.050,20,15
5,Si2p,94.000,20.000,11.750,0.100,20,2
[POINT INFO]
PointNumber,Xposition,Yposition
1,1024,1024
[PEAK DATA]
PointNumber,1
RegionName,C1s,,O1s,,Pt4f,,Cu2p3,,Si2p,
```

```
,Time (min),Data (CPS),Time (min),Data (CPS), ... ,Time (min),Data (CPS),
,0.000,46142,0.000,57711,0.000,207322,0.000,54401,0.000,12444,
,0.000,39895,0.000,55214,0.000,238795,0.000,71552,0.000,12498,
...
,32.000,1531,32.000,240005,32.000,1938,32.000,6482,32.000,48073,
,33.000,1582,33.000,242800,33.000,1089,33.000,4961,33.000,49444,
[SPECTRA DATA]
PointNumber,1
RegionName,C1s
Cycle,1,2,3,4,5,6,7,8,9,10,11, ... ,34,35,
Energy (eV),Data (Counts),Data (Counts) ...
,Data (Counts),Data (Counts),Data (Counts),Data (Counts),
298.000,108,70,66,57,30,29,23,18, ... ,14,20,17,21,12,23,29,9,12,17,23,24,19,15,
297.900,99,73,75,54,35,23,16,21, ... ,9,17,16,27,14,23,20,13,17,15,11,22,18,21,
...
278.100,85,76,74,48,41,24,23,26, ... ,15,19,21,14,18,16,10,17,18,17,13,18,18,13,
278.000,78,79,64,49,38,22,21,21, ... ,18,21,26,12,17,16,13,19,20,19,11,16,11,14,
RegionName,O1s
Cycle,1,2,3,4,5,6,7,8,9,10,11,12,13, ... ,27,28,29,30,31,32,33,34,35,
Energy (eV),Data (Counts),Data (Counts), ... ,Data (Counts),Data (Counts),
543.000,408,390,329,265,182,147,136,119, ... ,107,96,94,82,81,97,106,84,100,
542.900,399,416,375,261,185,132,130,130, ... ,98,97,98,107,93,102,79,93,78,85,
...
523.200,388,389,453,346,218,146,90,66,64, ... ,33,41,31,38,38,41,36,38,36,35,42,
523.100,405,402,445,364,226,153,97,70,66, ... ,43,35,37,31,38,31,42,38,40,39,
523.000,398,406,439,352,203,151,95,73,69, ... ,40,38,38,35,40,34,34,38,37,34,
RegionName,Pt4f
Cycle,1,2,3,4,5,6,7,8,9,10,11, ... ,22,23,24,25,26,27,28,29,30,31,32,33,34,35,
Energy (eV),Data (Counts),Data (Counts), ... ,Data (Counts),Data (Counts),
86.000,115,135,134,123,66,41,24,22,24,18, ... ,5,8,14,10,6,9,5,8,7,6,7,5,8,2,3,
85.900,84,134,149,109,73,39,25,23,16,14,8,8, ... ,10,7,7,6,9,11,4,7,10,1,6,
...
66.100,36,42,49,39,21,12,13,11,16,9,11, ... ,8,7,8,9,6,6,6,4,5,6,7,9,3,4,
66.000,28,40,43,39,27,17,14,9,13,8,9,8, ... ,10,10,8,5,4,7,3,7,8,5,9,5,6,
RegionName,Cu2p3
Cycle,1,2,3,4,5,6,7,8,9,10,11, ... ,23,24,25,26,27,28,29,30,31,32,33,34,35,
Energy (eV),Data (Counts),Data (Counts), ... ,Data (Counts),Data (Counts),
957.000,1170,1211,1263,1362,826,527,382,326, ... ,242,227,197,240,202,229,215,
956.950,1092,1185,1138,1397,867,525,385,335, ... ,247,235,245,209,232,224,234,
...
927.050,941,913,964,869,547,423,352,272,291, ... ,217,279,266,217,261,242,227,
927.000,954,956,948,864,522,368,346,299,257, ... ,265,232,253,246,259,268,252,
RegionName,Si2p
Cycle,1,2,3,4,5,6,7,8,9,10,11,12, ... ,25,26,27,28,29,30,31,32,33,34,35,
Energy (eV),Data (Counts),Data (Counts), ... ,Data (Counts),Data (Counts),
114.000,130,125,137,100,55,54,29,24, ... ,14,15,15,13,9,17,10,7,12,10,14,14,8,
113.900,133,128,135,93,51,34,31,19,17, ... ,14,8,10,10,11,10,9,7,9,14,18,7,
...
94.100,122,117,131,108,69,42,33,20, ... ,12,10,14,9,6,6,8,5,4,6,9,5,6,7,6,
94.000,123,122,140,111,63,37,29,23,20, ... ,12,8,7,8,6,6,3,4,11,5,7,5,5,
```

### 3.1.12 VGX-900 (\*.1)

#### Comment:

- VGX-900 files can be recorded with decreasing or increasing kinetic or binding energy
- 1. row: experimental method,
- 2. row: 12 characters start energy, 12 characters end energy, 12 characters step width, 12 characters number of scans, 12 characters time per step, 6 characters number of steps, 8 characters pass energy
- Example: multiregion measurement with 5 regions (survey, C 1s, N 1s, O 1s, Si 2p)
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\09-VGX-900 (.1)\ Install-Memory Card:\GX-900-MultiReg-BE-increasing-with-Excitation-energy.1

```

XPS-Spectrum
  0.00000  1100.00000  1.00000  2.00000  0.10000  1101  100.0 -
1486.6
          Survey
215
222
225
...
18590
18544
18749
  275.00000  305.00000  0.02500  10.00000  0.05000  1201  20.0 -
1486.6
          C1s
209
213
216
...
977
992
1119
997
  395.00000  420.00000  0.02500  20.00000  0.05000  1001  20.0 -
1486.6
          N1s
2834
2843
2850
...
3029
2946
2885
3075
  520.00000  550.00000  0.02500  5.00000  0.05000  1201  20.0 -
1486.6
          O1s
807
850
851
...
1197
1200
1193
  95.00000  120.00000  0.02500  10.00000  0.05000  1001  20.0 -
1486.6
Si
256
241
219
...
208
230
210
215

```

### 3.1.13 VAMAS

#### 3.1.13.1 Standard Format (\*.VMS;\*NPL)

Comment:

- ',NORM' in 7. row means ',Multiregion Measurement'
- Acquisition parameters saved in header of each region

- Example: multiregion measurement of GaAs with 8 regions (As 2p<sub>3/2</sub>, As 3d, C 1s, Ga 2p<sub>3/2</sub>, Ga 3d, O 1s, Survey, VB)
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\10-Vamas (.VMS)\VAMAS-MultiReg-GaAs.VMS

VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4

Institute ID

ESCALab250

vgengineer

1

As2p3

NORM

REGULAR

8

0

0

0

0

0

8

Region 1

sample id

2007

7

11

12

15

0

0

0

XPS

Al

1486.6

1.0E37

1.0E37

1.0E37

1.0E37

1.0E37

FAT

10

1

4.444

0

0

0

0

0

As2p3

-1

kinetic energy

eV

151.6

0.05

1

counts per channel

d

pulse counting

0.3

5

0

0

0

0

```
0
401
0
10000
16389.1800000041
16569.0600000015
16452.1600000039
16071.5800000038
15940.9000000052
...
12967.2800000033
12998.0600000011
12904.8600000032
Region 2
sample id
2007
7
11
11
45
43
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
As3d

-1
kinetic energy
eV
1436.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
281
0
10000
238.65999999962
239.639999999449
233.739999999547
245.17999999964
...
193.09999999989
```

```
200.540000000061
Region 3
sample id
2007
7
11
11
37
34
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
0
C1s

-1
kinetic energy
eV
1191.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
401
0
10000
2948.54000000032
2975.69999999348
3025.55999999944
3080.79999999792
...
3039.59999999812
3074.74000000033
3136.04000000021
Region 4
sample id
2007
7
11
12
26
15
0
0
```

```
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
Ga2p3

-1
kinetic energy
eV
356.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
401
0
10000
8753.799999999996
8611.96000000445
8614.64000000418
8670.04000000134
...
7040.82000000105
7134.219999999996
7143.42000000003
Region 5
sample id
2007
7
11
12
3
38
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
```

```
4.444
0
0
0
0
0
0
Ga3d

-1
kinetic energy
eV
1456.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
321
0
10000
113.8199999999877
99.29999999998113
103.6199999999768
...
43.79999999998772
35.3000000000432
40.7799999999868
Region 6
sample id
2007
7
11
11
54
25
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
0
O1s

-1
kinetic energy
eV
946.6
```

```
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
301
0
10000
6797.37999999294
6775.21999999325
6831.79999999088
...
6678.09999999377
6699.85999999812
6626.33999999272
Region 7
sample id
2007
7
11
11
26
13
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
50
1
4.444
0
0
0
0
0
0
Survey

-1
kinetic energy
eV
86.59999999999999
0.5
1
counts per channel
d
pulse counting
0.3
2
0
0
0
0
0
```

```
2801
0
10000
113668.31
113261.39
111981.53
111248.01
...
444.849999999974
197.139999999988
68.0399999999922
Region 8
sample id
2007
7
11
12
33
29
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
VB
-1
kinetic energy
eV
1476.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
241
0
10000
37.259999999985
30.539999999924
35.5399999999286
...
4.14000000000136
2.25999999999409
2.1800000000005
end of experiment
```

### 3.1.13.2 Parameter Dependent Measurement (Depth Profile) (\*.VMS)

Comment:

- SDP<sup>6</sup> in 7. row means profile (e.g. sputter depth profile, angle resolved measurement)
- Example consists of 21 spectra, i.e. 3 regions (O 1s, C 1s, Si 2p) with 7 steps (sputter time, angle etc.)
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\10-Vamas (.VMS)\Vamas-Profile-Si\_C\_O\_20-Parasteps\_KE-increasing\_Counts\_without\_Cor\_Par.VMS

```
VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4
Univ. Leipzig, Fachbereich Chemie
EscaLab 220-IXL
Ronald Hesse
C:\RH\DAT\SIDP
0
SDP
REGULAR
3
1
Etch Time
Seconds
0
0
0
0
21
Region 0

1998
12
21
9
47
2
255
0
XPS
0
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
C1s
C1s
-1
Kinetic Energy
eV
1196.6
0.1
```

```
1
Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
81
7149.84
14129.2
7388.86
7285.92
7355.6
...
7163.96
7177.98
7190.72
...
Region 0

1998
12
21
10
33
19
255
0
XPS
360
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
C1s
C1s
-1
Kinetic Energy
eV
1196.6
0.1
```

```
1
Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
81
7400.7
7973.76
7469.58
7452.52
...
7727.98
7659.92
Region 1

1998
12
21
9
47
3
255
0
XPS
0
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
01s
01s
-1
Kinetic Energy
eV
947.6
0.1
1

Counts
```

```
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
111
7487.76
33338.5
7731.46
...
7688.62
7509.76
7502.9
...
Region 1

1998
12
21
10
33
19
255
0
XPS
360
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
01s
01s
-1
Kinetic Energy
eV
947.6
0.1
1

Counts
pulse counting
0.3
```

```
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
111
7187.1
8566.98
7359.68
...
7362.26
7240
7220.72
7265.28
Region 2

1998
12
21
9
47
1
255
0
XPS
0
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
Si2p
Si2p
-1
Kinetic Energy
eV
1378.6
0.1
1

Counts
pulse counting
0.3
3
0
```

```
0
1
1
1
0
0
Cyclic
0
0
0
0
131
1785.06
18039.9
...
1837.52
1842.62
...
Region 2

1998
12
21
10
25
37
255
0
XPS
300
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
Si2p
Si2p
-1
Kinetic Energy
eV
1378.6
0.1
1

Counts
pulse counting
0.3
3
0
0
1
1
1
```

```
0
0
Cyclic
0
0
0
0
131
1976.72
25878.7
3811.28
3780.16
...
1976.72
1980.54
Region 2

1998
12
21
10
33
19
255
0
XPS
360
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
Si2p
Si2p
-1
Kinetic Energy
eV
1378.6
0.1
1

Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
```

```

0
0
0
0
131
1940.86
25983.9
3690
...
1969.58
1991.7
2053.38
end of experiment

```

### 3.1.13.3 Multipoint Measurement (Area Scan) (\*.VMS)

Comment:

- Multipoint measurement (area scan), MAP in the 6. row means: Mapping
- Example consists of 211 spectra, i.e. 3 regions (O 1s, Ag 3d, Bi 4f) at 70 recording points (210 single spectra with x and y position) and one survey
- sequence of spectra: region 1: O 1s 1. point, region 2: Ag 3d, 1. point, region 3: Bi 4f, 1. point, region 4: O1s, 2. point, ..., region 208: O 1s 70. point 70. region 209: Ag 3d, 70. point, region 210: Bi 4f, 70. point, region 211: survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\10-Vamas (.VMS)\Vamas-AreaScan-3Regions.VMS

```

VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4
Not Specified
Kratos Axis Ultra
Not Specified
/C=/data/Hirsch/test_RH_Matrix.dset
0
MAP
REGULAR
4
41
32768
32768
1
Etch Time
s
0
0
0
0
211
O 1s/2
Not Specified
2013
9
23
11
28
51
0
3
XPS      Spectrum
Acqn. Time(s): 65      Sweeps: 2      Anode:Mono (Al (Mono)) (150 W)
Step(meV) : 100.0
Dwell Time(ms): 180   Charge Neutraliser :On   Acquired On :13/09/23
11:28:51
XPS
51.31
1.241

```

0  
Mono (Al (Mono))  
1486.69  
150  
1E+37  
1E+37  
6000  
6000  
1E+37  
1E+37  
FAT  
80  
1E+37  
-4.479  
0  
1E+37  
1E+37  
1E+37  
1E+37  
0  
1s  
-1  
Kinetic Energy  
eV  
946.69  
0.1  
2  
Intensity  
d  
Transmission  
d  
pulse counting  
0.18  
2  
0  
1E+37  
1E+37  
1E+37  
0  
362  
1127  
2334  
0.709544  
0.712206  
1127  
0.709544  
1140  
0.709558  
1163  
0.709573  
1141  
0.709588  
1156  
0.709603  
...  
1281  
0.712162  
1316  
0.712177  
1330  
0.712192  
1333  
0.712206  
Ag 3d/3  
Not Specified  
2013  
9

23  
11  
28  
51  
0  
3  
XPS Spectrum  
Acqn. Time(s): 65 Sweeps: 2 Anode: Mono (Al (Mono)) (150 W)  
Step (meV): 100.0  
Dwell Time (ms): 180 Charge Neutraliser : On Acquired On : 13/09/23  
11:28:51  
XPS  
51.31  
1.241  
0  
Mono (Al (Mono))  
1486.69  
150  
1E+37  
1E+37  
6000  
6000  
1E+37  
1E+37  
FAT  
80  
1E+37  
-4.479  
0  
1E+37  
1E+37  
1E+37  
1E+37  
Ag  
3d  
-1  
Kinetic Energy  
eV  
1109.69  
0.1  
2  
Intensity  
d  
Transmission  
d  
pulse counting  
0.18  
2  
0  
1E+37  
1E+37  
1E+37  
0  
362  
359  
6763  
0.741829  
0.746462  
844  
0.741829  
845  
0.741855  
817  
0.741881  
840  
0.741907  
842

```
0.741932
...
398
0.74641
395
0.746436
383
0.746462
Bi 4f/4
Not Specified
2013
9
23
11
28
51
0
3
    XPS      Spectrum
    Acqn. Time(s): 98      Sweeps: 3      Anode:Mono(Al (Mono)) (150 W)
Step(meV): 100.0
    Dwell Time(ms): 180      Charge Neutraliser :On      Acquired On :13/09/23
11:28:51
XPS
51.31
1.241
0
Mono(Al (Mono))
1486.69
150
1E+37
1E+37
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
Bi
4f
-1
Kinetic Energy
eV
1317.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
3
0
1E+37
1E+37
1E+37
0
362
427
```

912  
0.783451  
0.786926  
517  
0.783451  
574  
0.783462  
516  
0.783473  
...  
603  
0.786891  
592  
0.786926  
O 1s/7  
Not Specified  
2013  
9  
23  
11  
35  
24  
0  
3  
XPS Spectrum  
Acqn. Time(s): 65 Sweeps: 2 Anode:Mono(Al (Mono))(150 W)  
Step(meV): 100.0 Charge Neutraliser :On Acquired On :13/09/23  
Dwell Time(ms): 180  
11:35:24  
XPS  
51.61  
1.241  
0  
Mono(Al (Mono))  
1486.69  
150  
1E+37  
1E+37  
6000  
6000  
1E+37  
1E+37  
FAT  
80  
1E+37  
-4.479  
0  
1E+37  
1E+37  
1E+37  
1E+37  
O  
1s  
-1  
Kinetic Energy  
eV  
946.69  
0.1  
2  
Intensity  
d  
Transmission  
d  
pulse counting  
0.18  
2  
0

1E+37  
1E+37  
1E+37  
0  
362  
989  
2326  
0.709544  
0.712206  
1099  
0.709544  
1017  
0.709558  
1099  
0.709573  
1078  
0.709588  
1082  
0.709603  
...  
1063  
0.712162  
1057  
0.712177  
1055  
0.712192  
990  
0.712206  
Ag 3d/8  
Not Specified  
2013  
9  
23  
11  
35  
24  
0  
3

XPS Spectrum

Acqn. Time(s): 33 Sweeps: 1 Anode: Mono (Al (Mono)) (150 W) Step(meV): 100.0

Dwell Time(ms): 180 Charge Neutraliser :On Acquired On :13/09/23 11:35:24

XPS

51.61

1.241

0

Mono (Al (Mono))

1486.69

150

1E+37

1E+37

6000

6000

1E+37

1E+37

FAT

80

1E+37

-4.479

0

1E+37

1E+37

1E+37

1E+37

Ag

3d

-1

Kinetic Energy

```
eV
1109.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
1
0
1E+37
1E+37
1E+37
0
362
177
2343
0.741829
0.746462
319
0.741829
327
0.741855
348
0.741881
354
0.741907
334
0.741932
304
0.741958
330
0.741984
333
0.74201
...
192
0.74641
187
0.746436
205
0.746462
Bi 4f/9
Not Specified
2013
9
23
11
35
24
0
3
XPS Spectrum
Acqn. Time(s): 98 Sweeps: 3 Anode:Mono (Al (Mono)) (150 W) Step(meV): 100.0
Dwell Time(ms): 180 Charge Neutraliser :On Acquired On :13/09/23 11:35:24
XPS
51.61
1.241
0
Mono (Al (Mono))
1486.69
150
1E+37
1E+37
```

```
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
Bi
4f
-1
Kinetic Energy
eV
1317.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
3
0
1E+37
1E+37
1E+37
0
362
406
1039
0.783451
0.786926
493
0.783451
484
0.783462
473
0.783473
...
77
0.786856
104
0.786891
76
0.786926
Survey_Ende/351
Not Specified
2013
9
23
17
52
17
0
3
XPS Spectrum
Acqn. Time(s): 60 Sweeps: 1 Anode:Mono(Al (Mono))(150 W) Step(meV): 1000.0
Dwell Time(ms): 50 Charge Neutraliser :On Acquired On :13/09/23 17:52:17
XPS
54.01
3.041
```

```
0
Mono (Al (Mono))
1486.69
150
1E+37
1E+37
6000
6000
1E+37
1E+37
FAT
160
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
Wide
None
-1
Kinetic Energy
eV
286.69
1
2
Intensity
d
Transmission
d
pulse counting
0.0498
1
0
1E+37
1E+37
1E+37
0
2412
0
5814
29.4792
42.7379
994
30.7448
971
30.7282
1020
30.7117
1006
30.6952
...
0
42.7379
end of experiment
```

### 3.1.14 NPL (\*.NPL)

#### Comment:

- Header contains all important acquisition parameters
- Example consists of 3 spectra (O 1s, C 1s, survey)
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\12-NPL (.NPL)\NPL-MultiReg-3Spectra.NPL

---

C:\ALI\AAL15\B1507.DAT

3 Spectra  
1 Levels  
1 Points

---

Region : 1 "C 1s" Level : 1 Point : 1  
301 Channels  
From : 1176.600  
To : 1206.600  
Step : 0.100  
Kinetic eV  
XPS  
CAE : 10  
WF : 3.95  
10 Scans  
Dwell Time : 100ms  
Al Source

---

2087.7  
2150

...  
836  
851.1  
840.1  
844.1  
848.4  
824.8

---

Region : 2 "O 1s" Level : 1 Point : 1  
251 Channels  
From : 936.600  
To : 961.600  
Step : 0.100  
Kinetic eV  
XPS  
CAE : 10  
WF : 3.95  
10 Scans  
Dwell Time : 100ms  
Al Source

---

3476.2  
3626.7  
3759.6

...  
3521.5  
3507.5  
3501.2

---

Region : 3 "wideAl" Level : 1 Point : 1  
2801 Channels  
From : 86.600  
To : 1486.600  
Step : 0.500  
Kinetic eV  
XPS  
CRR : 10  
WF : 3.95  
2 Scans  
Dwell Time : 50ms  
Al Source

---

1179.19  
1135.35  
...

451.644  
470.943

### 3.1.15 SPECSLAB (\*.EXP)

Comment:

- The region name are saved in “tag”
- Only the data set “original” is read
- Example shows 11 spectra: 2xsurvey, 3xAu 3d, 3xAu 4f, 3xO 1s
- Spectra names: Survey1, Survey2, Au 4f\_1, Au 3d\_1, O 1s\_1, Au 4f\_2, Au 3d\_2, O 1s\_2, Au 4f\_3, Au 3d\_3, O 1s\_3
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\13-Speclab(.EXP)\Speclab-MultiReg-Au\_Mg-Excit.EXP

```
#SPX
region: 1
method: XPS
active: 0
range: 200 1300 0.5
scans: 1
dwell: 0.1
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 192;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Survey1"
ManipulationProtocol:
```

```
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 10 22
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 2201 long 12558
46488
46693
45865
...
2176
2127
enddata
background: 2201 double 21247
46348.667
46211.736
46074.805
...
2157.193
2158.667
endbackground
original: 2201 long 12558
46488
46693
45865
...
2176
2127
endoriginal
endregion
region: 2
method: XPS
active: 0
range: 200 1560 0.5
scans: 1
dwell: 0.1
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Al;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 192;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
```

```
    ma_y = 0;
    ma_sample = 6;
    ma_z = 0;
    ma_tilt = 0;
    ma_rot = 0;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = 283;
    mi_acp_pascal = 1.7e-07;
    mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Survey2"
ManipulationProtocol:
{
    mp_nstrings = 3;
    mp_strings = {
        "Smooth Golay",
        "Smooth Golay",
        "Smooth Golay"
    }
}
measure_date: 13 09 2005 10 15
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 2721 long 13508
15347
15255
15413
...
265
252
enddata
background: 2721 double 24363
15425.250
15425.250
15375.775
...
257.420
256.000
endbackground
original: 2721 long 13508
15347
15255
15413
...
265
252
endoriginal
endregion
region: 3
method: XPS
active: 0
range: 1160 1173 0.1
scans: 3
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode = Mg;
    xrs_voltage = 0;
```

```
    xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
    ea_mode = esca_c_ep;
    ea_serial = 0;
    ea_vers = 0;
    ea_const = 24;
    ea_ampl_fact = 0;
    ea_particle_polarity = -1;
    ea_detector_U = 2249.9;
    ea_conversion_U = 0;
    ea_aperture = 13;
    ea_is_small_spot = 0;
}
Manipulator: Max
{
    ma_type = Max;
    ma_x = 0;
    ma_y = 0;
    ma_sample = 6;
    ma_z = 0;
    ma_tilt = 0;
    ma_rot = 0;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = 283;
    mi_acp_pascal = 1.7e-07;
    mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 4f_1"
ManipulationProtocol:
{
    mp_nstrings = 0;
    mp_strings = {
    }
}
measure_date: 13 09 2005 10 53
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 131 long 669
2168
2185
2279
...
1392
1339
1391
endoriginal
endregion
region: 4
method: XPS
active: 0
range: 880 935 0.1
scans: 3
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode = Mg;
```

```
xrs_voltage = 0;
xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 24;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 3d_1"
ManipulationProtocol:
{
  mp_nstrings = 5;
  mp_strings = {
    "Default Background applied",
    "Default Background applied",
    "No Background [1191.6..1191.6]",
    "Tougaard Background B/C 2866/1643 [1191.6..1191.6]",
    "Shirley Background [1191.6..1191.6]"
  }
}
measure_date: 13 09 2005 10 53
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 551 long 2755
3842
4039
3827
...
2509
2518
2565
enddata
background: 551 double 4959
3902.809
3902.490
3902.667
...
2534.058
2532.362
```

```
2530.667
endbackground
original: 551 long 2755
3842
4039
3827
...
2509
2518
2565
endoriginal
endregion
region: 5
method: XPS
active: 0
range: 690 725 0.1
scans: 3
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 24;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "0 1s_1"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 10 56
filename: "050913_Au_Mg_13"
```

```
visible: 0
depth: 1
sputter_def: 0
data: 351 long 1755
5390
5231
5249
...
4642
4894
4759
enddata
background: 351 double 3159
5290.000
5264.830
5239.660
...
4760.143
4762.571
4765.000
endbackground
original: 351 long 1755
5390
5231
5249
...
4642
4894
4759
endoriginal
endregion
region: 6
method: XPS
active: 1
range: 1160 1173 0.1
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode = Mg;
    xrs_voltage = 0;
    xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
    ea_mode = esca_c_ep;
    ea_serial = 0;
    ea_vers = 0;
    ea_const = 48;
    ea_ampl_fact = 0;
    ea_particle_polarity = -1;
    ea_detector_U = 2249.9;
    ea_conversion_U = 0;
    ea_aperture = 13;
    ea_is_small_spot = 0;
}
Manipulator: Max
{
    ma_type = Max;
    ma_x = 0;
    ma_y = 0;
    ma_sample = 6;
    ma_z = 0;
    ma_tilt = 0;
```

```
    ma_rot = 0;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = 283;
    mi_acp_pascal = 1.7e-07;
    mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 4f_2"
ManipulationProtocol:
{
    mp_nstrings = 0;
    mp_strings = {
    }
}
measure_date: 13 09 2005 11 10
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 131 long 720
6816
7071
6798
...
4423
4275
4408
enddata
background: 131 double 1179
6895.175
6894.786
6895.000
...
4368.547
4368.753
4368.667
endbackground
original: 131 long 720
6816
7071
6798
...
4248
4423
4275
4408
endoriginal
endregion
region: 7
method: XPS
active: 1
range: 880 935 0.1
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode = Mg;
    xrs_voltage = 0;
    xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
```

```
{
  ea_mode =  esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 48;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 3d 2"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 11 11
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 551 long 3022
9426
9444
9495
...
6275
6399
6238
enddata
background: 551 double 4959
9455.037
9455.052
9455.000
...
6177.532
6240.766
6304.000
endbackground
original: 551 long 3022
9426
9444
9495
...
6275
6399
```

```
6238
endoriginal
endregion
region: 8
method: XPS
active: 1
range: 690 725 0.1
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 48;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "O 1s_2"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 11 14
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 351 long 2081
10501
10265
10450
...
9563
```

```
10156
9816
enddata
background: 351 double 3463
10413.160
10413.160
10413.121
...
9768.989
9806.995
9845.000
endbackground
original: 351 long 2081
10501
10265
10450
...
9563
10156
9816
endoriginal
endregion
region: 9
method: XPS
active: 1
range: 1160 1173 0.2
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 192;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
```

```
flood_gun_U: 0
tag: "Au 4f_3"
ManipulationProtocol:
{
  mp_nstrings = 5;
  mp_strings = {
    "Default Background applied",
    "Default Background applied",
    "No Background [1191.6..1191.6]",
    "Tougaard Background B/C 2866/1643 [1191.6..1191.6]",
    "Shirley Background [1191.6..1191.6]"
  }
}
measure_date: 13 09 2005 11 20
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 66 long 430
67216
67186
67441
...
48517
47882
47434
enddata
background: 66 double 660
67360.999
67360.999
67360.651
...
47944.353
47941.887
47942.145
47944.333
endbackground
original: 66 long 430
67216
67186
67441
...
48517
47882
47434
endoriginal
endregion
region: 10
method: XPS
active: 1
range: 880 935 0.2
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
```

```
    ea_const = 192;
    ea_ampl_fact = 0;
    ea_particle_polarity = -1;
    ea_detector_U = 2249.9;
    ea_conversion_U = 0;
    ea_aperture = 13;
    ea_is_small_spot = 0;
}
Manipulator: Max
{
    ma_type = Max;
    ma_x = 0;
    ma_y = 0;
    ma_sample = 6;
    ma_z = 0;
    ma_tilt = 0;
    ma_rot = 0;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = 283;
    mi_acp_pascal = 1.7e-07;
    mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 3d 3"
ManipulationProtocol:
{
    mp_nstrings = 0;
    mp_strings = {
    }
}
}
measure_date: 13 09 2005 11 20
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 276 long 1709
77278
77950
77600
...
52072
52506
52648
enddata
background: 276 double 2760
77610.974
77609.295
77609.341
77608.179
77606.895
77605.696
...
52131.467
52270.067
52408.667
endbackground
original: 276 long 1709
77278
77950
77600
...
52072
52506
52648
```

```
endoriginal
endregion
region: 11
method: XPS
active: 1
range: 695 720 0.2
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 192;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "O 1s_3"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 11 22
filename: "050913_Au_Mg_13"
visible: 1
depth: 1
sputter_def: 0
data: 126 long 768
82388
82946
82067
...
78573
78518
```

```

78679
enddata
background: 126 double 1260
82467.000
82412.977
82358.954
...
78852.292
78721.146
78590.000
endbackground
original: 126 long 768
82388
82946
82067
...
78573
78518
78679
endoriginal
endregion

```

### 3.1.16 VSW-Tübingen (\*.DAT)

Comment:

- Regions separated by star
- Start- and endenergy given in KE
- Example: Multiregion measurement, 2 spectra (Ag 3d, Au 4f)
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\14-VSW-Tübingen  
(.DAT)\VSW-MultiReg-Ag3d-Au4f.DAT

```

PCF
EISCA
 5. 6.2003

Goetz,2,Ag3d,Au4f
frei
Referenz Au 123ø mm 474
Gesamtsignal
50.84 Prozent Totzeit
*
2
XPS
FAT
2
X-Ray
1
 1.0000000000E+01
 1.0000000000E+04
*
486
860.001
884.977
50.0
0.051
0.200
*
486
1144.999
1169.975
50.0
0.051
0.200
*

```



```
-
1000.00    58228
 999.75    58404
 999.50    58170
  ...
  1.00     1210
  0.75     1214
  0.50     1078
  0.25     1208
```

### 3.1.18 ScientaSES-Signals (\*.txt)

Comment::

- Excitation energy was transferred from the synchrotron in case ,Monochromator Energy' is zero
- Excitation energy in Line: 'Ph. energy=1099.995'
- Example: 2 regions, VB and Ce, La,\_Co
- Versions 1.2.2 and 1.3.1 are loadable
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\16-ScientaSES-Signals(.TXT)\ScientaSES-Signals-MultiReg-2Regions.TXT

[Info]

Number of Regions=2  
Version=1.2.2

[Region 1]

Region Name=014  
Dimension 1 name=Kinetic Energy [eV]  
Dimension 1 size=451  
Dimension 1 scale=1060.00000 1060.10000 1060.20000 1060.30000 1060.40000  
1060.50000 1060.60000 1060.70000 1060.80000 1060.90000 1061.00000 1061.10000  
1061.20000 1061.30000 1061.40000 1061.50000 1061.60000 1061.70000 1061.80000  
1061.90000 1062.00000 1062.10000 1062.20000 1062.30000 1062.40000 1062.50000  
1062.60000 1062.70000 1062.80000 1062.90000 1063.00000 1063.10000 1063.20000  
...  
1101.10000 1101.20000 1101.30000 1101.40000 1101.50000 1101.60000 1101.70000  
1101.80000 1101.90000 1102.00000 1102.10000 1102.20000 1102.30000 1102.40000  
1102.50000 1102.60000 1102.70000 1102.80000 1102.90000 1103.00000 1103.10000  
1103.20000 1103.30000 1103.40000 1103.50000 1103.60000 1103.70000 1103.80000  
1103.90000 1104.00000 1104.10000 1104.20000 1104.30000 1104.40000 1104.50000  
1104.60000 1104.70000 1104.80000 1104.90000 1105.00000

[Info 1]

Instrument=SES 2002-2MS201  
Location=WERA  
User=CP  
Sample=WERA20  
Comments=La0.9Ce0.1CoO3  
xsl=-240 50/50 size=5 slit=2.5

Date=8/15/2007  
Time=5:32:08 PM  
Region Name=VB\_1100  
Excitation Energy=0  
Energy Scale=Kinetic  
Acquisition Mode=Swept  
Center Energy=9  
Low Energy=1060  
High Energy=1105  
Energy Step=0.1  
Step Time=100  
Detector First X-Channel=1  
Detector Last X-Channel=471  
Detector First Y-Channel=127  
Detector Last Y-Channel=536

Number of Slices=1  
Lens Mode=Transmission  
Pass Energy=100  
Number of Sweeps=3  
Time per Spectrum Channel=24.3

[User Interface Information 1]  
Monochromator Energy= 0.0000  
[Manipulator]  
Z=-0.313  
Phi=-0.203  
Ph. energy=1099.995  
XSL=-239.962

[Data 1]  
1060.00000 46444.00000  
1060.10000 47000.00000  
1060.20000 52272.00000  
1060.30000 49488.00000  
1060.40000 42540.00000  
...  
1104.50000 552.00000  
1104.60000 556.00000  
1104.70000 956.00000  
1104.80000 748.00000  
1104.90000 120.00000  
1105.00000 556.00000

[Region 2]  
Region Name=014  
Dimension 1 name=Kinetic Energy [eV]  
Dimension 1 size=2201  
Dimension 1 scale=120.00000 120.10000 120.20000 120.30000 120.40000 120.50000  
120.60000 120.70000 120.80000 120.90000 121.00000 121.10000 121.20000 121.30000  
121.40000 121.50000 121.60000 121.70000 121.80000 121.90000 122.00000 122.10000  
...  
336.60000 336.70000 336.80000 336.90000 337.00000 337.10000 337.20000 337.30000  
337.40000 337.50000 337.60000 337.70000 337.80000 337.90000 338.00000 338.10000  
338.20000 338.30000 338.40000 338.50000 338.60000 338.70000 338.80000 338.90000  
339.00000 339.10000 339.20000 339.30000 339.40000 339.50000 339.60000 339.70000  
339.80000 339.90000 340.00000

[Info 2]  
Instrument=SES 2002-2MS201  
Location=WERA  
User=CP  
Sample=WERA20  
Comments=La0.9Ce0.1CoO3  
xsl=-240 50/50 size=5 slit=2.5

Date=8/15/2007  
Time=5:32:08 PM  
Region Name=Ce\_La\_Co\_1100  
Excitation Energy=0  
Energy Scale=Kinetic  
Acquisition Mode=Swept  
Center Energy=9  
Low Energy=120  
High Energy=340  
Energy Step=0.1  
Step Time=100  
Detector First X-Channel=1  
Detector Last X-Channel=471  
Detector First Y-Channel=127  
Detector Last Y-Channel=536  
Number of Slices=1  
Lens Mode=Transmission

```
Pass Energy=100
Number of Sweeps=3
Time per Spectrum Channel=24.3
```

```
[User Interface Information 2]
Monochromator Energy= 0.0000
[Manipulator]
Z=-0.313
Phi=-0.203
Ph. energy=1099.995
XSL=-239.962
```

```
[Data 2]
 120.00000 2291472.00000
 120.10000 2327004.00000
 ...
 339.90000 1192620.00000
 340.00000 1212936.00000
```

### 3.1.19 ScientaSES-Spectra (\*.txt)

Comment:

- ‚Number of Slices’ is the number of separate intensities per channel
- The sum of all intensities per slice or the intensities of slices gives the intensity shown in the spectrum
- Different versions changes the position of the different information (e.g. version 1.2.2 and version 1.2.5)
- Energy may be given in BE or KE
- Example with 1 region: Ag3d
- Versions 1.2.2, 1.2.5 and 1.3.1 are loadable
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\17-ScientaSES-Spectra(\*.TXT)\ScientaSES-Spectra-V1.2.2-BE-SingleReg-Ag3d.TXT

```
[Info]
Number of Regions=1
Version=1.2.2
```

```
[Region 1]
Region Name=Ag 3d5
Dimension 1 name=Binding Energy [eV]
Dimension 1 size=201
Dimension 1 scale=375.00000 374.95000 374.90000 ... 365.05000 365.00000
Dimension 2 name=Y-Scale [mm]
Dimension 2 size=100
Dimension 2 scale=-1.51287 -1.48119 -1.44950 ... 1.52871 1.56040 1.59208 1.62376
```

```
[Info 1]
Instrument=R3000-6MS014
Location=Scienta
User=Scienta
Sample=transmission
Comments=
Date=5/14/2009
Time=11:41:49 AM
Region Name=Ag 3d5
Excitation Energy=1486.6
Energy Scale=Binding
Acquisition Mode=Swept
Center Energy=9
Low Energy=1111.6
High Energy=1121.6
Energy Step=0.05
```

```

Step Time=200
Detector First X-Channel=19
Detector Last X-Channel=784
Detector First Y-Channel=210
Detector Last Y-Channel=609
Number of Slices=100
Lens Mode=Transmission
Pass Energy=50
Number of Sweeps=4
Time per Spectrum Channel=87.2

```

```

[User Interface Information 1]
R1=0.000
R2=0.000

```

```

[Data 1]
  375.00000  3781.00000  3519.00000  ... 4899.00000  5055.00000  4187.00000
  374.95000  4277.00000  3606.00000  ... 5074.00000  4701.00000  4456.00000
...
  365.05000  707.00000  718.00000  ... 803.00000  815.00000  1004.00000
  365.00000  762.00000  801.00000  ... 590.00000  1368.00000  906.00000

```

### 3.1.20 PHI Spectrometer

Comment:

- Header in ASCII from SOFH to EOFH
- Different software versions define the line numbers of acquisition information as well as the format of the saved intensities
- Intensities saved in cps
- Intensities saved on the end of the file as single float or double float numbers (number of bytes: 4x or 8x number of channels of all regions)

#### 3.1.20.1 Multiregion Measurements (\*.spe)

##### Software Version 1: SS 2.1.0.1

- Example of 2 regions: Te 3d<sub>5/2</sub>, Bi 4f
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg- V1-SS 2.1.0.1.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: Bi2Te3
SoftwareVersion: SS 2.1.0.1
InstrumentModel: PHI VersaProbe II
AcqFilename: C:\ZCH\120685\120685.11.BST 307 TP.spe
FileDate: 2012 8 16
AcqFileDate: 2012 8 16
Institution: PHI
Operator:
ExperimentID: 120685
EnergyReference: none 0.0
AnalyserWorkFcn: 4.218 eV
AnalyserRetardGain: 1.000207
PlatenID:
PhotoFilename: 120685.7.Low Mag.pho
SXIFilename:
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
IntensityRecal: no

```

IntensityCalCoeff: 100.000 0.330  
EnergyRecal: no  
ScanDeflectionSpan: 50 70  
ScanDeflectionOffset: 0 -20  
SCAMultiplierVoltage: 1650.0 V  
NarrowAcceptanceAngle: no  
PeakToNoiseRatioState: no  
DelayBeforeAcquire: 5 seconds  
C60IonGun: None  
BiasBoxMode: 0  
SemFieldOfView: 0.0000000  
EBeamCurrent: 0.0 nA  
ImageSizeXY: 0.0000 0.0000  
IonGunMode: Standby  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 2.000 kV  
FloatVolt: 0.0 V  
FloatEnable: no  
GridVolt: 150.0  
CondensorVolt: 1420.00  
ObjectiveVolt: 1344.00  
BendVolt: 26.00  
SputterRaster: 3.00 3.00 mm  
SputterRasterOffset: -0.690 -0.300 mm  
TargetSputterTime: 2.0 min  
SputterEmission: 15.00 mA  
DeflectionBias: 0.0 V  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvNumCycles: 15  
SurvTimePerStep: 50.000000  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 2197 3136  
PhotoOffsetInPixel: 1519 200  
PhotoSizeInMm: 35.000 50.000  
PhotoOffsetInMm: 0.008 0.008  
NoSpectralRegFull: 5  
SpectralRegDefFull: 1 1 Te3d5 52 301 -0.1000 597.0000 567.0000 596.0000 568.0000  
0.000000 5.85 AREA  
SpectralRegDef2Full: 1 30.0 1 0 8 1  
SpectralRegBackgroundFull: 1 0.0 582.0 0.0  
SpectralRegHeroFull: 1 582.0 0.0 0.0 0.0  
SpectralRegDefFull: 2 0 Sb3d5 51 201 -0.1000 545.0000 525.0000 544.0000 526.0000  
0.000000 5.85 AREA  
SpectralRegDef2Full: 2 20.0 1 0 8 1  
SpectralRegBackgroundFull: 2 0.0 535.0 0.0  
SpectralRegHeroFull: 2 535.0 0.0 0.0 0.0  
SpectralRegDefFull: 3 1 Bi4f 83 201 -0.1000 172.0000 152.0000 171.0000 153.0000  
0.000000 5.85 AREA  
SpectralRegDef2Full: 3 20.0 1 0 8 1  
SpectralRegBackgroundFull: 3 0.0 162.0 0.0  
SpectralRegHeroFull: 3 162.0 0.0 0.0 0.0  
SpectralRegDefFull: 4 0 Cls 6 201 -0.1000 298.0000 278.0000 297.0000 279.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 4 20.0 1 0 6 1  
SpectralRegBackgroundFull: 4 0.0 288.0 0.0  
SpectralRegHeroFull: 4 288.0 0.0 0.0 0.0  
SpectralRegDefFull: 5 0 O1s 8 201 -0.1000 543.0000 523.0000 542.0000 524.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 5 20.0 1 0 6 1  
SpectralRegBackgroundFull: 5 0.0 533.0 0.0  
SpectralRegHeroFull: 5 533.0 0.0 0.0 0.0  
NoSpectralReg: 2  
SpectralRegDef: 1 1 Te3d5 52 301 -0.1000 597.0000 567.0000 596.0000 568.0000  
6.000000 5.85 AREA

SpectralRegDef2: 1 30.0 1 0 8 1 0.00  
SpectralRegBackground: 1 0.0 582.0 0.0  
SpectralRegHero: 1 582.0 0.0 0.0 0.00  
SpectralRegDef: 2 1 Bi4f 83 201 -0.1000 172.0000 152.0000 171.0000 153.0000  
6.000000 5.85 AREA  
SpectralRegDef2: 2 20.0 1 0 8 1 0.00  
SpectralRegBackground: 2 0.0 162.0 0.0  
SpectralRegHero: 2 162.0 0.0 0.0 0.00  
NoSpatialArea: 1  
SpatialAreaDef: 1 1 1 (-279.7 -8247.6 18557.9 45.0 -90.1)  
SpatialAreaDesc: 1 Bi2Te3  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 0  
XrayPower: 25.61 W  
XrayBeamDiameter: 100.0 um  
XRayBeamVoltage: 15000.0 V  
XRayCondenserLensVoltage: 8230.0 V  
XRayObjectiveCoilCurrent: 0.748 A  
XRayBlankingVoltage: 325.0 V  
XRayFilamentCurrent: 1.576 A  
XRayStigmator: 0.0 0.0  
XRayHighPower: no  
EgunNeutMode: Off  
NeutralizerCurrent: 0.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: 0.0  
EgunNeutYSteering: 0.0  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
SxiPersistence: 1 V  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 1458.6 eV  
SxiPassEnergy: 376 eV  
SxiLens2: 476 V  
SxiLens3: 406 V  
SxiLensBias: 0 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 350.0 V  
SxiDisplayMode: 2  
Detector Acq Time: 20.0 (min)  
Number Of Channels: 16  
Channel Info: 1 1 1.698  
Channel Info: 2 1 1.467  
Channel Info: 3 1 1.392  
Channel Info: 4 1 1.320  
Channel Info: 5 1 1.251  
Channel Info: 6 1 1.103  
Channel Info: 7 1 1.074  
Channel Info: 8 1 1.026  
Channel Info: 9 1 1.001  
Channel Info: 10 1 0.941  
Channel Info: 11 1 0.824  
Channel Info: 12 1 0.819  
Channel Info: 13 1 0.750  
Channel Info: 14 1 0.650  
Channel Info: 15 1 0.674  
Channel Info: 16 1 1.266  
StagePosition: 8.0986 0.7914 18.5579 45.0062 -90.0500  
StageCurrentRotationSpeed: 0.6700  
DefectPosID: 1  
DefectPosComment: Bi2Te3  
DefectPosU: -0.2797

```

DefectPosV: 8.2476
DefectPosX: 8.0986
DefectPosY: 0.7914
DefectPosZ: 18.5579
DefectPosTilt: 45.0063
DefectPosRotation: -90.0500
DefectPosAligment: None
DefectPosReferenceImage: 120685.7.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
□ □ À □ □ □ □ □ □ □ -□ □ □ pnt sar +□'+□ä@c/s àø'□
f4 ´□ Ð □ □ □ □ □ □ □ É □ □ pnt sar
+□'+□ä@c/s àø'□ f4 $□ „□ Uå-D«:"D«J~D €□D«*"DUu"D Ð-D Ð~D
p"DU□"D«°•DUe"D«□•D«j`DUÅŽD«:'DUu'DU5"DUµ□DU□"DU...•D p'DUö'D 0"D δ□D
...

```

### Software Version 2: XPS V1.00

- Example of 3 regions: survey, Ag 3d, Au 4f
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V2-XPS V1.00.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
Comment:
SoftwareVersion: XPS V1.00
InstrumentModel: PHI Model 1600/3057
Institution:
FileDate: 2006 04 05
AcqFileDate: 2006 04 05
AcqFilename: C:\user_Data\stak\060404Ag_on_AuStandard0002.pdt
Operator:
ExperimentID:
PlatenID:
PlatenDesc:
StagePosition: 0.0 0.0 0.0 0.0 0.0
SampleID:
SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Al 1486.6 std
XrayPower: 400 W
XrayBeamDiameter: 0.0 um
NeutralizerEnergy: 0.0 eV
NeutralizerCurrent: 0.0 mA
SourceAnalyzerAngle: 54.7 d
AnalyzerSolidAngle: 7 sr
AnalyzerMode: FAT
AnalyzerWorkFcn: 3.5 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 3
SpectralRegDef: 1 1 SUR 111 1401 -1.000 1400.000 0.000 1400.000 0.000 0.320
187.85 none

```

```

SpectralRegDef: 2 2 Ag3d 47 201 -0.100 382.000 362.000 382.000 362.000 2.560
11.75 none
SpectralRegDef: 3 3 Au4f 79 201 -0.100 99.000 79.000 99.000 79.000 2.560 11.75
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
[] [] [] [] [] [] [] y[] [] [] chn sar c/s
f8 È+ 0[] [] [] [] É [] [] chn sar
c/s f8 H[] ø, [] [] [] É [] [] chn
sar c/s f8 H[] @3 [] [] [] çhR`ç8[]A[]
4±Mò[]AØÅ[]»0¹[]A»hèfàr[]AM[]G[]%¼ []AŽ.²%[]Ð A[] %ÚPÌ AÂèR[]fY A[] púyM AØEÍ`O? AíçnBü[]
...

```

### Software Version 3: XPS V1.20

- Example of 9 regions: Cu 2p, Ag 3p<sub>1/2</sub>, Ag 3d, Au 4f, C 1s, Au 3p, Au 4d<sub>3/2</sub>, Au 4d<sub>5/2</sub>, C 1s
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V3-XPS V1.20.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: A_2 after Ar sputter 2 min 3kV 2x2 detail
SoftwareVersion: XPS V1.20
InstrumentModel: PHI Model 5000
Institution:
FileDate: 2008 09 25
AcqFileDate: 2008 09 25
AcqFilename: C:\Data\Mennica\A_2_second-meas.0003.pdt
Operator:
ExperimentID:
PlatenID:
PlatenDesc:
StagePosition: 2.001 1.692 17.713 45.006 0.150
SampleID:
SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Al 1486.6 mono
XrayPower: 25.0W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 1.0 eV
NeutralizerCurrent: 5.0 mA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20 sr
AnalyserMode: FAT
AnalyserWorkFcn: 4.4 eV
IntensityRecal: no
IntensityCalCoeff: 33.698 0.024
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar+
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 2000.0 2000.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 9
SpectralRegDef: 1 1 Cu2p 29 351 -0.100 963.000 928.000 963.000 928.000 1.250
23.50 none
SpectralRegDef: 2 2 Ag3p1 47 161 -0.100 614.000 598.000 614.000 598.000 1.250
23.50 none
SpectralRegDef: 3 3 Ag3d 47 161 -0.100 378.000 362.000 378.000 362.000 1.250
23.50 none

```



```

NoSpectralReg: 5
SpectralRegDef: 1 1 Sc2p3 21 171 -0.100 412.000 395.000 412.000 395.000 0.740
11.75 none
SpectralRegDef: 2 2 Ge3d 32 681 -0.025 40.000 23.000 40.000 23.000 2.220 5.85
none
SpectralRegDef: 3 3 Gd3d 64 1001 -0.100 1275.000 1175.000 1275.000 1175.000
2.220 11.75 none
SpectralRegDef: 4 4 O1s 8 361 -0.050 541.000 523.000 541.000 523.000 0.740 11.75
none
SpectralRegDef: 5 5 C1s 6 151 -0.100 293.000 278.000 293.000 278.000 1.480 11.75
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
  à  «  chn  sar  c/s
f8 X  ð  ©  chn  sar
c/s      f8 H  H  é  chn
sar      c/s      f8 H  •  i
  chn  sar      c/s      f8 H
  ø;      -  chn  sar  c/s
f8 ,  G      ñ  d  ~  °  @  -  d  ã  ö  î  t  _  @  À  È  @  o
...

```

### Software Version 5: XPS V2.0

- Example of 1 regions: survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.(SPE))\PHI-MultiReg-V5-XPS V2.0.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: none
SoftwareVersion: XPS V2.0
InstrumentModel: PHI Quantum 2000
Institution: PHI
FileDate: 2006 1 19
AcqFileDate: 2006 1 19
AcqFilename: Schleifer001.spe
Operator:
ExperimentID: 2006-0067
PlatenID: 0067
PlatenDesc: none
StagePosition: 23.0921 6.2673 24.5600 45.0000 -0.0207
PhotoFilename: Schleifer001.pho
ActualPhotoFilename: /D=/Compass6.1.1/datafiles/photos/4_1137682717.pho
SXIFilename: Schleifer001.sxi
ActualSXIFilename: /D=/Compass6.1.1/datafiles/SXIs/1_1137687332.sxi
XraySource: Al 1486.6 mono
XrayPower: 19.47 W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 2.5 V
NeutralizerCurrent: 5.0 uA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 3.9 eV
IntensityRecal: no
IntensityCalCoeff: 23.460 0.183
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 4.000 keV
SputterCurrent: 15.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s

```

```

PreAcqSputterRate: 4.2 A/s
NoSpectralReg: 1
SpectralRegDef: 1 1 1su 111 1351 -1.0000 1345.0 -5.0 1345.0 -5.0 1.760000
117.40 AREA
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (22045.7 4351.8 24560.0 45.0 -0.3)
SpatialAreaDesc: 1 Nr1 Bahn sauber1
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH

```

```

□ □ ` □ □ □ □ □ □ □ G□ □ □ pnt 7777sar 7777 7777777c/s 7777777
77777f8 78* p i* □Δ>リ@ □*□リ@ ・・リ@
λeリ@ □Δレリ@ 瑾リ@ phリ@ ・{`リ@ 夕87リ@ 夕h湍@ ・□華@ □1Hリ@ □~暖@ @7
□リ@ 夕々リ@ @j、リ@ `DZリ@ >リ@ □!@リ@
・@リ@ □Nリ@ @:葦@ 瑜リ@ ・鯨@ `・@ `□袒@ @z□リ@ □リ・@ □聡リ@ □
・レリ@ 潦リ@ ・+レリ@ ・リ
...

```

### Software Version 6: XPS V3.5s

- Example of 1 region: survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V6-XPS V3.5S.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
Comment:
SoftwareVersion: XPS V3.5S
InstrumentModel: PHI Model 1600/3057 (Special)
Institution:
FileDate: 2005 06 12
AcqFileDate: 2005 06 12
AcqFilename: d:\xpsspe~1\zharni~2\2005\06112005\XPS2.PCS
Operator:
ExperimentID:
PlatenID:
PlatenDesc:
StagePosition:
SampleID:
SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Unknown 369.0 std
XrayPower: 400 W
XrayBeamDiameter: 0.0 um
NeutralizerEnergy: 0.0 eV
NeutralizerCurrent: 0.0 mA
SourceAnalyzerAngle: 54.7 d
AnalyzerSolidAngle: 7 sr
AnalyzerMode: FAT
AnalyzerWorkFcn: 3.6 eV
IntensityRecal: no
IntensityCalCoeff: 24.5 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 1.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 1
SpectralRegDef: 1 1 C1 6 401 -0.050 275.400 255.400 275.400 255.400 0.250 5.85
none

```

```

NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (127.0, 127.0, 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
  2005\06c\s05\XPS2.PCS f8 e~ p chn e~1\sar ni~2
  è³@ ø²@ ,´@ T´@ ì³@ "²@ □³@ ¬³@ $´@ •²@
  ³@ Ü³@ ð³@ Ø³@ ð³@ Ð³@ □´@ (´@ ´@ ô³@
...

```

### Software Version 7: EIS V2.1/EIS-Sphera V2.4

- Example of 4 regions: Ag survey and three Ag 3d spectra with different pass energy
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V7-EIS V2.1.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: Experiment Type: XPS
SoftwareVersion: EIS V2.1
FileDate: 02 11 28
XraySource: ?? 1486.7 std
XrayPower: 225 W
SourceAnalyserAngle: 0 d
AnalyserWorkFcn: 4.5 eV
IntensityRecal: no
IntensityCalCoeff: 6.55 0.45
EnergyRecal: no
NoSpectralReg: 4
SpectralRegDef: 1 1 Su1 111 1501 -0.5 750.0 0.0 750.0 0.0 0.202 80.00 AREA
SpectralRegDef: 2 2 Su2 111 301 -0.0200 371.0 365.0 371.0 365.0 1.375 40.00 AREA
SpectralRegDef: 3 3 Su3 111 301 -0.0200 371.0 365.0 371.0 365.0 1.188 20.00 AREA
SpectralRegDef: 4 4 Su4 111 301 -0.0200 371.0 365.0 371.0 365.0 1.095 10.00 AREA
NoSpatialArea: 0
EOFH
  f8 e. • f8 h x0 pts sar c/s
  sar c/s f8 h à9 pts sar pts
  À:Ú@ □Ú@ À-Ú@ €_Ú@ □Ú@ ÝÚ@ @ Ú@ À:Ú@ ÀÚ@ €íÚ@
...

```

### Software Version 8: Compass V7.2.2

- Example of 6 regions: Ni 2p, Al 2p, Al 2s, O 1s, C 1s, VB
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V8-Compass V7.2.2.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: Xu Sample-A
SoftwareVersion: Compass V7.2.2
InstrumentModel: PHI Quantera SXM
Institution: PHI
FileDate: 2006 7 3
AcqFileDate: 2006 7 3
AcqFilename: Xu-A_060703-02.spe
Operator:
ExperimentID: Ota
PlatenID: Platen 1

```

```

PlatenDesc: Xu_A-C
StagePosition: 21.4967 37.2531 24.0190 45.0000 -0.0066
PhotoFilename: Xu-A_060703-02.pho
ActualPhotoFilename: /C=/Program
Files/PHI/Compass7.2.1/datafiles/photos/3_1151890988.pho
SXIFilename: none
ActualSXIFilename:
XraySource: Al 1486.6 mono
XrayPower: 25.10 W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 0.0 V
NeutralizerCurrent: 0.0 uA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 4.125 eV
IntensityRecal: no
IntensityCalCoeff: 82.402 0.235
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 2.000 keV
SputterCurrent: 25.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0.2 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 Ni2p 28 401 -0.1250 890.0 840.0 890.0 844.0 12.000000
69.00 AREA
SpectralRegDef: 2 2 Al2p 13 241 -0.1250 85.0 55.0 75.0 68.0 12.000000
69.00 AREA
SpectralRegDef: 3 3 Al2s 13 321 -0.1250 130.0 90.0 110.0 90.0 12.000000
69.00 AREA
SpectralRegDef: 4 4 O1s 8 241 -0.1250 550.0 520.0 540.0 527.0 1.200000
69.00 AREA
SpectralRegDef: 5 5 C1s 6 241 -0.1250 300.0 270.0 300.0 275.0 1.200000
69.00 AREA
SpectralRegDef: 6 6 V11s 112 401 -0.1250 30.0 -20.0 30.0 -20.0 1.200000
69.00 AREA
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (21339.2 37232.7 24019.0 45.0 0.0)
SpatialAreaDesc: 1 sample-A
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH
□ □ @□ □ □ □ □ □ □ □ □ □ pnt a~o□sar □ □k□h
İ c/s Té□ □ Äçr□f8 ^
... P□ Ø
...

```

### Software Version 9: Compass V7.3

- Example of 1 region: survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V9-Compass V7.3.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: 10/21/08
SoftwareVersion: Compass V7.3
InstrumentModel: PHI Quantera SXM
Institution: PHI

```



```

SourceAnalyserAngle: 54.0 d
AnalyserMode: FAT
AnalyserWorkFcn: 4.5 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: 40Ar
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 10.0 0.0 um
PreAcqSputterTime: 152356 s
PreAcqSputterRate: 1.0 A/s
NoSpectralReg: 4
SpectralRegDef: 1 1 Ag1 47 200 -0.0250 371.0 366.0 371.0 366.0 1.200000 5.85
none
SpectralRegDef: 2 2 Ag1 47 200 -0.0250 371.0 366.0 371.0 366.0 0.900000 11.75
none
SpectralRegDef: 3 3 Ag1 47 200 -0.0250 371.0 366.0 371.0 366.0 0.600000 23.50
none
SpectralRegDef: 4 4 Ag1 47 120 -0.0500 371.0 365.0 371.0 365.0 0.300000 46.95
none
XrayScanIncXY: 0.0 0.0 um
NoSpatialArea: 1
SpatialAreaDef: 1 Full 1 (0.0 0.0 0.0 0.0 0.0)
EOFH
□ □ e□ □ □ □ □ □ □ È □ □ pnt □ sar 'p□ □ c/s □
□□ f4 □ •□ □ □ □ □ È □ □ pnt □ sar 'p□
...

```

### Software Version 11: XPS 3.3

- Example of 5 region: C 1s, O 1s, Au 4f, N 1s, Si 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V11-XPS V3.3.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
Comment:
SoftwareVersion: XPS V3.3
InstrumentModel: PHI Model 1600/3057
Institution:
FileDate: 2012 10 02
AcqFileDate: 2012 10 02
AcqFilename: c:\lab2012\bchornik\mkogan\MTXN_3.PCS
Operator:
ExperimentID:
PlatenID:
PlatenDesc:
StagePosition:
SampleID:
SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Al 1486.6 std
XrayPower: 400 W
XrayBeamDiameter: 0.0 um
NeutralizerEnergy: 0.0 eV
NeutralizerCurrent: 0.0 mA
SourceAnalyzerAngle: 54.7 d
AnalyzerSolidAngle:
AnalyzerMode: FAT
AnalyzerWorkFcn: 4.2 eV
IntensityRecal: no
IntensityCalCoeff: 24.5 0.207

```

```

EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 4.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 10000.0 10000.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 5
SpectralRegDef: 1 1 C1 6 101 -0.100 290.000 280.000 290.000 280.000 3.000 44.75
none
SpectralRegDef: 2 2 O 0 121 -0.100 539.000 527.000 539.000 527.000 0.750 44.75
none
SpectralRegDef: 3 3 Au1 79 121 -0.100 93.000 81.000 93.000 81.000 12.000 44.75
none
SpectralRegDef: 4 4 N 0 121 -0.100 407.000 395.000 407.000 395.000 75.000 44.75
none
SpectralRegDef: 5 5 Si1 14 66 -0.200 108.000 95.000 108.000 95.000 1.500 44.75
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (127.0, 127.0, 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
□ □ à□ □ □ □ □ □ e □ □ chn €âÈsar €/É îÈc/s
=É@ €□Éf8 (□ ð□
...

```

### Software Version 12: SS 2.6.1.2

- Example of 3 region: O 1s, Si 2p, Si 2s
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V12-SS 2.6.1.2.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: SiO2
SoftwareVersion: SS 2.6.1.2
InstrumentModel: PHI VersaProbe II With AES
AcqFilename: C:\Datafiles\service\AGL\2015\01\SiO2_25nm_01.111.Point 1.spe
FileDate: 2015 1 15
AcqFileDate: 2015 1 15
Institution: Physical Electronics GmbH
Operator: Andrey Lyapin
ExperimentID: 01
EnergyReference: none 0.0
AnalyserWorkFcn: 4.210 eV
AnalyserRetardGain: 1.000715
PlatenID: SiO2_25nm_01
PhotoFilename: SiO2_25nm_01.101.Low Mag.pho
SXIFilename:
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
IntensityRecal: no
IntensityCalCoeff: 56.591 0.222
EnergyRecal: no
ScanDeflectionSpan: 30 60
ScanDeflectionOffset: 0 18
SCAMultiplierVoltage: 2100.0 V
NarrowAcceptanceAngle: no
RefreshPersistence: 1
PeakToNoiseRatioState: yes
DelayBeforeAcquire: 10 seconds
C60IonGun: None
BiasBoxMode: 0
SemFieldOfView: 1300.000000

```

```
ImageSizeXY: 1300.0000 400.0000
IonGunMode: Neutralize
SputterIon: Ar+
SputterCurrent: 0.040 uA
SputterRate: 0.000 A/min
SputterEnergy: 0.210 kV
FloatVolt: -200.0 V
FloatEnable: yes
GridVolt: 120.0
CondensorVolt: 144.48
ObjectiveVolt: 191.10
BendVolt: 3.99
SputterRaster: 0.00 0.00 mm
SputterRasterOffset: -0.200 0.000 mm
TargetSputterTime: 1.0 min
SputterEmission: 7.00 mA
DeflectionBias: 71.0 V
XpsScanMode: scanned
AnalyserMode: FAT
SurvNumCycles: 12
SurvTimePerStep: 50.000000
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2771 2806
PhotoOffsetInPixel: 961 179
PhotoSizeInMm: 61.452 60.949
PhotoOffsetInMm: 0.011 0.011
NoSpectralRegFull: 3
SpectralRegDefFull: 1 1 Si2p 14 101 -0.2000 110.0000 90.0000 109.0000 91.0000
0.000000 23.50 HEIGHT
SpectralRegDef2Full: 1 20.0 3 0 6 500
SpectralRegBackgroundFull: 1 0.0 100.0 0.0
SpectralRegHeroFull: 1 100.0 0.0 0.0 0.00
SpectralRegIRFull: 1 0 0.000 0.000 0.0
SpectralRegDefFull: 2 1 O1s 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000
0.000000 23.50 HEIGHT
SpectralRegDef2Full: 2 20.0 1 0 6 500
SpectralRegBackgroundFull: 2 0.0 533.0 0.0
SpectralRegHeroFull: 2 533.0 0.0 0.0 0.00
SpectralRegIRFull: 2 0 0.000 0.000 0.0
SpectralRegDefFull: 3 1 Si2s 14 101 -0.2000 163.0000 143.0000 162.0000 144.0000
0.000000 23.50 HEIGHT
SpectralRegDef2Full: 3 20.0 3 0 6 500
SpectralRegBackgroundFull: 3 0.0 153.0 0.0
SpectralRegHeroFull: 3 153.0 0.0 0.0 0.00
SpectralRegIRFull: 3 0 0.000 0.000 0.0
NoSpectralReg: 3
SpectralRegDef: 1 1 Si2p 14 101 -0.2000 110.0000 90.0000 109.0000 91.0000
1.500000 23.50 HEIGHT
SpectralRegDef2: 1 20.0 3 0 6 500
SpectralRegBackground: 1 0.0 100.0 0.0
SpectralRegHero: 1 100.0 0.0 0.0 0.00
SpectralRegIR: 1 0 0.000 0.000 0.0
SpectralRegDef: 2 1 O1s 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000
0.600000 23.50 HEIGHT
SpectralRegDef2: 2 20.0 1 0 6 500
SpectralRegBackground: 2 0.0 533.0 0.0
SpectralRegHero: 2 533.0 0.0 0.0 0.00
SpectralRegIR: 2 0 0.000 0.000 0.0
SpectralRegDef: 3 1 Si2s 14 101 -0.2000 163.0000 143.0000 162.0000 144.0000
10.500000 23.50 HEIGHT
SpectralRegDef2: 3 20.0 3 0 6 500
SpectralRegBackground: 3 0.0 153.0 0.0
SpectralRegHero: 3 153.0 0.0 0.0 0.00
SpectralRegIR: 3 0 0.000 0.000 0.0
NoSpatialArea: 1
```

SpatialAreaDef: 1 1 4 (-4373.3 -5907.8 16187.4 45.0 -0.1) (-3073.3 -5907.8  
16187.4 45.0 -0.1) (-3073.3 -5507.8 16187.4 45.0 -0.1) (-4373.3 -5507.8 16187.4  
45.0 -0.1)  
SpatialAreaDesc: 1 Tool matching VP II  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 6  
XrayPower: 90.80 W  
XrayBeamDiameter: 100.0 um  
XRayBeamVoltage: 20000.0 V  
XRayCondenserLensVoltage: 9550.0 V  
XRayObjectiveCoilCurrent: 0.938 A  
XRayBlankingVoltage: 430.0 V  
XRayFilamentCurrent: 1.645 A  
XRayStigmator: 0.0 0.0  
XRayHighPower: yes  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 3.00 V  
EgunNeutExtractor: 40.0 V  
EgunNeutXSteering: 0.0  
EgunNeutYSteering: -3.0  
EgunNeutFilament: 0.90 A  
EgunNeutPulseLength: 50.0 msec  
SxiPersistence: 4 V  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 534.0 eV  
SxiPassEnergy: 376 eV  
SxiLens2: -711 V  
SxiLens3: -673 V  
SxiLensBias: 200 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 439.8 V  
SxiDisplayMode: 0  
Detector Acq Time: 100.0 (min)  
Number Of Channels: 16  
Channel Info: 1 1 1.600  
Channel Info: 2 1 1.237  
Channel Info: 3 1 1.144  
Channel Info: 4 1 1.112  
Channel Info: 5 1 1.029  
Channel Info: 6 1 0.973  
Channel Info: 7 1 0.953  
Channel Info: 8 1 0.959  
Channel Info: 9 1 1.096  
Channel Info: 10 1 1.081  
Channel Info: 11 1 0.916  
Channel Info: 12 1 0.804  
Channel Info: 13 1 0.770  
Channel Info: 14 1 0.722  
Channel Info: 15 1 0.750  
Channel Info: 16 1 0.820  
StagePosition: -4.2486 6.0367 16.1874 45.0031 -0.0500  
StageCurrentRotationSpeed: 1.0000  
DefectPosID: 1  
DefectPosComment: Tool matching VP II  
DefectPosU: -3.7246  
DefectPosV: 5.7082  
DefectPosX: -4.2486  
DefectPosY: 6.0367  
DefectPosZ: 16.1874  
DefectPosTilt: 45.0031  
DefectPosRotation: -0.0500  
DefectPosAlignent: None

DefectPosReferenceImage: SiO2\_25nm\_01.101.Low Mag.pho  
 Deconvolution: no  
 DeconvolutionPassEnergy: 23.50 eV  
 XRaySetting: 100u100W\_HP  
 EOFH

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### Software Version 13: SS 2.7.1.22

- Example of 5 regions: O 1s, B 1s, Ru 3d, S 2p, Au 4f
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V13-SS 2.7.1.22.SPE

SOFH  
 Platform: PC  
 Technique: XPS  
 FileType: SPECTRUM  
 FileDesc:  
 SoftwareVersion: SS 2.7.1.22  
 InstrumentModel: PHI VersaProbe II  
 AcqFilename: C:\ZCH\160977\160977.9.AT.spe  
 FileDate: 2016 8 17  
 AcqFileDate: 2016 8 17  
 Institution: PHI  
 Operator:  
 ExperimentID: 160977  
 EnergyReference: none 0.0  
 AnalyserWorkFcn: 4.184 eV  
 AnalyserRetardGain: 1.000227  
 PlatenID: FC  
 PhotoFilename: 160977.1.Low Mag.pho  
 SXIFilename:  
 SourceAnalyserAngle: 45.0 d  
 AnalyserSolidAngle: 0.38 sr  
 IntensityRecal: no  
 IntensityCalCoeff: -0.019 0.005  
 EnergyRecal: no  
 ScanDeflectionSpan: 50 60  
 ScanDeflectionOffset: 0 0  
 SCAMultiplierVoltage: 1800.0 V  
 NarrowAcceptanceAngle: no  
 PeakToNoiseRatioState: no  
 DelayBeforeAcquire: 5 seconds  
 C60IonGun: None  
 BiasBoxMode: 0  
 SemFieldOfView: 0.0000000  
 ImageSizeXY: 0.0000 0.0000  
 IonGunMode: Neutralize  
 SputterIon: Ar+  
 SputterCurrent: 0.000 uA  
 SputterRate: 0.000 A/min  
 SputterEnergy: 0.110 kV  
 FloatVolt: -100.0 V  
 FloatEnable: yes  
 GridVolt: 100.0  
 CondensorVolt: 74.80  
 ObjectiveVolt: 101.20  
 BendVolt: 1.60  
 SputterRaster: 0.00 0.00 mm  
 SputterRasterOffset: 0.500 -0.150 mm  
 TargetSputterTime: 1.0 min  
 SputterEmission: 7.00 mA  
 DeflectionBias: 71.0 V  
 XpsScanMode: scanned  
 AnalyserMode: FAT  
 SurvNumCycles: 20  
 SurvTimePerStep: 100.000000

```
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2197 3136
PhotoOffsetInPixel: 1519 200
PhotoSizeInMm: 35.000 50.000
PhotoOffsetInMm: 0.008 0.008
NoSpectralRegFull: 6
SpectralRegDefFull: 1 1 O1s 8 151 -0.1000 540.0000 525.0000 539.0000 526.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 1 15.0 3 0 6 1
SpectralRegBackgroundFull: 1 0.0 532.5 0.0
SpectralRegHeroFull: 1 532.5 0.0 0.0 0.0
SpectralRegIRFull: 1 0 0.000 0.000 0.0
SpectralRegDefFull: 2 1 N1s 7 201 -0.1000 412.0000 392.0000 411.0000 393.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 2 20.0 5 0 6 1
SpectralRegBackgroundFull: 2 0.0 402.0 0.0
SpectralRegHeroFull: 2 402.0 0.0 0.0 0.00
SpectralRegIRFull: 2 0 0.000 0.000 0.0
SpectralRegDefFull: 3 0 C1s 6 151 -0.1000 293.0000 278.0000 292.0000 279.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 3 15.0 1 0 6 1
SpectralRegBackgroundFull: 3 0.0 285.5 0.0
SpectralRegHeroFull: 3 285.5 0.0 0.0 0.00
SpectralRegIRFull: 3 0 0.000 0.000 0.0
SpectralRegDefFull: 4 1 Ru3d 44 221 -0.1000 294.0000 272.0000 293.0000 273.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 4 22.0 5 0 6 1
SpectralRegBackgroundFull: 4 0.0 283.0 0.0
SpectralRegHeroFull: 4 283.0 0.0 0.0 0.00
SpectralRegIRFull: 4 0 0.000 0.000 0.0
SpectralRegDefFull: 5 1 S2p 16 201 -0.1000 175.0000 155.0000 174.0000 156.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 5 20.0 3 0 6 1
SpectralRegBackgroundFull: 5 0.0 165.0 0.0
SpectralRegHeroFull: 5 165.0 0.0 0.0 0.00
SpectralRegIRFull: 5 0 0.000 0.000 0.0
SpectralRegDefFull: 6 1 Au4f 79 121 -0.1000 90.0000 78.0000 89.0000 79.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 6 12.0 1 0 6 1
SpectralRegBackgroundFull: 6 0.0 84.0 0.0
SpectralRegHeroFull: 6 84.0 0.0 0.0 0.00
SpectralRegIRFull: 6 0 0.000 0.000 0.0
NoSpectralReg: 5
SpectralRegDef: 1 1 O1s 8 151 -0.1000 540.0000 525.0000 539.0000 526.0000
36.000000 23.50 AREA
SpectralRegDef2: 1 15.0 3 0 6 1
SpectralRegBackground: 1 0.0 532.5 0.0
SpectralRegHero: 1 532.5 0.0 0.0 0.00
SpectralRegIR: 1 0 0.000 0.000 0.0
SpectralRegDef: 2 1 N1s 7 201 -0.1000 412.0000 392.0000 411.0000 393.0000
60.000000 23.50 AREA
SpectralRegDef2: 2 20.0 5 0 6 1
SpectralRegBackground: 2 0.0 402.0 0.0
SpectralRegHero: 2 402.0 0.0 0.0 0.00
SpectralRegIR: 2 0 0.000 0.000 0.0
SpectralRegDef: 3 1 Ru3d 44 221 -0.1000 294.0000 272.0000 293.0000 273.0000
60.000000 23.50 AREA
SpectralRegDef2: 3 22.0 5 0 6 1
SpectralRegBackground: 3 0.0 283.0 0.0
SpectralRegHero: 3 283.0 0.0 0.0 0.00
SpectralRegIR: 3 0 0.000 0.000 0.0
SpectralRegDef: 4 1 S2p 16 201 -0.1000 175.0000 155.0000 174.0000 156.0000
36.000000 23.50 AREA
SpectralRegDef2: 4 20.0 3 0 6 1
SpectralRegBackground: 4 0.0 165.0 0.0
SpectralRegHero: 4 165.0 0.0 0.0 0.00
SpectralRegIR: 4 0 0.000 0.000 0.0
```

SpectralRegDef: 5 1 Au4f 79 121 -0.1000 90.0000 78.0000 89.0000 79.0000  
12.000000 23.50 AREA  
SpectralRegDef2: 5 12.0 1 0 6 1  
SpectralRegBackground: 5 0.0 84.0 0.0  
SpectralRegHero: 5 84.0 0.0 0.0 0.00  
SpectralRegIR: 5 0 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 1 1 (11792.6 6044.0 18280.0 45.0 -90.0)  
SpatialAreaDesc: 1  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 7  
XrayPower: 51.88 W  
XrayBeamDiameter: 5.0 um  
XRayBeamVoltage: 18000.0 V  
XRayCondenserLensVoltage: 9900.0 V  
XRayObjectiveCoilCurrent: 0.780 A  
XRayBlankingVoltage: 370.0 V  
XRayFilamentCurrent: 1.620 A  
XRayStigmator: 0.0 0.0  
XRayHighPower: no  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: -11.0  
EgunNeutYSteering: -6.0  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
SxiPersistence: 1  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 1458.6 eV  
SxiPassEnergy: 376 eV  
SxiLens2: 476 V  
SxiLens3: 406 V  
SxiLensBias: 0 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 350.0 V  
SxiDisplayMode: 2  
Detector Acq Time: 50.0 (min)  
Number Of Channels: 16  
Channel Info: 1 1 1.541  
Channel Info: 2 1 1.377  
Channel Info: 3 1 1.296  
Channel Info: 4 1 1.178  
Channel Info: 5 1 1.110  
Channel Info: 6 1 1.021  
Channel Info: 7 1 0.991  
Channel Info: 8 1 0.996  
Channel Info: 9 1 0.999  
Channel Info: 10 1 0.989  
Channel Info: 11 1 0.748  
Channel Info: 12 1 0.886  
Channel Info: 13 1 0.816  
Channel Info: 14 1 0.735  
Channel Info: 15 1 0.779  
Channel Info: 16 1 1.312  
StagePosition: -5.6880 -11.6231 18.2804 45.0031 -90.0500  
StageCurrentRotationSpeed: 0.6700  
DefectPosID: 1  
DefectPosComment:  
DefectPosU: 11.7936  
DefectPosV: -6.0449  
DefectPosX: -5.6880

```

DefectPosY: -11.6231
DefectPosZ: 18.2804
DefectPosTilt: 45.0031
DefectPosRotation: -90.0500
DefectPosAligment: None
DefectPosReferenceImage: 160977.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 200u50W15KV
EOFH
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```

### Software Version 14: SS 2.8.0.30

- Example of 1 region: C 1s
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V14-SS 2.8.9.30.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: Graphite
SoftwareVersion: SS 2.8.0.30
InstrumentModel: PHI VersaProbe II
AcqFilename: G:\Datafiles\JWKim\field_study\0612\sample.120.spe
FileDate: 2018 6 12
AcqFileDate: 2018 6 12
Institution: KRISS
Operator:
ExperimentID: 0612
EnergyReference: none 0.0
AnalyserWorkFcn: 4.389 eV
AnalyserRetardGain: 1.000035
PlatenID: Graphene
PhotoFilename: HATCN.114.pho
SXIFilename:
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 0.38 sr
IntensityRecal: no
IntensityCalCoeff: 82.808 0.246
EnergyRecal: no
ScanDeflectionSpan: 40 60
ScanDeflectionOffset: 0 0
SCAMultiplierVoltage: 1750.0 V
NarrowAcceptanceAngle: no
PeakToNoiseRatioState: no
DelayBeforeAcquire: 5 seconds
C60IonGun: None
BiasBoxMode: 0
TFParameters: 0, 1, 2, 93.73, 7.481, 1, 1
SemFieldOfView: 0.0000000
ImageSizeXY: 0.0000 0.0000
IonGunMode: Off
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 0.100 kV
FloatVolt: 0.0 V
FloatEnable: no
GridVolt: 150.0
CondensorVolt: 0.00
ObjectiveVolt: 0.00
BendVolt: 0.00
SputterRaster: 0.00 0.00 mm
SputterRasterOffset: 0.000 0.000 mm

```

TargetSputterTime: 10.0 min  
SputterEmission: 0.00 mA  
DeflectionBias: 0.0 V  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvNumCycles: 2  
SurvTimePerStep: 20.000000  
NoSpectralRegFull: 13  
SpectralRegDefFull: 1 0 Suls 111 3001 -0.4000 1199.0000 -1.0000 1198.0000 0.0000  
0.000000 93.90 AREA  
SpectralRegDef2Full: 1 1200.0 1 0 2 1  
SpectralRegBackgroundFull: 1 0.0 599.0 0.0  
SpectralRegHeroFull: 1 599.0 0.0 0.0 0.00  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
SpectralRegDefFull: 2 0 Au4f 79 161 -0.1250 99.0000 79.0000 98.0000 80.0000  
0.000000 58.70 AREA  
SpectralRegDef2Full: 2 20.0 1 0 2 1  
SpectralRegBackgroundFull: 2 0.0 89.0 0.0  
SpectralRegHeroFull: 2 89.0 0.0 0.0 0.00  
SpectralRegIRFull: 2 0 0.000 0.000 0.0  
SpectralRegDefFull: 3 0 P2p 15 301 -0.0500 141.0000 126.0000 140.0000 127.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 3 15.0 1 0 6 1  
SpectralRegBackgroundFull: 3 0.0 133.5 0.0  
SpectralRegHeroFull: 3 133.5 0.0 0.0 0.00  
SpectralRegIRFull: 3 0 0.000 0.000 0.0  
SpectralRegDefFull: 4 1 Cls 6 501 -0.0500 303.0000 278.0000 302.0000 279.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 4 25.0 5 0 6 1  
SpectralRegBackgroundFull: 4 0.0 290.5 0.0  
SpectralRegHeroFull: 4 290.5 0.0 0.0 0.00  
SpectralRegIRFull: 4 0 0.000 0.000 0.0  
SpectralRegDefFull: 5 0 O1s 8 301 -0.0500 540.0000 525.0000 539.0000 526.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 5 15.0 6 0 6 1  
SpectralRegBackgroundFull: 5 0.0 532.5 0.0  
SpectralRegHeroFull: 5 532.5 0.0 0.0 0.00  
SpectralRegIRFull: 5 0 0.000 0.000 0.0  
SpectralRegDefFull: 6 0 N1s 7 161 -0.1250 411.0000 391.0000 410.0000 392.0000  
0.000000 58.70 AREA  
SpectralRegDef2Full: 6 20.0 2 0 2 1  
SpectralRegBackgroundFull: 6 0.0 401.0 0.0  
SpectralRegHeroFull: 6 401.0 0.0 0.0 0.00  
SpectralRegIRFull: 6 0 0.000 0.000 0.0  
SpectralRegDefFull: 7 0 F1s 9 401 -0.0500 699.0000 679.0000 698.0000 680.0000  
0.000000 46.95 AREA  
SpectralRegDef2Full: 7 20.0 4 0 4 1  
SpectralRegBackgroundFull: 7 0.0 689.0 0.0  
SpectralRegHeroFull: 7 689.0 0.0 0.0 0.00  
SpectralRegIRFull: 7 0 0.000 0.000 0.0  
SpectralRegDefFull: 8 0 Ag4d 47 481 -0.0250 9.0000 -3.0000 8.0000 -2.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 8 12.0 1 0 6 1  
SpectralRegBackgroundFull: 8 0.0 3.0 0.0  
SpectralRegHeroFull: 8 3.0 0.0 0.0 0.00  
SpectralRegIRFull: 8 0 0.000 0.000 0.0  
SpectralRegDefFull: 9 0 WF(-2V) -1 161 -0.0250 1482.0000 1478.0000 1481.0000  
1479.0000 0.000000 2.95 AREA  
SpectralRegDef2Full: 9 4.0 1 0 8 1  
SpectralRegBackgroundFull: 9 0.0 1480.0 0.0  
SpectralRegHeroFull: 9 1480.0 0.0 0.0 0.00  
SpectralRegIRFull: 9 0 0.000 0.000 0.0  
SpectralRegDefFull: 10 0 WF(-2.5V) -1 161 -0.0250 1481.5000 1477.5000 1480.5000  
1478.5000 0.000000 2.95 AREA  
SpectralRegDef2Full: 10 4.0 1 0 8 1  
SpectralRegBackgroundFull: 10 0.0 1479.5 0.0  
SpectralRegHeroFull: 10 1479.5 0.0 0.0 0.00

```
SpectralRegIRFull: 10 0 0.000 0.000 0.0
SpectralRegDefFull: 11 0 WF(-5V) -1 161 -0.0250 1479.0000 1475.0000 1478.0000
1476.0000 0.000000 2.95 AREA
SpectralRegDef2Full: 11 4.0 1 0 8 1
SpectralRegBackgroundFull: 11 0.0 1477.0 0.0
SpectralRegHeroFull: 11 1477.0 0.0 0.0 0.00
SpectralRegIRFull: 11 0 0.000 0.000 0.0
SpectralRegDefFull: 12 0 WF(-10V) -1 161 -0.0250 1474.0000 1470.0000 1473.0000
1471.0000 0.000000 2.95 AREA
SpectralRegDef2Full: 12 4.0 1 0 8 1
SpectralRegBackgroundFull: 12 0.0 1472.0 0.0
SpectralRegHeroFull: 12 1472.0 0.0 0.0 0.00
SpectralRegIRFull: 12 0 0.000 0.000 0.0
SpectralRegDefFull: 13 0 WF(-15V) -1 161 -0.0250 1469.0000 1465.0000 1468.0000
1466.0000 0.000000 2.95 AREA
SpectralRegDef2Full: 13 4.0 1 0 8 1
SpectralRegBackgroundFull: 13 0.0 1467.0 0.0
SpectralRegHeroFull: 13 1467.0 0.0 0.0 0.00
SpectralRegIRFull: 13 0 0.000 0.000 0.0
NoSpectralReg: 1
SpectralRegDef: 1 1 C1s 6 501 -0.0500 303.0000 278.0000 302.0000 279.0000
1.200000 23.50 AREA
SpectralRegDef2: 1 25.0 5 0 6 1
SpectralRegBackground: 1 0.0 290.5 0.0
SpectralRegHero: 1 290.5 0.0 0.0 0.00
SpectralRegIR: 1 0 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 4 1 (-2604.6 -9759.6 15724.3 45.0 -0.1)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 2
XrayPower: 25.14 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 15000.0 V
XRayCondenserLensVoltage: 8420.0 V
XRayObjectiveCoilCurrent: 0.740 A
XRayBlankingVoltage: 250.0 V
XRayFilamentCurrent: 1.550 A
XRayStigmator: 0.0 0.0
XRayHighPower: no
EgunNeutMode: Off
NeutralizerCurrent: 20.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 30.0 V
EgunNeutXSteering: -21.5
EgunNeutYSteering: -8.0
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 285.0 eV
SxiPassEnergy: 376 eV
SxiLens2: -898 V
SxiLens3: -850 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 250.0 V
SxiDisplayMode: 1
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.816
Channel Info: 2 1 1.428
Channel Info: 3 1 1.393
```

```

Channel Info: 4 1 1.255
Channel Info: 5 1 1.298
Channel Info: 6 1 0.991
Channel Info: 7 1 1.100
Channel Info: 8 1 0.958
Channel Info: 9 1 0.968
Channel Info: 10 1 0.794
Channel Info: 11 1 0.821
Channel Info: 12 1 0.766
Channel Info: 13 1 0.772
Channel Info: 14 1 0.704
Channel Info: 15 1 0.751
Channel Info: 16 1 1.563
StagePosition: -2.9096 11.3670 15.7243 45.0094 -0.1000
StageCurrentRotationSpeed: 1.0000
DefectPosID: 4
DefectPosComment:
DefectPosU: -2.6046
DefectPosV: 9.7596
DefectPosX: -2.9096
DefectPosY: 11.3670
DefectPosZ: 15.7243
DefectPosTilt: 45.0094
DefectPosRotation: -0.1000
DefectPosAligment: None
DefectPosReferenceImage: HATCN.114.pho
GCIBSputterRate: 0.0 A/min
GCIBBeam: 3.500 kV
GCIBIonization: 150.0 V
GCIBExtractor: 1.90 kV
GCIBRasterSize: 3.0 3.0 mm
GCIBRasterOffset: 2.0 1.8 mm
GCIBWien: 12.00 V
GCIBBend: -73.00 V
GCIBEmission: 20.00 mA
GCIBMagnet: 25.0 A
GCIBObjective: 52.00 Percent
GCIBFocus: 79.30 Percent
GCIBGasPressure: 650.00 kPa
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 100u25W15KV
EOFH
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```

### Software Version 15: SS 4.1.4.3

- Example of 1 region: Survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V14-SS 4.1.4.3.SPE

```

SOFH
Platform: PC
Technique: XPS
TechniqueEx: XPS
FileType: SPECTRUM
FileDesc:
SoftwareVersion: SS 4.1.4.3
InstrumentModel: PHI Quantes
AcqFilename:
C:\Datafiles\quantex_I\xknigge\Daten\20210719_XPS_Co304\Co304.117.13.Co304_H2O_m_1.spe
FileDate: 2021 7 19
AcqFileDate: 2021 7 19
Institution: PHI
Operator:
ExperimentID:
EnergyReference: none 0.0

```

AnalyserWorkFcn: 4.375 eV  
AnalyserRetardGain: 1.000302  
PlatenID: NSIT\_Co304\_  
PlatenDesc:  
PhotoFilename: C:\Datafiles\Service\Install\1 Inch Puck.106.pho  
SXIFilename:  
SourceAnalyserAngle: 45.0 d  
AnalyserSolidAngle: 0.38 sr  
IntensityRecal: no  
IntensityCalCoeff: 312.723 1.455  
EnergyRecal: no  
ScanDeflectionSpan: 200 150  
ScanDeflectionOffset: -10 30  
SCAMultiplierVoltage: 2000.0 V  
NarrowAcceptanceAngle: no  
PeakToNoiseRatioState: no  
DelayBeforeAcquire: 15 seconds  
C60IonGun: None  
TFParameters: 0, 1, 2, 93.73, 7.481, 1, 1  
SemFieldOfView: 0.0000000  
ImageSizeXY: 0.0000 0.0000  
IonGunMode: Neutralize  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 0.001 kV  
FloatVolt: 0.0 V  
FloatEnable: no  
GridVolt: 120.0  
CondensorVolt: 0.00  
ObjectiveVolt: 0.00  
BendVolt: 0.00  
SputterRaster: 0.00 0.00 mm  
SputterRasterOffset: 0.000 0.000 mm  
TargetSputterTime: 1.0 min  
SputterEmission: 0.00 mA  
DeflectionBias: 0.0 V  
IonGunGasPressure: 0.000 mPa  
NeutIon: Ar+  
NeutCurrent: 0.000 uA  
NeutRate: 0.000 A/min  
NeutEnergy: 0.110 kV  
NeutFloatVolt: -100.0 V  
NeutFloatEnable: yes  
NeutGridVolt: 120.0  
NeutCondensorVolt: 82.50  
NeutObjectiveVolt: 72.05  
NeutBendVolt: 6.60  
NeutRaster: 0.00 0.00 mm  
NeutRasterOffset: -0.050 0.410 mm  
NeutTargetTimedOnTime: 2.0 min  
NeutEmission: 5.00 mA  
NeutDeflectionBias: 20.0 V  
NeutIonGunGasPressure: 2.600 mPa  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvNumCycles: 1  
SurvTimePerStep: 50.000000  
NoSpectralRegFull: 1  
SpectralRegDefFull: 1 1 Su1s 111 1101 -1.0000 1100.0000 0.0000 1100.0000 0.0000  
0.000000 280.00 TOTAL  
SpectralRegDef2Full: 1 1100.0 5 0 2 1  
SpectralRegBackgroundFull: 1 0.0 550.0 0.0  
SpectralRegHeroFull: 1 550.0 0.0 0.0 0.00  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
NoSpectralReg: 1

SpectralRegDef: 1 1 Suls 111 1101 -1.0000 1100.0000 0.0000 1100.0000 0.0000  
0.500000 280.00 TOTAL  
SpectralRegDef2: 1 1100.0 5 0 2 1  
SpectralRegBackground: 1 0.0 550.0 0.0  
SpectralRegHero: 1 550.0 0.0 0.0 0.0  
SpectralRegIR: 1 1 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 Point13 1 (-24191.1 -19291.8 24116.0 45.0 360.0)  
SpatialAreaDesc: 1 microwave H2O  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 1  
XrayPower: 24.00 W  
XrayBeamDiameter: 100.0 um  
XRayBeamVoltage: 15000.0 V  
XRayCondenserLensVoltage: 8340.0 V  
XRayObjectiveCoilCurrent: 0.719 A  
XRayBlankingVoltage: 300.0 V  
XRayFilamentCurrent: 1.520 A  
XRayStigmator: 0.3 0.4  
XRayOffsetInUm: 0 -20  
XRayMagFactor: 0.138 0.140  
XRayDelayFactor: 2000 1000  
XRayRotationInDeg: -21.00 V  
XRayHighPower: no  
XRayEmissionControl: yes  
XRayEmissionCurrent: 3.000 mA  
XRayStepDelayReadBeam: 5  
XRayStepsPerDiameter: 1.0  
XRayInterlaceInterval: 1  
XRayMaxFilamentCurrent: 1.600 A  
XRaySetting: 100u25W15KV  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: 1.1  
EgunNeutYSteering: -7.9  
EgunNeutFilament: 1.10 A  
EgunNeutPulseLength: 10.0 msec  
EgunNeutPulseFrequency: 30  
SxiPersistence: 1  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 1456.0 eV  
SxiPassEnergy: 0 eV  
SxiLens2: -286 V  
SxiLens3: -286 V  
SxiLens4: -281 V  
SxiLens5: -281 V  
SxiRotator: 0.00 A  
SxiLensBias: 200 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 70.0 V  
SxiDisplayMode: 2  
Detector Acq Time: 30.0 (min)  
Number Of Channels: 32  
Channel Info: 1 1 1.216  
Channel Info: 2 1 1.234  
Channel Info: 3 1 1.163  
Channel Info: 4 1 1.133  
Channel Info: 5 1 1.038  
Channel Info: 6 1 1.113  
Channel Info: 7 1 1.031  
Channel Info: 8 1 1.119



**Software Version 16: SS 3.10.2.1**

- Example of 1 region: Survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V16-SS 3.10.2.1.SPE

SOFH  
 Platform: PC  
 Technique: XPS  
 TechniqueEx: AES  
 FileType: SPECTRUM  
 FileDesc: FCM\_E1  
 SoftwareVersion: SS 3.10.2.1  
 InstrumentModel: PHI Quantera SXM  
 AcqFilename: C:\Messdaten\2022\2022\_054FCM\2022\_054FCM.201.FCM\_E1.spe  
 FileDate: 2022 3 10  
 AcqFileDate: 2022 3 10  
 Institution: PHI  
 Operator:  
 ExperimentID: 1  
 EnergyReference: none 0.0  
 AnalyserWorkFcn: 3.825 eV  
 AnalyserRetardGain: 0.999426  
 PlatenID: 2022\_054FCM  
 PlatenDesc:  
 PhotoFilename: 2022\_054FCM.101.Std Photo.pho  
 SXIFilename:  
 SourceAnalyserAngle: 45.0 d  
 AnalyserSolidAngle: 0.38 sr  
 IntensityRecal: no  
 IntensityCalCoeff: 27.040 0.169  
 EnergyRecal: no  
 ScanDeflectionSpan: 100 60  
 ScanDeflectionOffset: 33 -3  
 SCAMultiplierVoltage: 1890.0 V  
 NarrowAcceptanceAngle: no  
 PeakToNoiseRatioState: no  
 DelayBeforeAcquire: 2 seconds  
 C60IonGun: None  
 TFCParameters: 0, 1, 2, 93.73, 7.481, 1, 1  
 SemFieldOfView: 0.0000000  
 ImageSizeXY: 0.0000 0.0000  
 IonGunMode: Neutralize  
 SputterIon: Ar+  
 SputterCurrent: 0.000 uA  
 SputterRate: 0.000 A/min  
 SputterEnergy: 0.110 kV  
 FloatVolt: -102.0 V  
 FloatEnable: yes  
 GridVolt: 120.0  
 CondensorVolt: 78.43  
 ObjectiveVolt: 102.63  
 BendVolt: 3.22  
 SputterRaster: 0.00 0.00 mm  
 SputterRasterOffset: 0.900 -0.800 mm  
 TargetSputterTime: 0.2 min  
 SputterEmission: 3.00 mA  
 DeflectionBias: 0.0 V  
 IonGunGasPressure: 0.000 mPa  
 XpsScanMode: scanned  
 AnalyserMode: FAT  
 SurvNumCycles: 7  
 SurvTimePerStep: 20.000000  
 NoSpectralRegFull: 7  
 SpectralRegDefFull: 1 1 Suls 111 3501 -0.4000 1405.0000 5.0000 1404.0000 6.0000  
 0.000000 112.00 HEIGHT  
 SpectralRegDef2Full: 1 1400.0 2 0 1 400  
 SpectralRegBackgroundFull: 1 0.0 705.0 0.0

```
SpectralRegHeroFull: 1 705.0 0.0 0.0 0.00
SpectralRegIRFull: 1 0 0.000 0.000 0.0
SpectralRegDefFull: 2 0 Cu2p3 29 126 -0.2000 950.0000 925.0000 949.0000 926.0000
0.000000 26.00 HEIGHT
SpectralRegDef2Full: 2 25.0 10 0 1 500
SpectralRegBackgroundFull: 2 0.0 937.5 0.0
SpectralRegHeroFull: 2 937.5 0.0 0.0 0.00
SpectralRegIRFull: 2 0 0.000 0.000 0.0
SpectralRegDefFull: 3 0 Cu_LMM 29 63 -0.4000 583.0000 558.0000 582.0000 559.0000
0.000000 112.00 HEIGHT
SpectralRegDef2Full: 3 25.0 5 0 1 500
SpectralRegBackgroundFull: 3 0.0 570.5 0.0
SpectralRegHeroFull: 3 570.5 0.0 0.0 0.00
SpectralRegIRFull: 3 0 0.000 0.000 0.0
SpectralRegDefFull: 4 0 C1s 6 76 -0.2000 292.0000 277.0000 291.0000 278.0000
0.000000 26.00 HEIGHT
SpectralRegDef2Full: 4 15.0 8 0 1 400
SpectralRegBackgroundFull: 4 0.0 284.5 0.0
SpectralRegHeroFull: 4 284.5 0.0 0.0 0.00
SpectralRegIRFull: 4 0 0.000 0.000 0.0
SpectralRegDefFull: 5 0 N1s 7 81 -0.2000 408.0000 392.0000 407.0000 393.0000
0.000000 26.00 HEIGHT
SpectralRegDef2Full: 5 16.0 7 0 1 400
SpectralRegBackgroundFull: 5 0.0 400.0 0.0
SpectralRegHeroFull: 5 400.0 0.0 0.0 0.00
SpectralRegIRFull: 5 0 0.000 0.000 0.0
SpectralRegDefFull: 6 0 Si2p 14 151 -0.1000 107.0000 92.0000 106.0000 93.0000
0.000000 26.00 HEIGHT
SpectralRegDef2Full: 6 15.0 3 0 1 350
SpectralRegBackgroundFull: 6 0.0 99.5 0.0
SpectralRegHeroFull: 6 99.5 0.0 0.0 0.00
SpectralRegIRFull: 6 0 0.000 0.000 0.0
SpectralRegDefFull: 7 0 O1s 8 151 -0.1000 538.0000 523.0000 537.0000 524.0000
0.000000 26.00 HEIGHT
SpectralRegDef2Full: 7 15.0 2 0 1 400
SpectralRegBackgroundFull: 7 0.0 530.5 0.0
SpectralRegHeroFull: 7 530.5 0.0 0.0 0.00
SpectralRegIRFull: 7 0 0.000 0.000 0.0
NoSpectralReg: 1
SpectralRegDef: 1 1 Su1s 111 3501 -0.4000 1405.0000 5.0000 1404.0000 6.0000
0.280000 112.00 HEIGHT
SpectralRegDef2: 1 1400.0 2 0 1 400
SpectralRegBackground: 1 0.0 705.0 0.0
SpectralRegHero: 1 705.0 0.0 0.0 0.00
SpectralRegIR: 1 1 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 Point13 1 (-25240.7 21146.3 24270.0 45.0 360.0)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 0
XrayPower: 43.82 W
XrayBeamDiameter: 200.0 um
XrayBeamVoltage: 15000.0 V
XrayCondenserLensVoltage: 7600.0 V
XrayObjectiveCoilCurrent: 0.736 A
XrayBlankingVoltage: 300.0 V
XrayFilamentCurrent: 1.616 A
XrayStigmator: -0.1 0.0
XrayOffsetInUm: -20 -30
XrayMagFactor: 0.330 0.330
XrayDelayFactor: 1000 2000
XrayRotationInDeg: -21.00 V
XrayHighPower: no
XrayEmissionControl: yes
XrayEmissionCurrent: 4.000 mA
XrayStepDelayReadBeam: 5
```

XRayStepsPerDiameter: 1.0  
XRayInterlaceInterval: 1  
XRayMaxFilamentCurrent: 1.700 A  
XRaySetting: 200u50W15KV  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: -14.0  
EgunNeutYSteering: -14.2  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
EgunNeutPulseFrequency: 30  
SxiPersistence: 1  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.60  
SxiBindingEnergy: 410.0 eV  
SxiPassEnergy: 280 eV  
SxiLens2: -287 V  
SxiLens3: -287 V  
SxiLens4: -670 V  
SxiLens5: -670 V  
SxiRotator: 0.00 A  
SxiLensBias: 200 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 200.0 V  
SxiDisplayMode: 2  
Detector Acq Time: 30.0 (min)  
Number Of Channels: 32  
Channel Info: 1 1 1.253  
Channel Info: 2 1 1.147  
Channel Info: 3 1 1.145  
Channel Info: 4 1 1.080  
Channel Info: 5 1 1.133  
Channel Info: 6 1 1.115  
Channel Info: 7 1 1.133  
Channel Info: 8 1 1.111  
Channel Info: 9 1 1.105  
Channel Info: 10 1 1.097  
Channel Info: 11 1 1.056  
Channel Info: 12 1 1.017  
Channel Info: 13 1 1.029  
Channel Info: 14 1 1.019  
Channel Info: 15 1 1.020  
Channel Info: 16 1 1.009  
Channel Info: 17 1 1.005  
Channel Info: 18 1 0.968  
Channel Info: 19 1 0.984  
Channel Info: 20 1 0.966  
Channel Info: 21 1 0.964  
Channel Info: 22 1 0.954  
Channel Info: 23 1 0.967  
Channel Info: 24 1 0.917  
Channel Info: 25 1 0.933  
Channel Info: 26 1 0.912  
Channel Info: 27 1 0.907  
Channel Info: 28 1 0.862  
Channel Info: 29 1 0.879  
Channel Info: 30 1 0.866  
Channel Info: 31 1 0.906  
Channel Info: 32 1 0.847  
StagePosition: -24.9525 -21.5285 24.2765 45.0000 359.9623  
StageCurrentRotationSpeed: 0.5000  
DefectPosID: 13  
DefectPosName: FCM\_E1

```

DefectPosComment:
DefectPosU: -25.2406
DefectPosV: -21.1443
DefectPosX: -24.9525
DefectPosY: -21.5285
DefectPosZ: 24.2765
DefectPosTilt: 45.0000
DefectPosRotation: 359.9623
DefectPosAlignment: Standard
DefectPosReferenceImage: 2022_054FCM.101.Std Photo.pho
Deconvolution: no
DeconvolutionPassEnergy: 13.00 eV
AutoEGunNeut: yes
AutoEGunNeutSetting: E-Neut
AutoIonNeut: yes
AutoIonNeutSetting: I-Neut
AutoZAlign: yes
AutoZAlignSetting: 100u25W15KV
AutoZAlignHPSetting: 100u100W20KV_HP
Presputter: no
PresputterTime: 0.20 (min)
AutoBeamPark: no
AutoBeamParkSetting: Park_20u4.5W15KV
EOFH

```

```

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```

...

### Software Version 17: SS 3.2.1.10

- Example of 1 region: Survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V17-SS 3.2.1.10.SPE

```

SOFH
Platform: PC
Technique: XPS
TechniqueEx: XPS
FileType: SPECTRUM
FileDesc: 1.CS1
SoftwareVersion: SS 3.2.1.10
InstrumentModel: PHI VersaProbe II
AcqFilename: D:\Datafiles\Data PHI-VP\INE VP\IMKORB\GGG40.9.spe
FileDate: 2021 10 11
AcqFileDate: 2021 10 11
Institution: PHI
ExperimentID: IMKORB
EnergyReference: none 0.0
AnalyserWorkFcn: 4.254 eV
AnalyserRetardGain: 1.000592
PlatenID: IMKORB-1
PhotoFilename: GGG40.8.pho
SXIFilename:
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 0.38 sr
IntensityRecal: no
IntensityCalCoeff: 62.470 0.355
EnergyRecal: no
ScanDeflectionSpan: 80 30
ScanDeflectionOffset: 10 5
SCAMultiplierVoltage: 1900.0 V
NarrowAcceptanceAngle: no
PeakToNoiseRatioState: no
DelayBeforeAcquire: 2 seconds
C60IonGun: None
BiasBoxMode: 0
TFParameters: 0,
1, 18, 93.73, 46.67, 23.33, 9.342, 4.671, 2.919, 156.3, 77.82, 38.91, 15.58, 7.788, 4.867, 240

```

.2,119.6,59.8,23.94,11.97,7.481,0.6962,0.8969,0.9582,1,0.9227,0.7902,0.4567,0.78  
21,0.8461,0.9791,1,0.9653,0.3922,0.5496,0.7675,0.9008,0.964,1  
SemFieldOfView: 0.0000000  
ImageSizeXY: 0.0000 0.0000  
IonGunMode: Standby  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 0.110 kV  
FloatVolt: -104.0 V  
FloatEnable: yes  
GridVolt: 102.0  
CondensorVolt: 71.50  
ObjectiveVolt: 100.10  
BendVolt: 1.43  
SputterRaster: 0.00 0.00 mm  
SputterRasterOffset: 0.700 0.500 mm  
TargetSputterTime: 0.0 min  
SputterEmission: 0.00 mA  
DeflectionBias: 73.0 V  
IonGunGasPressure: 0.000 mPa  
NeutIon: Ar+  
NeutCurrent: 0.000 uA  
NeutRate: 0.000 A/min  
NeutEnergy: 0.110 kV  
NeutFloatVolt: -104.0 V  
NeutFloatEnable: yes  
NeutGridVolt: 102.0  
NeutCondensorVolt: 71.50  
NeutObjectiveVolt: 100.10  
NeutBendVolt: 1.43  
NeutRaster: 0.00 0.00 mm  
NeutRasterOffset: 0.700 0.500 mm  
NeutTargetTimedOnTime: 0.0 min  
NeutEmission: 0.00 mA  
NeutDeflectionBias: 73.0 V  
NeutIonGunGasPressure: 0.000 mPa  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvNumCycles: 16  
SurvTimePerStep: 50.000000  
NoSpectralRegFull: 19  
SpectralRegDefFull: 1 1 Su1s 111 1694 -0.8000 1350.0000 -5.0000 1349.0000 -  
4.0000 0.000000 187.85 AREA  
SpectralRegDef2Full: 1 1355.0 1 0 1 400  
SpectralRegBackgroundFull: 1 0.0 672.5 0.0  
SpectralRegHeroFull: 1 672.5 0.0 0.0 0.00  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
SpectralRegDefFull: 2 0 Cu2p3 29 51 -0.1000 935.0000 930.0000 934.0000 931.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 2 5.0 2 0 4 300  
SpectralRegBackgroundFull: 2 0.0 932.5 0.0  
SpectralRegHeroFull: 2 932.5 0.0 0.0 0.00  
SpectralRegIRFull: 2 0 0.000 0.000 0.0  
SpectralRegDefFull: 3 0 Cu2p3 29 51 -0.1000 935.0000 930.0000 934.0000 931.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 3 5.0 1 0 4 300  
SpectralRegBackgroundFull: 3 0.0 932.5 0.0  
SpectralRegHeroFull: 3 932.5 0.0 0.0 0.00  
SpectralRegIRFull: 3 0 0.000 0.000 0.0  
SpectralRegDefFull: 4 0 Au4f7 79 41 -0.1000 86.0000 82.0000 85.0000 83.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 4 4.0 2 0 4 400  
SpectralRegBackgroundFull: 4 0.0 84.0 0.0  
SpectralRegHeroFull: 4 84.0 0.0 0.0 0.00  
SpectralRegIRFull: 4 0 0.000 0.000 0.0

SpectralRegDefFull: 5 0 Au4f7 79 41 -0.1000 86.0000 82.0000 85.0000 83.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 5 4.0 1 0 4 300  
SpectralRegBackgroundFull: 5 0.0 84.0 0.0  
SpectralRegHeroFull: 5 84.0 0.0 0.0 0.00  
SpectralRegIRFull: 5 0 0.000 0.000 0.0  
SpectralRegDefFull: 6 0 Ag3d5 47 66 -0.1000 371.5000 365.0000 370.5000 366.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 6 6.5 2 0 4 400  
SpectralRegBackgroundFull: 6 0.0 368.3 0.0  
SpectralRegHeroFull: 6 368.3 0.0 0.0 0.00  
SpectralRegIRFull: 6 0 0.000 0.000 0.0  
SpectralRegDefFull: 7 0 Ag3d5 47 41 -0.1000 370.0000 366.0000 369.0000 367.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 7 4.0 1 0 4 400  
SpectralRegBackgroundFull: 7 0.0 368.0 0.0  
SpectralRegHeroFull: 7 368.0 0.0 0.0 0.00  
SpectralRegIRFull: 7 0 0.000 0.000 0.0  
SpectralRegDefFull: 8 0 Mg1s 12 91 -0.1000 1306.0000 1297.0000 1305.0000  
1298.0000 0.000000 23.50 AREA  
SpectralRegDef2Full: 8 9.0 2 0 4 300  
SpectralRegBackgroundFull: 8 0.0 1301.5 0.0  
SpectralRegHeroFull: 8 1301.5 0.0 0.0 0.00  
SpectralRegIRFull: 8 0 0.000 0.000 0.0  
SpectralRegDefFull: 9 0 Cu2p1 29 171 -0.1000 964.0000 947.0000 963.0000 948.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 9 17.0 2 0 4 300  
SpectralRegBackgroundFull: 9 0.0 955.5 0.0  
SpectralRegHeroFull: 9 955.5 0.0 0.0 0.00  
SpectralRegIRFull: 9 0 0.000 0.000 0.0  
SpectralRegDefFull: 10 0 Cs3d5 55 101 -0.1000 727.0000 717.0000 726.0000  
718.0000 0.000000 23.50 AREA  
SpectralRegDef2Full: 10 10.0 1 0 4 300  
SpectralRegBackgroundFull: 10 0.0 722.0 0.0  
SpectralRegHeroFull: 10 722.0 0.0 0.0 0.00  
SpectralRegIRFull: 10 0 0.000 0.000 0.0  
SpectralRegDefFull: 11 0 Fe2p3 26 401 -0.1000 740.0000 700.0000 739.0000  
701.0000 0.000000 23.50 AREA  
SpectralRegDef2Full: 11 40.0 3 0 4 300  
SpectralRegBackgroundFull: 11 0.0 720.0 0.0  
SpectralRegHeroFull: 11 720.0 0.0 0.0 0.00  
SpectralRegIRFull: 11 0 0.000 0.000 0.0  
SpectralRegDefFull: 12 0 I3d5 53 121 -0.1000 623.0000 611.0000 622.0000 612.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 12 12.0 4 0 4 300  
SpectralRegBackgroundFull: 12 0.0 617.0 0.0  
SpectralRegHeroFull: 12 617.0 0.0 0.0 0.00  
SpectralRegIRFull: 12 0 0.000 0.000 0.0  
SpectralRegDefFull: 13 0 O1s 8 63 -0.8000 573.0000 523.0000 572.0000 524.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 13 50.0 1 0 4 300  
SpectralRegBackgroundFull: 13 0.0 548.0 0.0  
SpectralRegHeroFull: 13 548.0 0.0 0.0 0.00  
SpectralRegIRFull: 13 0 0.000 0.000 0.0  
SpectralRegDefFull: 14 0 Sn3d5 50 91 -0.1000 488.0000 479.0000 487.0000 480.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 14 9.0 4 0 4 300  
SpectralRegBackgroundFull: 14 0.0 483.5 0.0  
SpectralRegHeroFull: 14 483.5 0.0 0.0 0.00  
SpectralRegIRFull: 14 0 0.000 0.000 0.0  
SpectralRegDefFull: 15 0 U4f7 92 271 -0.1000 401.0000 374.0000 400.0000 375.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 15 27.0 4 0 4 300  
SpectralRegBackgroundFull: 15 0.0 387.5 0.0  
SpectralRegHeroFull: 15 387.5 0.0 0.0 0.00  
SpectralRegIRFull: 15 0 0.000 0.000 0.0

```
SpectralRegDefFull: 16 0 Cls 6 151 -0.1000 292.0000 277.0000 291.0000 278.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 16 15.0 4 0 4 300
SpectralRegBackgroundFull: 16 0.0 284.5 0.0
SpectralRegHeroFull: 16 284.5 0.0 0.0 0.00
SpectralRegIRFull: 16 0 0.000 0.000 0.0
SpectralRegDefFull: 17 0 Cl2p 17 81 -0.1000 201.0000 193.0000 200.0000 194.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 17 8.0 4 0 4 300
SpectralRegBackgroundFull: 17 0.0 197.0 0.0
SpectralRegHeroFull: 17 197.0 0.0 0.0 0.00
SpectralRegIRFull: 17 0 0.000 0.000 0.0
SpectralRegDefFull: 18 0 Zr3d 40 111 -0.1000 186.0000 175.0000 185.0000 176.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 18 11.0 1 0 4 300
SpectralRegBackgroundFull: 18 0.0 180.5 0.0
SpectralRegHeroFull: 18 180.5 0.0 0.0 0.00
SpectralRegIRFull: 18 0 0.000 0.000 0.0
SpectralRegDefFull: 19 0 S2p 16 81 -0.1000 167.0000 159.0000 166.0000 160.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 19 8.0 2 0 4 300
SpectralRegBackgroundFull: 19 0.0 163.0 0.0
SpectralRegHeroFull: 19 163.0 0.0 0.0 0.00
SpectralRegIRFull: 19 0 0.000 0.000 0.0
NoSpectralReg: 1
SpectralRegDef: 1 1 Suls 111 1694 -0.8000 1350.0000 -5.0000 1349.0000 -4.0000
0.800000 187.85 AREA
SpectralRegDef2: 1 1355.0 1 0 1 400
SpectralRegBackground: 1 0.0 672.5 0.0
SpectralRegHero: 1 672.5 0.0 0.0 0.00
SpectralRegIR: 1 1 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 1 1 (-2897.0 -6519.0 16089.5 45.0 -0.1)
SpatialAreaDesc: 1 CS1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.7 mono
XrayAnodePosition: 4
XrayPower: 34.83 W
XrayBeamDiameter: 200.0 um
XRayBeamVoltage: 15000.0 V
XRayCondenserLensVoltage: 7750.0 V
XRayObjectiveCoilCurrent: 0.785 A
XRayBlankingVoltage: 330.0 V
XRayFilamentCurrent: 1.588 A
XRayStigmator: 0.0 0.0
XRayOffsetInUm: 130 150
XRayMagFactor: 0.361 0.356
XRayDelayFactor: 2000 1000
XRayRotationInDeg: -21.50 V
XRayHighPower: no
XRayEmissionControl: yes
XRayEmissionCurrent: 4.000 mA
XRayStepDelayReadBeam: 5
XRayStepsPerDiameter: 1.0
XRayInterlaceInterval: 1
XRayMaxFilamentCurrent: 1.650 A
XRaySetting: 180u35W15KV_new
EgunNeutMode: Neutralize
NeutralizerCurrent: 18.0 uA
NeutralizerEnergy: 1.30 V
EgunNeutExtractor: 45.0 V
EgunNeutXSteering: 0.0
EgunNeutYSteering: -2.0
EgunNeutFilament: 0.90 A
EgunNeutPulseLength: 10.0 msec
EgunNeutPulseFrequency: 2
SxiPersistence: 1
```

```

SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.50
SxiBindingEnergy: 550.0 eV
SxiPassEnergy: 376 eV
SxiLens2: -699 V
SxiLens3: -662 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 400.0 V
SxiDisplayMode: 1
Detector Acq Time: 100.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.909
Channel Info: 2 1 1.404
Channel Info: 3 1 1.353
Channel Info: 4 1 1.252
Channel Info: 5 1 1.141
Channel Info: 6 1 1.063
Channel Info: 7 1 1.019
Channel Info: 8 1 0.958
Channel Info: 9 1 0.961
Channel Info: 10 1 0.909
Channel Info: 11 1 0.817
Channel Info: 12 1 0.757
Channel Info: 13 1 0.725
Channel Info: 14 1 0.695
Channel Info: 15 1 0.739
Channel Info: 16 1 1.896
StagePosition: -2.8425 6.6240 16.0895 45.0031 -0.0500
StageCurrentRotationSpeed: 1.0000
DefectPosID: 1
DefectPosComment: CS1
DefectPosU: -2.8979
DefectPosV: 6.5180
DefectPosX: -2.8425
DefectPosY: 6.6240
DefectPosZ: 16.0895
DefectPosTilt: 45.0031
DefectPosRotation: -0.0500
DefectPosAligment: None
DefectPosReferenceImage: GGG40.8.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
AutoIonNeut: yes
Presputter: no
EOFH
□ □ ` □ □ □ □ □ □ ž □ □ □ pnt □ sar
...

```

### 3.1.20.2 PHI Spectrometer/Profile (\*.pro)

Comment:

- With respect to the multiregion files (\*.spe) the header contains additional profile information (e.g. number of parameter steps, sputter time)

#### Software Version 1: SS 2.1.0.1

- Example. sputter depth profile with 21 sputter steps and 3 regions: F 1s, O 1s, La 3d<sub>5/2</sub>
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V1-SS 2.1.0.1.PRO

SOFH

Platform: PC  
Technique: XPS  
FileType: DEPTHPRO  
FileDesc:  
SoftwareVersion: SS 2.1.0.1  
InstrumentModel: PHI VersaProbe II  
AcqFilename: C:\ZCH\120530\Temp120530.26.50\_PVD\_12\_1.pro  
FileDate: 2012 8 22  
AcqFileDate: 2012 8 22  
Institution: PHI  
Operator:  
ExperimentID: 120530  
EnergyReference: none 0.0  
AnalyserWorkFcn: 4.218 eV  
AnalyserRetardGain: 1.000207  
PlatenID:  
PhotoFilename: 120530.20.Low Mag.pho  
SXIFilename:  
SourceAnalyserAngle: 45.0 d  
AnalyserSolidAngle: 20.0 sr  
IntensityRecal: no  
IntensityCalCoeff: 100.000 0.330  
EnergyRecal: no  
ScanDeflectionSpan: 50 70  
ScanDeflectionOffset: 0 -20  
SCAMultiplierVoltage: 1650.0 V  
NarrowAcceptanceAngle: no  
PeakToNoiseRatioState: no  
DelayBeforeAcquire: 5 seconds  
C60IonGun: None  
BiasBoxMode: 0  
SemFieldOfView: 0.0000000  
EBeamCurrent: 0.0 nA  
ImageSizeXY: 0.0000 0.0000  
IonGunMode: Neutralize  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 0.110 kV  
FloatVolt: -100.0 V  
FloatEnable: yes  
GridVolt: 120.0  
CondensorVolt: 73.70  
ObjectiveVolt: 102.30  
BendVolt: 1.43  
SputterRaster: 0.00 0.00 mm  
SputterRasterOffset: 2.350 0.100 mm  
TargetSputterTime: 2.0 min  
SputterEmission: 7.00 mA  
DeflectionBias: 78.0 V  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvTimePerStep: 50.000000  
NoDPDataCyc: 21  
NoPreSputterCyc: 1  
ProfSputterDelay: 5.0  
ProfXrayOffDuringSputter: no  
ProfZalarHighAccuracyInterval: 20  
SampleRotation: off  
DepthRecal: no  
SputterMode: Alternating  
NoDepthReg: 1  
DepthCalDef: 1 Layer1 1 0.0000 0.0000 Ar+ 10.00 0.50 20 2KV3x3 2.000 150 15.00 0  
0 1420 1344 26 3.0 3.0 -0.69 -0.30 0.00 0.00 Ar  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 2197 3136  
PhotoOffsetInPixel: 1519 200

PhotoSizeInMm: 35.000 50.000  
PhotoOffsetInMm: 0.008 0.008  
NoSpectralRegFull: 3  
SpectralRegDefFull: 1 1 F1s 9 101 -0.2000 699.0000 679.0000 698.0000 680.0000  
0.000000 46.95 AREA  
SpectralRegDef2Full: 1 20.0 1 0 4 1  
SpectralRegBackgroundFull: 1 0.0 689.0 0.0  
SpectralRegHeroFull: 1 689.0 0.0 0.0 0.00  
SpectralRegDefFull: 2 1 O1s 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000  
0.000000 46.95 AREA  
SpectralRegDef2Full: 2 20.0 1 0 4 1  
SpectralRegBackgroundFull: 2 0.0 533.0 0.0  
SpectralRegHeroFull: 2 533.0 0.0 0.0 0.00  
SpectralRegDefFull: 3 1 La3d5 57 126 -0.2000 850.0000 825.0000 849.0000 826.0000  
0.000000 46.95 AREA  
SpectralRegDef2Full: 3 25.0 1 0 4 1  
SpectralRegBackgroundFull: 3 0.0 837.5 0.0  
SpectralRegHeroFull: 3 837.5 0.0 0.0 0.00  
NoSpectralReg: 3  
SpectralRegDef: 1 1 F1s 9 101 -0.2000 699.0000 679.0000 698.0000 680.0000  
0.200000 46.95 AREA  
SpectralRegDef2: 1 20.0 1 0 4 1 0.00  
SpectralRegBackground: 1 0.0 689.0 0.0  
SpectralRegHero: 1 689.0 0.0 0.0 0.00  
SpectralRegDef: 2 1 O1s 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000  
0.200000 46.95 AREA  
SpectralRegDef2: 2 20.0 1 0 4 1 0.00  
SpectralRegBackground: 2 0.0 533.0 0.0  
SpectralRegHero: 2 533.0 0.0 0.0 0.00  
SpectralRegDef: 3 1 La3d5 57 126 -0.2000 850.0000 825.0000 849.0000 826.0000  
0.200000 46.95 AREA  
SpectralRegDef2: 3 25.0 1 0 4 1 0.00  
SpectralRegBackground: 3 0.0 837.5 0.0  
SpectralRegHero: 3 837.5 0.0 0.0 0.00  
NoSpatialArea: 1  
SpatialAreaDef: 1 1 1 (10354.5 2256.9 18760.0 45.0 -90.0)  
SpatialAreaDesc: 1  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 0  
XrayPower: 25.61 W  
XrayBeamDiameter: 100.0 um  
XRayBeamVoltage: 15000.0 V  
XRayCondenserLensVoltage: 8230.0 V  
XRayObjectiveCoilCurrent: 0.748 A  
XRayBlankingVoltage: 325.0 V  
XRayFilamentCurrent: 1.577 A  
XRayStigmator: 0.0 0.0  
XRayHighPower: no  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 0.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 40.0 V  
EgunNeutXSteering: 1.0  
EgunNeutYSteering: 4.0  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
SxiPersistence: 1 V  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 694.0 eV  
SxiPassEnergy: 188 eV  
SxiLens2: -591 V  
SxiLens3: -560 V  
SxiLensBias: 0 V

```

SxiShutterBias: yes
SxiShutterBiasVoltage: 349.9 V
SxiDisplayMode: 1
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.698
Channel Info: 2 1 1.467
Channel Info: 3 1 1.392
Channel Info: 4 1 1.320
Channel Info: 5 1 1.251
Channel Info: 6 1 1.103
Channel Info: 7 1 1.074
Channel Info: 8 1 1.026
Channel Info: 9 1 1.001
Channel Info: 10 1 0.941
Channel Info: 11 1 0.824
Channel Info: 12 1 0.819
Channel Info: 13 1 0.750
Channel Info: 14 1 0.650
Channel Info: 15 1 0.674
Channel Info: 16 1 1.266
StagePosition: -2.6672 -9.4501 18.7598 45.0094 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 1
DefectPosComment:
DefectPosU: 10.3546
DefectPosV: -2.2577
DefectPosX: -2.6672
DefectPosY: -9.4501
DefectPosZ: 18.7598
DefectPosTilt: 45.0094
DefectPosRotation: -90.0500
DefectPosAlignment: None
DefectPosReferenceImage: 120530.20.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
□ □ à□ □ □ □ □ □ □ e □ □ pnt cyc c/s
ñDnw□ □ f4 5$! ð□ □ □ □ □ e □ □ pnt cyc
...

```

### Software Version 2: XPS V1.30

- Example. sputter depth profile with 41 sputter steps (sputter time: 30 s, -30 ... 1170) and 6 regions: C 1s, O 1s, Ni 2p<sub>3/2</sub>, Fe 2p<sub>3/2</sub>, Cr 2p<sub>3/2</sub>, Mo 3d,
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V2-XPS V1.30.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
Comment: Nr 3 TP
SoftwareVersion: XPS V1.30
InstrumentModel: PHI Model 1600/3057
Institution:
FileDate: 2009 07 05
AcqFileDate: 2009 07 05
AcqFilename: C:\XPS_Data\Besmehn\19650018.pdt
Operator:
ExperimentID:
PlatenID:
PlatenDesc: Nr 3 TP
StagePosition: 0.0 0.0 0.0 0.0 0.0
SampleID:

```

```

SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Al 1486.7 mono
XrayPower: 300 W
XrayBeamDiameter: 0.0 um
NeutralizerEnergy: 1.0 eV
NeutralizerCurrent: 20.0 mA
SourceAnalyzerAngle: 90.0 d
AnalyzerSolidAngle: 7 sr
AnalyzerMode: FAT
AnalyzerWorkFcn: 3.7 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 C1s 6 261 -0.050 291.000 278.000 291.000 278.000 0.200 11.75
HEIGHT
SpectralRegDef: 2 2 O1s 8 261 -0.050 539.000 526.000 539.000 526.000 0.200 11.75
HEIGHT
SpectralRegDef: 3 3 Ni2p3 28 441 -0.050 871.000 849.000 871.000 849.000 0.200
11.75 HEIGHT
SpectralRegDef: 4 4 Fe2p3 26 401 -0.050 723.000 703.000 723.000 703.000 0.300
11.75 HEIGHT
SpectralRegDef: 5 5 Cr2p3 24 361 -0.050 588.000 570.000 588.000 570.000 0.200
11.75 HEIGHT
SpectralRegDef: 6 6 Mo3d 42 361 -0.050 240.000 222.000 240.000 222.000 0.300
11.75 HEIGHT
NoDPDataCyc: 41
NoPreSputterCyc: 2
SputterInterval: 30.000 s
SputterMode: alt
SampleRotation: off
DepthRecal: no
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
□ □ □ □ □ □ □ □ □ ) □ □ cyc reg
...

```

### Software Version 3: XPS V2.0

- Example. sputter depth profile with 11 steps and 6 regions: C 1s, O 1s, Cu 2p, N 1s, Ag 3d, S 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V3-XPS V2.0.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
FileDesc: none
SoftwareVersion: XPS V2.0
InstrumentModel: PHI Quantum 2000
Institution: PHI
FileDate: 2006 1 30
AcqFileDate: 2006 1 30
AcqFilename: Profilschleifer001.pro
Operator: ro
ExperimentID: 2006-0067

```

```

PlatenID: 0067b
PlatenDesc: none
StagePosition: 7.4316 38.0950 8.6000 45.0000 -0.0207
PhotoFilename: Profilschleifer001.pProfilschleifer001.sxi
ActualPhotoFilename: /D=/Compass6.1.1/datafiles/photos/1_1138109828.pho
SXIFilename: Profilschleifer001.sxi
ActualSXIFilename: /D=/Compass6.1.1/datafiles/SXIs/1_1138176141.sxi
XraySource: Al 1486.6 mono
XrayPower: 19.47 W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 2.5 V
NeutralizerCurrent: 5.0 uA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 3.9 eV
IntensityRecal: no
IntensityCalCoeff: 23.460 0.183
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 1.000 keV
SputterCurrent: 15.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0.4 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 Cu2p 29 161 -0.0500 936.0 928.0 936.0 928.0 13.199999
23.50 AREA
SpectralRegDef: 2 2 C1s 6 201 -0.0500 290.0 280.0 290.0 280.0 15.840002 23.50
AREA
SpectralRegDef: 3 3 O1s 8 201 -0.0500 537.0 527.0 537.0 527.0 26.399998 23.50
AREA
SpectralRegDef: 4 4 N1s 7 161 -0.0500 403.0 395.0 403.0 395.0 13.199999 23.50
AREA
SpectralRegDef: 5 5 Ag3d 47 301 -0.0500 379.0 364.0 375.0 364.0 10.559999
23.50 AREA
SpectralRegDef: 6 6 S2p 16 201 -0.0500 166.0 156.0 166.0 158.0 26.399998 23.50
AREA
NoDPDataCyc: 11
NoPreSputterCyc: 1
SputterMode: alt
SampleRotation: off
DepthRecal: no
NoDepthReg: 10
DepthCalDef: 1 Layer1 2 0.4000
DepthCalDef: 2 Layer2 3 0.4000
DepthCalDef: 3 Layer3 4 0.4000
DepthCalDef: 4 Layer4 5 0.4000
DepthCalDef: 5 Layer5 6 0.4000
DepthCalDef: 6 Layer6 7 0.4000
DepthCalDef: 7 Layer7 8 0.4000
DepthCalDef: 8 Layer8 9 0.4000
DepthCalDef: 9 Layer9 10 0.4000
DepthCalDef: 10 Layer10 11 0.4000
LayerRegionFlags: Cycle 1 0 0 0 0 0 0
LayerRegionFlags: Cycle 2 0 0 0 0 0 0
LayerRegionFlags: Cycle 3 0 0 0 0 0 0
LayerRegionFlags: Cycle 4 0 0 0 0 0 0
LayerRegionFlags: Cycle 5 0 0 0 0 0 0
LayerRegionFlags: Cycle 6 0 0 0 0 0 0
LayerRegionFlags: Cycle 7 0 0 0 0 0 0
LayerRegionFlags: Cycle 8 0 0 0 0 0 0
LayerRegionFlags: Cycle 9 0 0 0 0 0 0
LayerRegionFlags: Cycle 10 0 0 0 0 0 0
LayerRegionFlags: Cycle 11 0 0 0 0 0 0
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (6185.8 36097.0 8600.0 45.0 -0.3)

```

SpatialAreaDesc: 1 Nr1 Schleifer Stelle1

SpatialHRPhotoCor: 1 (0.0 0.0)

EOFH

```

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  □ □ □ cyc 7777reg 7777 7777777s 77777777777777f8 7□□ □□ □ □ □ □
    □

```

...

#### Software Version 4: Without software specification

- Example. sputter depth profile with 20 sputter steps (step width: 3, from -3 to 54) and 12 regions: C 1s, O 1s, F 1s, Na 1s, Si 2p, Cr 2p, Fe 2p, Ni 2p, N 1s, Mo 3d, Cu 2p, Mn 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V4-without\_software\_specification.PRO

SOFH

Platform: PC

Technique: XPS

FileType: DEPTHPRO

FileDesc: 1) ASF III Lu Einbau 2005 IV

FileDate: 108 7 21

AcqFileDate: 108 7 21

AcqFilename: ham26\_2.pro

ScanMode: scan

StagePosition: 0.0 0.0 0.0 45.0 0.0

XraySource: Al 1486.6 mono

XrayPower: 300.00 W

NeutralizerEnergy: 0.0 eV

NeutralizerCurrent: 0.0 mA

SourceAnalyserAngle: 90.0 d

AnalyserMode: FAT

AnalyserWorkFcn: 4.5 eV

IntensityRecal: no

IntensityCalCoeff: 24.500 0.207

EnergyRecal: no

EnergyReference: none 0.0

SputterIon: 3He

SputterEnergy: 3.000 keV

SputterCurrent: 0.0 nA

SputterRaster: 10.0 0.0 um

PreAcqSputterTime: 6 s

PreAcqSputterRate: 1.0 A/s

NoSpectralReg: 12

SpectralRegDef: 1 1 C1 6 200 -0.1000 295.0 275.0 295.0 280.0 0.100000 23.50 none

SpectralRegDef: 2 2 O1 8 200 -0.1000 540.0 520.0 540.0 525.0 0.100000 23.50 none

SpectralRegDef: 3 3 F1 9 200 -0.1000 695.0 675.0 695.0 680.0 0.100000 23.50 none

SpectralRegDef: 4 4 Na1 11 200 -0.1000 1081.0 1061.0 1081.0 1066.0 0.100000

23.50 none

SpectralRegDef: 5 5 Si1 14 200 -0.1000 110.0 90.0 110.0 95.0 0.100000 23.50 none

SpectralRegDef: 6 6 Cr1 24 400 -0.1000 605.0 565.0 605.0 567.0 0.100000 23.50

none

SpectralRegDef: 7 7 Fe1 26 400 -0.1000 735.0 695.0 735.0 700.0 0.100000 23.50

none

SpectralRegDef: 8 8 Ni1 28 500 -0.1000 890.0 840.0 890.0 844.0 0.100000 23.50

none

SpectralRegDef: 9 9 N1 7 200 -0.1000 410.0 390.0 410.0 394.0 0.100000 23.50 none

SpectralRegDef: 10 10 Mo1 42 200 -0.1000 240.0 220.0 240.0 223.0 0.100000 23.50

none

SpectralRegDef: 11 11 Cu1 29 500 -0.1000 970.0 920.0 970.0 924.0 0.100000 23.50

none

SpectralRegDef: 12 12 Mn1 25 400 -0.1000 670.0 630.0 670.0 632.0 0.100000 23.50

none

NoDPDataCyc: 20

NoPreSputterCyc: 2

SputterInterval: 3.000 s

SputterMode: alt

```

SampleRotation: off
DepthRecal: no
NoSpatialArea: 1
SpatialAreaDef: 1 Full 1 (0.0 0.0 0.0 0.0 0.0)
EOFH
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```

### Software Version 5: XPS V1.3.6

- Example. sputter depth profile with 7 sputter steps (step width: 60 s, from 0 to 360) and 5 regions: Cu 2p, Ni 2p, Ti 2p, O 1s, Si 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V5-XPS V1.3.6.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
FileDesc: TiNiCu 50 nm. Neut OFF. Sputt 2kV1x1. 2min interval
SoftwareVersion: XPS V1.3.6
InstrumentModel: PHI Model 5000
Institution:
FileDate: 2011 08 15
AcqFileDate: 2011 08 15
AcqFilename: D:\Data\Dennis Koenig\August 2011\TiNiCu_50nm_0001.pdt
Operator:
ExperimentID:
PlatenID:
PlatenDesc:
StagePosition: 9.249 -23.414 16.765 44.997 -177.750
SampleID:
SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Al 1486.6 mono
XrayPower: 50.4W
XrayBeamDiameter: 200.0 um
NeutralizerEnergy: 1.0 eV
NeutralizerCurrent: 20.0 mA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20 sr
AnalyserMode: FAT
AnalyserWorkFcn: 4.1 eV
LensConstant: 1
IntensityRecal: no
IntensityCalCoeff: 78.606 0.454
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 2.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 1000.0 1000.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 5
SpectralRegDef: 1 1 Cu2p 29 391 -0.100 965.000 926.000 965.000 926.000 0.750
23.50 AREA
SpectralRegDef: 2 2 Ni2p 28 431 -0.100 888.000 845.000 888.000 845.000 0.750
23.50 AREA
SpectralRegDef: 3 3 Ti2p 22 231 -0.100 471.000 448.000 471.000 448.000 0.750
23.50 AREA
SpectralRegDef: 4 4 O1s 8 161 -0.100 540.000 524.000 540.000 524.000 0.750 23.50
AREA
SpectralRegDef: 5 5 Si2p 14 181 -0.100 112.000 94.000 112.000 94.000 0.750 23.50
AREA

```

```

NoDPDataCyc: 7
NoPreSputterCyc: 1
SputterInterval: 60.000 s
SputterMode: alt
SampleRotation: off
DepthRecal: no
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDesc: 1
EOFH
□ □ □ □ □ □ □ □ □ □ cyc reg s
f8 □ □ ° □ □ □ □ □ □ □ □ □ □ cyc reg
c/s * eV f8 □ □ È □ □ □ □ □ □ □ □ # □ □ □ chn
...

```

### Software Version 6: SS 2.6.1.2

- Example of 1 regions: survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V6-SS-2.6.1.2.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
FileDesc: 25nm-Si
SoftwareVersion: SS 2.6.1.2
InstrumentModel: PHI VersaProbe II
AcqFilename: G:\Datafiles\ASKim\20150625-GCIB test\Temp20kV.2+1_1.pro
FileDate: 2015 6 25
AcqFileDate: 2015 6 25
Institution: KRISS
Operator: Ansoon Kim
ExperimentID: 20150625-GCIB test
EnergyReference: none 0.0
AnalyserWorkFcn: 4.435 eV
AnalyserRetardGain: 1.000087
PlatenID: 25nm-Si
PhotoFilename: 20kV.1.pho
SXIFilename:
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
IntensityRecal: no
IntensityCalCoeff: 82.808 0.246
EnergyRecal: no
ScanDeflectionSpan: 40 60
ScanDeflectionOffset: 0 0
SCAMultiplierVoltage: 1750.0 V
NarrowAcceptanceAngle: no
PeakToNoiseRatioState: no
DelayBeforeAcquire: 5 seconds
C60IonGun: None
BiasBoxMode: 0
SemFieldOfView: 0.000000
ImageSizeXY: 0.0000 0.0000
IonGunMode: Neutralize
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 0.110 kV
FloatVolt: -100.0 V
FloatEnable: yes
GridVolt: 120.0
CondensorVolt: 68.97
ObjectiveVolt: 101.31
BendVolt: 2.08
SputterRaster: 0.00 0.00 mm

```

SputterRasterOffset: 0.390 0.520 mm  
TargetSputterTime: 2.0 min  
SputterEmission: 7.00 mA  
DeflectionBias: 70.0 V  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvTimePerStep: 20.000000  
NoDPDataCyc: 72  
NoPreSputterCyc: 2  
ProfSputterDelay: 0.0  
ProfXrayOffDuringSputter: no  
ProfSourceBlankDuringSputter: no  
ProfZalarHighAccuracyInterval: 20  
SampleRotation: off  
DepthRecal: no  
SputterMode: AlternatingZalar  
NoDepthReg: 2  
DepthCalDef: 1 Layer1 1 0.0000 0.0000 Ar+ 150.00 2.50 60 '20kV' 20.000 150.0  
20.0 25.0 4.10 43.50 75.10 -7.00 -407.00 2.0 2.0 1.70 2.40 650.00 GCIB  
DepthCalDef: 2 Layer2 61 0.0000 0.0000 Ar+ 20.00 2.00 10 'PREVIOUS' 3.000 120  
7.00 0 0 2040 2049 36 2.0 2.0 0.19 0.21 0.00 0.00 Ar  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 1880 2005  
PhotoOffsetInPixel: 788 83  
PhotoSizeInMm: 56.129 59.691  
PhotoOffsetInMm: 0.015 0.015  
NoSpectralRegFull: 3  
SpectralRegDefFull: 1 1 Si2p 14 161 -0.1250 109.0000 89.0000 108.0000 90.0000  
0.000000 117.40 AREA  
SpectralRegDef2Full: 1 20.0 2 0 1 1  
SpectralRegBackgroundFull: 1 0.0 99.0 0.0  
SpectralRegHeroFull: 1 99.0 0.0 0.0 0.00  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
SpectralRegDefFull: 2 1 O1s 8 121 -0.1250 540.0000 525.0000 539.0000 526.0000  
0.000000 117.40 AREA  
SpectralRegDef2Full: 2 15.0 2 0 1 1  
SpectralRegBackgroundFull: 2 0.0 532.5 0.0  
SpectralRegHeroFull: 2 532.5 0.0 0.0 0.00  
SpectralRegIRFull: 2 0 0.000 0.000 0.0  
SpectralRegDefFull: 3 1 C1s 6 121 -0.1250 293.0000 278.0000 292.0000 279.0000  
0.000000 117.40 AREA  
SpectralRegDef2Full: 3 15.0 2 0 1 1  
SpectralRegBackgroundFull: 3 0.0 285.5 0.0  
SpectralRegHeroFull: 3 285.5 0.0 0.0 0.00  
SpectralRegIRFull: 3 0 0.000 0.000 0.0  
NoSpectralReg: 3  
SpectralRegDef: 1 1 Si2p 14 161 -0.1250 109.0000 89.0000 108.0000 90.0000  
0.040000 117.40 AREA  
SpectralRegDef2: 1 20.0 2 0 1 1  
SpectralRegBackground: 1 0.0 99.0 0.0  
SpectralRegHero: 1 99.0 0.0 0.0 0.00  
SpectralRegIR: 1 0 0.000 0.000 0.0  
SpectralRegDef: 2 1 O1s 8 121 -0.1250 540.0000 525.0000 539.0000 526.0000  
0.040000 117.40 AREA  
SpectralRegDef2: 2 15.0 2 0 1 1  
SpectralRegBackground: 2 0.0 532.5 0.0  
SpectralRegHero: 2 532.5 0.0 0.0 0.00  
SpectralRegIR: 2 0 0.000 0.000 0.0  
SpectralRegDef: 3 1 C1s 6 121 -0.1250 293.0000 278.0000 292.0000 279.0000  
0.040000 117.40 AREA  
SpectralRegDef2: 3 15.0 2 0 1 1  
SpectralRegBackground: 3 0.0 285.5 0.0  
SpectralRegHero: 3 285.5 0.0 0.0 0.00  
SpectralRegIR: 3 0 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 1 1 (900.0 3596.7 15893.6 45.0 -0.1)  
SpatialAreaDesc: 1

SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 1  
XrayPower: 49.04 W  
XrayBeamDiameter: 200.0 um  
XRayBeamVoltage: 15000.0 V  
XRayCondenserLensVoltage: 8000.0 V  
XRayObjectiveCoilCurrent: 0.718 A  
XRayBlankingVoltage: 280.0 V  
XRayFilamentCurrent: 1.604 A  
XRayStigmator: 0.0 0.0  
XRayHighPower: no  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: 34.8  
EgunNeutYSteering: -36.8  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
SxiPersistence: 1 V  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 410.0 eV  
SxiPassEnergy: 376 eV  
SxiLens2: -804 V  
SxiLens3: -761 V  
SxiLensBias: 0 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 410.0 V  
SxiDisplayMode: 2  
Detector Acq Time: 20.0 (min)  
Number Of Channels: 16  
Channel Info: 1 1 1.569  
Channel Info: 2 1 1.232  
Channel Info: 3 1 1.265  
Channel Info: 4 1 1.217  
Channel Info: 5 1 1.162  
Channel Info: 6 1 1.078  
Channel Info: 7 1 1.056  
Channel Info: 8 1 0.979  
Channel Info: 9 1 0.965  
Channel Info: 10 1 0.909  
Channel Info: 11 1 0.855  
Channel Info: 12 1 0.804  
Channel Info: 13 1 0.762  
Channel Info: 14 1 0.726  
Channel Info: 15 1 0.765  
Channel Info: 16 1 1.574  
StagePosition: 0.9371 -3.3933 15.8977 45.0062 -0.1500  
StageCurrentRotationSpeed: 1.0000  
DefectPosID: 1  
DefectPosComment:  
DefectPosU: 0.9045  
DefectPosV: -3.5956  
DefectPosX: 0.9371  
DefectPosY: -3.3933  
DefectPosZ: 15.8977  
DefectPosTilt: 45.0063  
DefectPosRotation: -0.1500  
DefectPosAligment: None  
DefectPosReferenceImage: 20kV.1.pho  
Deconvolution: no  
DeconvolutionPassEnergy: 2.95 eV  
XRaySetting: 200u50W15KV

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### Software Version 7: SS 2.5.0.9

- Example of 1 regions: survey
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V7-SS.2.5.0.9.PRO

SOFH  
 Platform: PC  
 Technique: XPS  
 FileType: SPECTRUM  
 FileDesc:  
 SoftwareVersion: SS 2.5.0.9  
 InstrumentModel: PHI VersaProbe II  
 AcqFilename: C:\ZCH\140420.14.7P APTES Toluol MP1.spe  
 FileDate: 2014 3 27  
 AcqFileDate: 2014 3 27  
 Institution: PHI  
 Operator:  
 ExperimentID: ZCH  
 EnergyReference: none 0.0  
 AnalyserWorkFcn: 4.132 eV  
 AnalyserRetardGain: 1.000186  
 PlatenID:  
 PhotoFilename: 140420.1.Low Mag.pho  
 SXIFilename:  
 SourceAnalyserAngle: 45.0 d  
 AnalyserSolidAngle: 20.0 sr  
 IntensityRecal: no  
 IntensityCalCoeff: 100.000 0.330  
 EnergyRecal: no  
 ScanDeflectionSpan: 50 70  
 ScanDeflectionOffset: 0 2  
 SCAMultiplierVoltage: 1700.0 V  
 NarrowAcceptanceAngle: no  
 PeakToNoiseRatioState: no  
 DelayBeforeAcquire: 5 seconds  
 C60IonGun: None  
 BiasBoxMode: 0  
 SemFieldOfView: 1400.000000  
 EBeamCurrent: -2.2 nA  
 ImageSizeXY: 1400.0000 200.0000  
 IonGunMode: Neutralize  
 SputterIon: Ar+  
 SputterCurrent: 0.000 uA  
 SputterRate: 0.000 A/min  
 SputterEnergy: 0.110 kV  
 FloatVolt: -100.0 V  
 FloatEnable: yes  
 GridVolt: 120.0  
 CondensorVolt: 69.30  
 ObjectiveVolt: 101.20  
 BendVolt: 1.43  
 SputterRaster: 0.00 0.00 mm  
 SputterRasterOffset: 1.950 -0.200 mm  
 TargetSputterTime: 10.0 min  
 SputterEmission: 7.00 mA  
 DeflectionBias: 71.0 V  
 XpsScanMode: scanned  
 AnalyserMode: FAT  
 SurvNumCycles: 15  
 SurvTimePerStep: 50.000000  
 PhotoZoomMode: Low Magnification  
 PhotoSizeInPixel: 2197 3136  
 PhotoOffsetInPixel: 1519 200

PhotoSizeInMm: 35.000 50.000  
PhotoOffsetInMm: -38.354 -50.000  
NoSpectralRegFull: 1  
SpectralRegDefFull: 1 1 survey 111 938 -0.8000 745.0000 -5.0000 744.0000 -4.0000  
0.000000 187.85 AREA  
SpectralRegDef2Full: 1 750.0 1 0 1 1  
SpectralRegBackgroundFull: 1 0.0 370.0 0.0  
SpectralRegHeroFull: 1 370.0 0.0 0.0 0.00  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
NoSpectralReg: 1  
SpectralRegDef: 1 1 survey 111 938 -0.8000 745.0000 -5.0000 744.0000 -4.0000  
0.750000 187.85 AREA  
SpectralRegDef2: 1 750.0 1 0 1 1  
SpectralRegBackground: 1 0.0 370.0 0.0  
SpectralRegHero: 1 370.0 0.0 0.0 0.00  
SpectralRegIR: 1 0 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 13 4 (8215.5 5905.4 19312.7 46.0 -90.1) (9615.5 5905.4 19312.7  
46.0 -90.1) (9615.5 6105.4 19312.7 46.0 -90.1) (8215.5 6105.4 19312.7 46.0 -  
90.1)  
SpatialAreaDesc: 1  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 1  
XrayPower: 92.65 W  
XrayBeamDiameter: 100.0 um  
XRayBeamVoltage: 20000.0 V  
XRayCondenserLensVoltage: 9250.0 V  
XRayObjectiveCoilCurrent: 0.929 A  
XRayBlankingVoltage: 400.0 V  
XRayFilamentCurrent: 1.621 A  
XRayStigmator: 0.0 0.0  
XRayHighPower: yes  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.01 V  
EgunNeutExtractor: 50.0 V  
EgunNeutXSteering: 2.0  
EgunNeutYSteering: 4.1  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
SxiPersistence: 1 V  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 534.0 eV  
SxiPassEnergy: 188 eV  
SxiLens2: -711 V  
SxiLens3: -673 V  
SxiLensBias: 0 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 342.0 V  
SxiDisplayMode: 1  
Detector Acq Time: 20.0 (min)  
Number Of Channels: 16  
Channel Info: 1 1 1.661  
Channel Info: 2 1 1.490  
Channel Info: 3 1 1.499  
Channel Info: 4 1 1.268  
Channel Info: 5 1 1.149  
Channel Info: 6 1 1.100  
Channel Info: 7 1 1.148  
Channel Info: 8 1 1.079  
Channel Info: 9 1 1.118  
Channel Info: 10 1 1.021  
Channel Info: 11 1 0.942



SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 0.110 kV  
FloatVolt: -100.0 V  
FloatEnable: yes  
GridVolt: 120.0  
CondensorVolt: 74.80  
ObjectiveVolt: 101.20  
BendVolt: 1.60  
SputterRaster: 0.00 0.00 mm  
SputterRasterOffset: 0.500 -0.150 mm  
TargetSputterTime: 1.0 min  
SputterEmission: 7.00 mA  
DeflectionBias: 71.0 V  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvTimePerStep: 100.000000  
NoDPDataCyc: 30  
NoPreSputterCyc: 0  
ProfSputterDelay: 5.0  
ProfXrayOffDuringSputter: no  
ProfSourceBlankDuringSputter: no  
ProfZalarHighAccuracyInterval: 20  
SampleRotation: off  
DepthRecal: no  
SputterMode: Alternating  
NoDepthReg: 1  
DepthCalDef: 1 Layer1 1 0.0000 0.0000 Ar+ 30.00 1.00 30 '500V3x3' 1.000 150  
15.00 -500 1 595 925 19 3.0 3.0 -3.01 -0.01 0.00 0.00 Ar  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 2197 3136  
PhotoOffsetInPixel: 1519 200  
PhotoSizeInMm: 35.000 50.000  
PhotoOffsetInMm: 0.008 0.008  
NoSpectralRegFull: 4  
SpectralRegDefFull: 1 1 Sc2p 21 401 -0.0500 410.0000 390.0000 409.0000 391.0000  
0.000000 11.75 AREA  
SpectralRegDef2Full: 1 20.0 5 0 6 1  
SpectralRegBackgroundFull: 1 0.0 400.0 0.0  
SpectralRegHeroFull: 1 400.0 0.0 0.0 0.00  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
SpectralRegDefFull: 2 1 O1s 8 141 -0.1000 537.0000 523.0000 536.0000 524.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 2 14.0 2 0 6 1  
SpectralRegBackgroundFull: 2 0.0 530.0 0.0  
SpectralRegHeroFull: 2 530.0 0.0 0.0 0.00  
SpectralRegIRFull: 2 0 0.000 0.000 0.0  
SpectralRegDefFull: 3 1 Ga3d 31 201 -0.1000 34.0000 14.0000 33.0000 15.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 3 20.0 3 0 6 1  
SpectralRegBackgroundFull: 3 0.0 24.0 0.0  
SpectralRegHeroFull: 3 24.0 0.0 0.0 0.00  
SpectralRegIRFull: 3 0 0.000 0.000 0.0  
SpectralRegDefFull: 4 1 Gd4d 64 351 -0.1000 167.0000 132.0000 166.0000 133.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 4 35.0 3 0 6 1  
SpectralRegBackgroundFull: 4 0.0 149.5 0.0  
SpectralRegHeroFull: 4 149.5 0.0 0.0 0.00  
SpectralRegIRFull: 4 0 0.000 0.000 0.0  
NoSpectralReg: 4  
SpectralRegDef: 1 1 Sc2p 21 401 -0.0500 410.0000 390.0000 409.0000 391.0000  
3.000000 11.75 AREA  
SpectralRegDef2: 1 20.0 5 0 6 1  
SpectralRegBackground: 1 0.0 400.0 0.0  
SpectralRegHero: 1 400.0 0.0 0.0 0.00  
SpectralRegIR: 1 0 0.000 0.000 0.0

SpectralRegDef: 2 1 O1s 8 141 -0.1000 537.0000 523.0000 536.0000 524.0000  
1.200000 23.50 AREA  
SpectralRegDef2: 2 14.0 2 0 6 1  
SpectralRegBackground: 2 0.0 530.0 0.0  
SpectralRegHero: 2 530.0 0.0 0.0 0.00  
SpectralRegIR: 2 0 0.000 0.000 0.0  
SpectralRegDef: 3 1 Ga3d 31 201 -0.1000 34.0000 14.0000 33.0000 15.0000 1.800000  
23.50 AREA  
SpectralRegDef2: 3 20.0 3 0 6 1  
SpectralRegBackground: 3 0.0 24.0 0.0  
SpectralRegHero: 3 24.0 0.0 0.0 0.00  
SpectralRegIR: 3 0 0.000 0.000 0.0  
SpectralRegDef: 4 1 Gd4d 64 351 -0.1000 167.0000 132.0000 166.0000 133.0000  
1.800000 23.50 AREA  
SpectralRegDef2: 4 35.0 3 0 6 1  
SpectralRegBackground: 4 0.0 149.5 0.0  
SpectralRegHero: 4 149.5 0.0 0.0 0.00  
SpectralRegIR: 4 0 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 1 4 (4058.7 -1.0 18872.0 45.0 -90.1) (5458.7 -1.0 18872.0 45.0  
-90.1) (5458.7 199.0 18872.0 45.0 -90.1) (4058.7 199.0 18872.0 45.0 -90.1)  
SpatialAreaDesc: 1  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 6  
XrayPower: 99.17 W  
XrayBeamDiameter: 100.0 um  
XrayBeamVoltage: 20000.0 V  
XrayCondenserLensVoltage: 9750.0 V  
XrayObjectiveCoilCurrent: 0.945 A  
XrayBlankingVoltage: 470.0 V  
XrayFilamentCurrent: 1.699 A  
XrayStigmator: 0.0 0.0  
XrayHighPower: yes  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: -11.0  
EgunNeutYSteering: -6.0  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
SxiPersistence: 1  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 531.0 eV  
SxiPassEnergy: 376 eV  
SxiLens2: -713 V  
SxiLens3: -675 V  
SxiLensBias: 0 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 350.0 V  
SxiDisplayMode: 2  
Detector Acq Time: 50.0 (min)  
Number Of Channels: 16  
Channel Info: 1 1 1.541  
Channel Info: 2 1 1.377  
Channel Info: 3 1 1.296  
Channel Info: 4 1 1.178  
Channel Info: 5 1 1.110  
Channel Info: 6 1 1.021  
Channel Info: 7 1 0.991  
Channel Info: 8 1 0.996  
Channel Info: 9 1 0.999  
Channel Info: 10 1 0.989

```

Channel Info: 11 1 0.748
Channel Info: 12 1 0.886
Channel Info: 13 1 0.816
Channel Info: 14 1 0.735
Channel Info: 15 1 0.779
Channel Info: 16 1 1.312
StagePosition: -0.1024 -4.4896 18.8720 45.0062 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 1
DefectPosComment:
DefectPosU: 4.7587
DefectPosV: -0.0990
DefectPosX: -0.1024
DefectPosY: -4.4895
DefectPosZ: 18.8720
DefectPosTilt: 45.0031
DefectPosRotation: -90.0500
DefectPosAlignment: None
DefectPosReferenceImage: 160987.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 100u100W20kV_HP
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### Software Version 9: SS 3.9.1.5

- Example. sputter depth profile with 32 sputter steps (32 steps) and one survey region per step
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V9-SS 3.9.1.5.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
FileDesc: Referenzmessungen.35 nm MgF2 / 30 nm LaF3 / 35 nm MgF2 / SiO2 (Quarz)
SoftwareVersion: SS 3.9.1.5
InstrumentModel: PHI Quantera SXM
AcqFilename:
C:\Messdaten\2018\0_Referenzmessungen\TempReferenzmessungen.103.Quarz_1.pro
FileDate: 2018 10 12
AcqFileDate: 2018 10 12
Institution: PHI
Operator:
ExperimentID: 1
EnergyReference: none 0.0
AnalyserWorkFcn: 4.075 eV
AnalyserRetardGain: 0.999938
PlatenID: Referenzmessungen
PlatenDesc:
PhotoFilename: Referenzmessungen.101.Std Photo.pho
SXIFilename:
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 0.38 sr
IntensityRecal: no
IntensityCalCoeff: 13.947 0.139
EnergyRecal: no
ScanDeflectionSpan: 85 71
ScanDeflectionOffset: 35 -21
SCAMultiplierVoltage: 1850.0 V
NarrowAcceptanceAngle: no
PeakToNoiseRatioState: yes
DelayBeforeAcquire: 10 seconds
C60IonGun: None
TFParameters: 0, 1, 2, 93.73, 7.481, 1, 1
SemFieldOfView: 0.0000000
ImageSizeXY: 0.0000 0.0000
IonGunMode: Neutralize

```

SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 4.000 kV  
FloatVolt: 0.0 V  
FloatEnable: no  
GridVolt: 170.0  
CondensorVolt: 2796.00  
ObjectiveVolt: 2976.00  
BendVolt: 157.20  
SputterRaster: 2.50 2.50 mm  
SputterRasterOffset: 0.640 -0.080 mm  
TargetSputterTime: 0.2 min  
SputterEmission: 15.00 mA  
DeflectionBias: 0.0 V  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvTimePerStep: 10.000000  
NoDPDataCyc: 37  
NoPreSputterCyc: 1  
ProfSputterDelay: 5.0  
ProfXrayOffDuringSputter: no  
ProfSourceBlankDuringSputter: no  
ProfZalarHighAccuracyInterval: 20  
SampleRotation: off  
DepthRecal: no  
SputterMode: Alternating  
NoDepthReg: 2  
DepthCalDef: 1 Layer2 1 0.0000 0.0000 Ar+ 0.20 0.20 1 '4KV\_Base' 4.000 170 15.00  
0 0 2796 2976 157 2.5 2.5 0.64 -0.08 0.00 0.00 Ar  
DepthCalDef: 2 Layer2 2 0.0000 0.0000 Ar+ 15.00 0.30 50 'PREVIOUS' 4.000 170  
15.00 0 0 2796 2976 157 2.5 2.5 0.64 -0.08 0.00 0.00 Ar  
NoSpectralRegFull: 1  
SpectralRegDefFull: 1 1 Sur -1 2751 -0.4000 1106.2000 6.2000 1105.2000 7.2000  
0.000000 112.00 HEIGHT  
SpectralRegDef2Full: 1 1100.0 15 0 1 400  
SpectralRegBackgroundFull: 1 0.0 556.2 0.0  
SpectralRegHeroFull: 1 556.2 0.0 0.0 0.0  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
NoSpectralReg: 1  
SpectralRegDef: 1 1 Sur -1 2751 -0.4000 1106.2000 6.2000 1105.2000 7.2000  
0.150000 112.00 HEIGHT  
SpectralRegDef2: 1 1100.0 15 0 1 400  
SpectralRegBackground: 1 0.0 556.2 0.0  
SpectralRegHero: 1 556.2 0.0 0.0 0.0  
SpectralRegIR: 1 1 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 Point1 1 (8587.6 23526.6 18521.0 45.0 359.9)  
SpatialAreaDesc: 1 35 nm MgF2 / 30 nm LaF3 / 35 nm MgF2 / SiO2 (Quarz)  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 10  
XrayPower: 26.54 W  
XrayBeamDiameter: 96.6 um  
XrayBeamVoltage: 15000.0 V  
XrayCondenserLensVoltage: 8450.0 V  
XrayObjectiveCoilCurrent: 0.820 A  
XrayBlankingVoltage: 310.0 V  
XrayFilamentCurrent: 1.450 A  
XrayStigmator: -0.1 0.0  
XrayOffsetInUm: 50 -50  
XrayMagFactor: 0.360 0.358  
XrayDelayFactor: 1000 2000  
XrayRotationInDeg: -20.50 V  
XrayHighPower: no  
XrayEmissionControl: yes  
XrayEmissionCurrent: 4.000 mA

```
XRayStepDelayReadBeam: 5
XRayStepsPerDiameter: 1.0
XRayInterlaceInterval: 1
XRayMaxFilamentCurrent: 1.650 A
XRaySetting: 100u25W15KV
EgunNeutMode: Neutralize
NeutralizerCurrent: 20.0 uA
NeutralizerEnergy: 1.10 V
EgunNeutExtractor: 45.0 V
EgunNeutXSteering: 2.8
EgunNeutYSteering: 0.3
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
EgunNeutPulseFrequency: 30
SxiPersistence: 1
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.60
SxiBindingEnergy: 1458.0 eV
SxiPassEnergy: 280 eV
SxiLens2: 476 V
SxiLens3: 406 V
SxiLens4: -250 V
SxiLens5: 0 V
SxiRotator: 0.75 A
SxiLensBias: 200 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 200.0 V
SxiDisplayMode: 2
Detector Acq Time: 30.0 (min)
Number Of Channels: 32
Channel Info: 1 1 1.158
Channel Info: 2 1 1.081
Channel Info: 3 1 1.074
Channel Info: 4 1 1.039
Channel Info: 5 1 1.097
Channel Info: 6 1 1.085
Channel Info: 7 1 1.090
Channel Info: 8 1 1.092
Channel Info: 9 1 1.082
Channel Info: 10 1 1.072
Channel Info: 11 1 1.046
Channel Info: 12 1 1.019
Channel Info: 13 1 1.030
Channel Info: 14 1 1.011
Channel Info: 15 1 1.021
Channel Info: 16 1 1.015
Channel Info: 17 1 1.006
Channel Info: 18 1 0.982
Channel Info: 19 1 0.992
Channel Info: 20 1 0.977
Channel Info: 21 1 0.960
Channel Info: 22 1 0.965
Channel Info: 23 1 0.952
Channel Info: 24 1 0.938
Channel Info: 25 1 0.941
Channel Info: 26 1 0.929
Channel Info: 27 1 0.910
Channel Info: 28 1 0.899
Channel Info: 29 1 0.910
Channel Info: 30 1 0.911
Channel Info: 31 1 0.955
Channel Info: 32 1 0.907
StagePosition: 9.3693 -22.6066 18.5206 45.0031 359.9401
StageCurrentRotationSpeed: 2.0000
DefectPosID: 1
```

DefectPosName: Quarz  
 DefectPosComment: 35 nm MgF2 / 30 nm LaF3 / 35 nm MgF2 / SiO2 (Quarz)  
 DefectPosU: 8.5876  
 DefectPosV: -23.5266  
 DefectPosX: 9.3693  
 DefectPosY: -22.6066  
 DefectPosZ: 18.5206  
 DefectPosTilt: 45.0031  
 DefectPosRotation: 359.9401  
 DefectPosAlignment: Standard  
 DefectPosReferenceImage: Referenzmessungen.101.Std Photo.pho  
 Deconvolution: no  
 DeconvolutionPassEnergy: 13.00 eV  
 AutoEGunNeut: yes  
 AutoEGunNeutSetting: E-Neut  
 AutoIonNeut: yes  
 AutoIonNeutSetting: I-Neut  
 AutoZAlign: no  
 AutoZAlignSetting: 100u25W15KV  
 AutoZAlignHPSetting: 100u100W20KV\_HP  
 Presputter: no  
 PresputterSetting: 2KV3x3  
 PresputterTime: 2.00 (min)  
 AutoBeamPark: no  
 AutoBeamParkSetting: Park\_20u4.5W15KV  
 EOFH

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### Software Version 10: SS 3.10.2.1

- Example. sputter depth profile with 27 sputter steps, 2 regions: O 1s, Si 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.PRO)\PHI-Profile-V10-SS-3.10.2.1.PRO

SOFH  
 Platform: PC  
 Technique: XPS  
 TechniqueEx: AES  
 FileType: DEPTHPRO  
 FileDesc: SiO2 6 (15 nm).2kV 1x1 mit 1/0,2 min, 03.03.22  
 SoftwareVersion: SS 3.10.2.1  
 InstrumentModel: PHI Quantera SXM  
 AcqFilename:  
 C:\Messdaten\Geraeteueberpruefung\2022\2022\_02\TempFaraday2.121.SiO2 6 (15 nm)\_1.pro  
 FileDate: 2022 3 3  
 AcqFileDate: 2022 3 3  
 Institution: PHI  
 Operator:  
 ExperimentID: 1  
 EnergyReference: none 0.0  
 AnalyserWorkFcn: 3.825 eV  
 AnalyserRetardGain: 0.999426  
 PlatenID: Faraday2  
 PlatenDesc:  
 PhotoFilename: Faraday2.101.Std Photo.pho  
 SXIFilename:  
 SourceAnalyserAngle: 45.0 d  
 AnalyserSolidAngle: 0.38 sr  
 IntensityRecal: no  
 IntensityCalCoeff: 27.040 0.169  
 EnergyRecal: no  
 ScanDeflectionSpan: 100 60  
 ScanDeflectionOffset: 33 -3  
 SCAMultiplierVoltage: 1890.0 V  
 NarrowAcceptanceAngle: no  
 PeakToNoiseRatioState: no  
 DelayBeforeAcquire: 2 seconds

```
C60IonGun: None
TFParameters: 0, 1, 2, 93.73, 7.481, 1, 1
SemFieldOfView: 0.0000000
ImageSizeXY: 0.0000 0.0000
IonGunMode: Neutralize
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 2.000 kV
FloatVolt: 0.0 V
FloatEnable: no
GridVolt: 150.0
CondensorVolt: 1596.00
ObjectiveVolt: 1458.00
BendVolt: -68.80
SputterRaster: 1.70 1.70 mm
SputterRasterOffset: -0.320 0.040 mm
TargetSputterTime: 1.0 min
SputterEmission: 15.00 mA
DeflectionBias: 0.0 V
IonGunGasPressure: 0.000 mPa
XpsScanMode: scanned
AnalyserMode: FAT
SurvTimePerStep: 50.000000
NoDPDataCyc: 27
NoPreSputterCyc: 1
ProfSputterDelay: 5.0
ProfXrayOffDuringSputter: no
ProfSourceBlankDuringSputter: no
ProfZalarHighAccuracyInterval: 20
SampleRotation: off
DepthRecal: no
SputterMode: Alternating
NoDepthReg: 1
DepthCalDef: 1 Layer2 1 0.0000 0.0000 Ar+ 6.00 0.20 30 '2KV1x1_SGS_80nA' 2.000
150 15.00 0 0 1596 1458 -69 1.7 1.7 -0.32 0.04 0.00 0.00 Ar
NoSpectralRegFull: 2
SpectralRegDefFull: 1 1 O1s 8 201 -0.1000 544.0000 524.0000 543.0000 525.0000
0.000000 26.00 HEIGHT
SpectralRegDef2Full: 1 20.0 2 0 1 350
SpectralRegBackgroundFull: 1 0.0 534.0 0.0
SpectralRegHeroFull: 1 534.0 0.0 0.0 0.00
SpectralRegIRFull: 1 0 0.000 0.000 0.0
SpectralRegDefFull: 2 1 Si2p 14 151 -0.1000 107.0000 92.0000 106.0000 93.0000
0.000000 26.00 HEIGHT
SpectralRegDef2Full: 2 15.0 2 0 1 350
SpectralRegBackgroundFull: 2 0.0 99.5 0.0
SpectralRegHeroFull: 2 99.5 0.0 0.0 0.00
SpectralRegIRFull: 2 0 0.000 0.000 0.0
NoSpectralReg: 2
SpectralRegDef: 1 1 O1s 8 201 -0.1000 544.0000 524.0000 543.0000 525.0000
0.100000 26.00 HEIGHT
SpectralRegDef2: 1 20.0 2 0 1 350
SpectralRegBackground: 1 0.0 534.0 0.0
SpectralRegHero: 1 534.0 0.0 0.0 0.00
SpectralRegIR: 1 1 0.000 0.000 0.0
SpectralRegDef: 2 1 Si2p 14 151 -0.1000 107.0000 92.0000 106.0000 93.0000
0.100000 26.00 HEIGHT
SpectralRegDef2: 2 15.0 2 0 1 350
SpectralRegBackground: 2 0.0 99.5 0.0
SpectralRegHero: 2 99.5 0.0 0.0 0.00
SpectralRegIR: 2 1 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 Point11 1 (30701.3 -3914.0 24444.0 45.0 360.0)
SpatialAreaDesc: 1 2kV 1x1 mit 1/0,2 min, 03.03.22
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
```

XrayAnodePosition: 0  
XrayPower: 43.82 W  
XrayBeamDiameter: 200.0 um  
XrayBeamVoltage: 15000.0 V  
XrayCondenserLensVoltage: 7600.0 V  
XrayObjectiveCoilCurrent: 0.736 A  
XrayBlankingVoltage: 300.0 V  
XrayFilamentCurrent: 1.613 A  
XrayStigmator: -0.1 0.0  
XrayOffsetInUm: -20 -30  
XrayMagFactor: 0.330 0.330  
XrayDelayFactor: 1000 2000  
XrayRotationInDeg: -21.00 V  
XrayHighPower: no  
XrayEmissionControl: yes  
XrayEmissionCurrent: 4.000 mA  
XrayStepDelayReadBeam: 5  
XrayStepsPerDiameter: 1.0  
XrayInterlaceInterval: 1  
XrayMaxFilamentCurrent: 1.700 A  
XraySetting: 200u50W15KV  
EgunNeutMode: Neutralize  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: -14.0  
EgunNeutYSteering: -14.2  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
EgunNeutPulseFrequency: 30  
SxiPersistence: 1  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.60  
SxiBindingEnergy: 1458.0 eV  
SxiPassEnergy: 280 eV  
SxiLens2: 476 V  
SxiLens3: 406 V  
SxiLens4: -250 V  
SxiLens5: 0 V  
SxiRotator: 0.75 A  
SxiLensBias: 200 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 200.0 V  
SxiDisplayMode: 2  
Detector Acq Time: 30.0 (min)  
Number Of Channels: 32  
Channel Info: 1 1 1.253  
Channel Info: 2 1 1.147  
Channel Info: 3 1 1.145  
Channel Info: 4 1 1.080  
Channel Info: 5 1 1.133  
Channel Info: 6 1 1.115  
Channel Info: 7 1 1.133  
Channel Info: 8 1 1.111  
Channel Info: 9 1 1.105  
Channel Info: 10 1 1.097  
Channel Info: 11 1 1.056  
Channel Info: 12 1 1.017  
Channel Info: 13 1 1.029  
Channel Info: 14 1 1.019  
Channel Info: 15 1 1.020  
Channel Info: 16 1 1.009  
Channel Info: 17 1 1.005  
Channel Info: 18 1 0.968  
Channel Info: 19 1 0.984

```

Channel Info: 20 1 0.966
Channel Info: 21 1 0.964
Channel Info: 22 1 0.954
Channel Info: 23 1 0.967
Channel Info: 24 1 0.917
Channel Info: 25 1 0.933
Channel Info: 26 1 0.912
Channel Info: 27 1 0.907
Channel Info: 28 1 0.862
Channel Info: 29 1 0.879
Channel Info: 30 1 0.866
Channel Info: 31 1 0.906
Channel Info: 32 1 0.847
StagePosition: 30.3196 5.1688 24.4505 45.0000 359.9623
StageCurrentRotationSpeed: 0.5000
DefectPosID: 11
DefectPosName: SiO2 6 (15 nm)
DefectPosComment: 2kV 1x1 mit 1/0,2 min, 03.03.22
DefectPosU: 30.7012
DefectPosV: 3.9120
DefectPosX: 30.3196
DefectPosY: 5.1688
DefectPosZ: 24.4505
DefectPosTilt: 45.0000
DefectPosRotation: 359.9623
DefectPosAlignment: Standard
DefectPosReferenceImage: Faraday2.101.Std Photo.pho
Deconvolution: no
DeconvolutionPassEnergy: 13.00 eV
AutoEGunNeut: yes
AutoEGunNeutSetting: E-Neut
AutoIonNeut: yes
AutoIonNeutSetting: I-Neut
AutoZAlign: no
AutoZAlignSetting: 100u25W15KV
AutoZAlignHPSetting: 100u100W20KV_HP
Presputter: no
PresputterTime: 1.00 (min)
AutoBeamPark: no
AutoBeamParkSetting: Park_20u4.5W15KV
EOFH
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```

### 3.1.20.3 PHI Spectrometer/Angle Resolved Profile (\*.ang)

Comment:

- With respect to the multi region files (\*.spe) the header contains additional profile information (e.g. angle values)

#### Software Version 1: SS 2.1.0.1

- Example. angle resolved measurement with 15 angles (angle steps: 5°, 15°...85°) and 6 regions: Si 2p, Ti 2p, O 1s, Hf 4f, Ni 2p<sub>3/2</sub>, Al 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.ANG)\PHI-Profile-V1-SS 2.1.0.1.ANG

```

SOFH
Platform: PC
Technique: XPS
FileType: ANGLEPRO
FileDesc:
SoftwareVersion: SS 2.1.0.1
InstrumentModel: PHI VersaProbe II

```

AcqFilename: C:\ZCH\120749\Temp120749.23.AN20120601C01\_1\_1.ang  
FileDate: 2012 11 14  
AcqFileDate: 2012 11 14  
Institution: PHI  
Operator:  
ExperimentID: 120749  
EnergyReference: none 0.0  
AnalyserWorkFcn: 4.218 eV  
AnalyserRetardGain: 1.000207  
PlatenID:  
PhotoFilename: 120749.17.Low Mag.pho  
SXIFilename:  
SourceAnalyserAngle: 45.0 d  
AnalyserSolidAngle: 20.0 sr  
IntensityRecal: no  
IntensityCalCoeff: 100.000 0.204  
EnergyRecal: no  
ScanDeflectionSpan: 50 70  
ScanDeflectionOffset: 0 -20  
SCAMultiplierVoltage: 1650.0 V  
NarrowAcceptanceAngle: yes  
PeakToNoiseRatioState: no  
DelayBeforeAcquire: 5 seconds  
C60IonGun: None  
BiasBoxMode: 0  
SemFieldOfView: 0.0000000  
EBeamCurrent: 0.0 nA  
ImageSizeXY: 0.0000 0.0000  
IonGunMode: Off  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 4.000 kV  
FloatVolt: 0.0 V  
FloatEnable: no  
GridVolt: 150.0  
CondensorVolt: 2780.00  
ObjectiveVolt: 2688.00  
BendVolt: 52.00  
SputterRaster: 3.00 3.00 mm  
SputterRasterOffset: -0.810 -0.310 mm  
TargetSputterTime: 2.0 min  
SputterEmission: 0.00 mA  
DeflectionBias: 0.0 V  
XpsScanMode: scanned  
AnalyserMode: FAT  
SurvNumCycles: 15  
SurvTimePerStep: 50.000000  
NoPolarAngles: 15  
PolarAngles: 15.0 20.0 25.0 30.0 35.0 40.0 45.0 50.0 55.0 60.0 65.0 70.0 75.0  
80.0 85.0  
PolarAngleCycles: 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 2197 3136  
PhotoOffsetInPixel: 1519 200  
PhotoSizeInMm: 35.000 50.000  
PhotoOffsetInMm: 0.008 0.008  
NoSpectralRegFull: 7  
SpectralRegDefFull: 1 1 Si2p 14 76 -0.2000 110.0000 95.0000 109.0000 96.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 1 15.0 20 0 6 1  
SpectralRegBackgroundFull: 1 0.0 102.5 0.0  
SpectralRegHeroFull: 1 102.5 0.0 0.0 0.00  
SpectralRegDefFull: 2 1 Ti2p 22 101 -0.2000 468.0000 448.0000 467.0000 449.0000  
0.000000 23.50 AREA  
SpectralRegDef2Full: 2 20.0 25 0 6 1  
SpectralRegBackgroundFull: 2 0.0 458.0 0.0

```
SpectralRegHeroFull: 2 458.0 0.0 0.0 0.00
SpectralRegDefFull: 3 1 O1s 8 61 -0.2000 539.0000 527.0000 538.0000 528.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 3 12.0 10 0 6 1
SpectralRegBackgroundFull: 3 0.0 533.0 0.0
SpectralRegHeroFull: 3 533.0 0.0 0.0 0.00
SpectralRegDefFull: 4 0 N1s 7 61 -0.2000 405.0000 393.0000 404.0000 394.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 4 12.0 20 0 6 1
SpectralRegBackgroundFull: 4 0.0 399.0 0.0
SpectralRegHeroFull: 4 399.0 0.0 0.0 0.00
SpectralRegDefFull: 5 1 Hf4f 72 86 -0.2000 26.0000 9.0000 25.0000 10.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 5 17.0 25 0 6 1
SpectralRegBackgroundFull: 5 0.0 17.5 0.0
SpectralRegHeroFull: 5 17.5 0.0 0.0 0.00
SpectralRegDefFull: 6 1 Ni2p3 28 86 -0.2000 865.0000 848.0000 864.0000 849.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 6 17.0 10 0 6 1
SpectralRegBackgroundFull: 6 0.0 856.5 0.0
SpectralRegHeroFull: 6 856.5 0.0 0.0 0.00
SpectralRegDefFull: 7 1 Al2p 13 76 -0.2000 83.0000 68.0000 82.0000 69.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 7 15.0 10 0 6 1
SpectralRegBackgroundFull: 7 0.0 75.5 0.0
SpectralRegHeroFull: 7 75.5 0.0 0.0 0.00
NoSpectralReg: 6
SpectralRegDef: 1 1 Si2p 14 76 -0.2000 110.0000 95.0000 109.0000 96.0000
6.000000 23.50 AREA
SpectralRegDef2: 1 15.0 20 0 6 1 0.00
SpectralRegBackground: 1 0.0 102.5 0.0
SpectralRegHero: 1 102.5 0.0 0.0 0.00
SpectralRegDef: 2 1 Ti2p 22 101 -0.2000 468.0000 448.0000 467.0000 449.0000
7.500000 23.50 AREA
SpectralRegDef2: 2 20.0 25 0 6 1 0.00
SpectralRegBackground: 2 0.0 458.0 0.0
SpectralRegHero: 2 458.0 0.0 0.0 0.00
SpectralRegDef: 3 1 O1s 8 61 -0.2000 539.0000 527.0000 538.0000 528.0000
3.000000 23.50 AREA
SpectralRegDef2: 3 12.0 10 0 6 1 0.00
SpectralRegBackground: 3 0.0 533.0 0.0
SpectralRegHero: 3 533.0 0.0 0.0 0.00
SpectralRegDef: 4 1 Hf4f 72 86 -0.2000 26.0000 9.0000 25.0000 10.0000 7.500000
23.50 AREA
SpectralRegDef2: 4 17.0 25 0 6 1 0.00
SpectralRegBackground: 4 0.0 17.5 0.0
SpectralRegHero: 4 17.5 0.0 0.0 0.00
SpectralRegDef: 5 1 Ni2p3 28 86 -0.2000 865.0000 848.0000 864.0000 849.0000
3.000000 23.50 AREA
SpectralRegDef2: 5 17.0 10 0 6 1 0.00
SpectralRegBackground: 5 0.0 856.5 0.0
SpectralRegHero: 5 856.5 0.0 0.0 0.00
SpectralRegDef: 6 1 Al2p 13 76 -0.2000 83.0000 68.0000 82.0000 69.0000 3.000000
23.50 AREA
SpectralRegDef2: 6 15.0 10 0 6 1 0.00
SpectralRegBackground: 6 0.0 75.5 0.0
SpectralRegHero: 6 75.5 0.0 0.0 0.00
NoSpatialArea: 1
SpatialAreaDef: 1 2 1 (-7006.4 -3844.4 12719.4 45.0 -0.1)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 0
XrayPower: 25.61 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 15000.0 V
XRayCondenserLensVoltage: 8230.0 V
```



- Example. angle resolved measurement with 3 angles and 8 regions: C 1s, O 1s, N 1s, P 2p, Si 2p, Al 2p, Ti 2p<sub>3/2</sub>, Cl 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.ANG)\PHI-Profile-V3-XPS V1.20.ANG

SOFH  
Platform: PC  
Technique: XPS  
FileType: ANGLEPRO  
FileDesc: Probe 3 Wafer Kammstrukturen  
SoftwareVersion: XPS V1.20  
InstrumentModel: PHI Model 5000  
Institution:  
FileDate: 2008 10 09  
AcqFileDate: 2008 10 09  
AcqFilename: D:\Lyapin\Data\DEMOS\2008\_09\_18\080918\_0028.pdt  
Operator:  
ExperimentID:  
PlatenID:  
PlatenDesc:  
StagePosition: 1.121 0.146 16.814 89.994 42.200  
SampleID:  
SampleDesc:  
PhotoFilename: none  
SXIFilename: none  
XraySource: Al 1486.6 mono  
XrayPower: 1.2W  
XrayBeamDiameter: 5.0 um  
NeutralizerEnergy: 1.4 eV  
NeutralizerCurrent: 20.0 mA  
SourceAnalyserAngle: 45.0 d  
AnalyserSolidAngle: 20 sr  
AnalyserMode: FAT  
AnalyserWorkFcn: 4.2 eV  
IntensityRecal: no  
IntensityCalCoeff: 20.719 0.079  
EnergyRecal: no  
EnergyReference: none 0.0  
SputterIon: C60  
SputterEnergy: 0.000 keV  
SputterCurrent: 0.0 nA  
SputterRaster: 0.0 0.0 um  
PreAcqSputterTime: 0 s  
PreAcqSputterRate: 0 A/s  
NoSpectralReg: 8  
SpectralRegDef: 1 1 C1s 6 201 -0.100 298.000 278.000 298.000 278.000 0.050 23.50  
AREA  
SpectralRegDef: 2 2 O1s 8 201 -0.100 543.000 523.000 543.000 523.000 0.050 23.50  
AREA  
SpectralRegDef: 3 3 N1s 7 201 -0.100 411.000 391.000 411.000 391.000 0.500 23.50  
AREA  
SpectralRegDef: 4 4 P2p 15 201 -0.100 143.000 123.000 143.000 123.000 0.050  
23.50 AREA  
SpectralRegDef: 5 5 Si2p 14 201 -0.100 114.000 94.000 114.000 94.000 0.050 23.50  
AREA  
SpectralRegDef: 6 6 Al2p 13 201 -0.100 88.000 68.000 88.000 68.000 0.050 23.50  
AREA  
SpectralRegDef: 7 7 Ti2p3 22 251 -0.100 476.000 451.000 476.000 451.000 0.750  
23.50 AREA  
SpectralRegDef: 8 8 Cl2p 17 201 -0.100 213.000 193.000 213.000 193.000 0.050  
23.50 AREA  
NoPolarAngles: 3  
PolarIncrement: 5 d  
PolarMode: irreg  
NoSpatialArea: 1  
SpatialAreaDef: 1 Area1 1 (580.0 1044.0 0.0 90.0 45.0)



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**Software Version 5: XPS V2.0**

- Example. angle resolved measurement with 5 angles and 6 regions: Cu 2p, C 1s, O 1s, N 1s, Ag 3d, S 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.ANG)\PHI-Profile-V5-XPS V2.0.ANG

```

SOFH
Platform: PC
Technique: XPS
FileType: ANGLEPRO
FileDesc: none
SoftwareVersion: XPS V2.0
InstrumentModel: PHI Quantum 2000
Institution: PHI
FileDate: 2006 1 25
AcqFileDate: 2006 1 25
AcqFilename: Winkelschleifer003.ang
Operator: ng
ExperimentID: 2006-0067
PlatenID: 0067b
PlatenDesc: none
StagePosition: 60.5992 38.3998 8.3400 45.0000 -0.0207
PhotoFilename: Winkelschleifer003.pWinkelschleifer003.sxi
ActualPhotoFilename: /D=/Compass6.1.1/datafiles/photos/1_1138109828.pho
SXIFilename: Winkelschleifer003.sxi
ActualSXIFilename: /D=/Compass6.1.1/datafiles/SXIs/1_1138176890.sxi
XraySource: Al 1486.6 mono
XrayPower: 19.47 W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 2.5 V
NeutralizerCurrent: 5.0 uA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 3.9 eV
IntensityRecal: no
IntensityCalCoeff: 23.460 0.183
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 1.000 keV
SputterCurrent: 15.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0.4 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 Cu2p 29 461 -0.0500 950.0 927.0 940.0 927.0 5.760000
23.50 AREA
SpectralRegDef: 2 2 C1s 6 301 -0.0500 295.0 280.0 295.0 280.0 5.760000 23.50
AREA
SpectralRegDef: 3 3 O1s 8 261 -0.0500 540.0 527.0 539.0 527.0 7.200000 23.50
AREA
SpectralRegDef: 4 4 N1s 7 241 -0.0500 406.0 394.0 404.0 394.0 5.760000 23.50
AREA
SpectralRegDef: 5 5 Ag3d 47 401 -0.0500 380.0 360.0 380.0 364.0 7.200000
23.50 AREA
SpectralRegDef: 6 6 S2p 16 301 -0.0500 170.0 155.0 170.0 158.0 10.800000 23.50
AREA
NoPolarAngles: 5
NoSpatialArea: 1
SpatialAreaDef: 1 Point3 1 (59385.6 36657.7 8340.0 45.0 -0.3)
SpatialAreaDesc: 1 Nr3 Schleifer Stelle1
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH

```

```

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ììììììììf8 ìğ □□ □ □ □ □ □ □ □ □ ang ììììreg ìììì
ìììììììc/s *
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```

### Software Version 10: Without software specification

- Example. angle resolved measurement with 5 angles and 5 regions: C 1s, P 2p, O 1s, Ti 2p, N 1s
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Profile(.ANG)\PHI-Profile-V10-without\_software\_specification.ANG

```

SOFH
Platform: PC
Technique: XPS
FileType: ANGLEPRO
FileDesc: DMAEMA-co-DMMEP_30_70 gammasterilisiert
FileDate: 111 2 8
AcqFileDate: 111 2 8
AcqFilename: MS_D16_7.ang
ScanMode: scan
StagePosition: 0.0 0.0 0.0 45.0 0.0
XraySource: Al 1486.6 mono
XrayPower: 300.00 W
NeutralizerEnergy: 0.0 eV
NeutralizerCurrent: 0.0 mA
SourceAnalyserAngle: 90.0 d
AnalyserMode: FAT
AnalyserWorkFcn: 4.5 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: 3He
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 10.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 1.0 A/s
NoSpectralReg: 5
SpectralRegDef: 1 1 C1 6 161 -0.1250 300.0 280.0 300.0 280.0 0.500000 58.70 none
SpectralRegDef: 2 2 P1 15 161 -0.1250 147.0 127.0 147.0 127.0 2.500000 58.70
none
SpectralRegDef: 3 3 O1 8 161 -0.1250 545.0 525.0 545.0 525.0 2.500000 58.70 none
SpectralRegDef: 4 4 Ti1 22 201 -0.1250 476.0 451.0 476.0 451.0 2.500000 58.70
none
SpectralRegDef: 5 5 N1 7 161 -0.1250 414.0 394.0 414.0 394.0 2.500000 58.70 none
NoPolarAngles: 5
PolarAngles: 15 30 45 60 75
NoSpatialArea: 1
SpatialAreaDef: 1 Full 1 (0.0 0.0 0.0 0.0 0.0)
EOFH
□ □ □ □ □ □ □ □ □ □ ; □ □ pnt □ □ ang A□ □ c/s ð
Ìú□ f4 "
...

```

### 3.1.20.4 PHI Spectrometer/Mapping (\*.map)

Comment:

- With respect to the multi region files (\*.spe) the header contains additional profile and mapping information (e.g. angle values, number and position of mapping points)

### Software Version 12: SS 2.6.1.2

- Example. snap shot mapping of 168x156 points of one region (S i2p)

- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Mapping(.MAP)\PHI-Mapping-168x156-V12-SS 2.6.1.2.MAP

SOFH  
Platform: PC  
Technique: XPS  
FileType: MAP  
FileDesc: ASKim150122-1  
SoftwareVersion: SS 2.6.1.2  
InstrumentModel: PHI VersaProbe II  
AcqFilename: G:\Datafiles\ASKim\ASKim150122-1.14\_1.map  
FileDate: 2015 1 22  
AcqFileDate: 2015 1 22  
Institution: PHI  
Operator:  
ExperimentID: ASKim  
EnergyReference: none 0.0  
AnalyserWorkFcn: 4.435 eV  
AnalyserRetardGain: 1.000087  
PlatenID: ASKim150122-1  
PhotoFilename:  
SXIFilename: ASKim150122-1.13.sxi  
SourceAnalyserAngle: 45.0 d  
AnalyserSolidAngle: 20.0 sr  
IntensityRecal: no  
IntensityCalCoeff: 82.808 0.246  
EnergyRecal: no  
ScanDeflectionSpan: 40 60  
ScanDeflectionOffset: 0 0  
SCAMultiplierVoltage: 1750.0 V  
NarrowAcceptanceAngle: no  
PeakToNoiseRatioState: no  
DelayBeforeAcquire: 5 seconds  
C60IonGun: None  
BiasBoxMode: 0  
SemFieldOfView: 168.0000000  
ImageSizeXY: 168.0000 156.0000  
IonGunMode: Standby  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 1.000 kV  
FloatVolt: 0.0 V  
FloatEnable: no  
GridVolt: 120.0  
CondensorVolt: 710.00  
ObjectiveVolt: 672.00  
BendVolt: 15.00  
SputterRaster: 3.00 3.00 mm  
SputterRasterOffset: 0.050 -0.050 mm  
TargetSputterTime: 2.0 min  
SputterEmission: 7.00 mA  
DeflectionBias: 0.0 V  
XpsScanMode: unscanned  
AnalyserMode: FAT  
SurvNumCycles: 1  
SurvTimePerStep: 20.000000  
NoMapPixelsXY: 265 246  
MapFramesPerFCC: 1  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 1880 2005  
PhotoOffsetInPixel: 788 83  
PhotoSizeInMm: 56.129 59.691  
PhotoOffsetInMm: 0.015 0.015  
NoSpectralRegFull: 2

SpectralRegDefFull: 1 1 Si2p 14 32 -0.2000 105.1000 98.9000 102.7500 101.2500  
0.000000 46.95 AREA  
SpectralRegDef2Full: 1 6.2 2 0 4 1  
SpectralRegBackgroundFull: 1 0.0 102.0 0.0  
SpectralRegHeroFull: 1 102.0 0.0 0.0 0.00  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
SpectralRegDefFull: 2 1 Ta4f 73 32 -0.2000 28.1000 21.9000 25.7500 24.2500  
0.000000 46.95 AREA  
SpectralRegDef2Full: 2 6.2 2 0 4 1  
SpectralRegBackgroundFull: 2 0.0 25.0 0.0  
SpectralRegHeroFull: 2 25.0 0.0 0.0 0.00  
SpectralRegIRFull: 2 0 0.000 0.000 0.0  
NoSpectralReg: 1  
SpectralRegDef: 1 1 Si2p 14 32 -0.2000 105.1000 98.9000 102.7500 101.2500  
0.004000 46.95 AREA  
SpectralRegDef2: 1 6.2 2 0 4 1  
SpectralRegBackground: 1 0.0 102.0 0.0  
SpectralRegHero: 1 102.0 0.0 0.0 0.00  
SpectralRegIR: 1 0 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 2-1 4 (3518.4 1465.2 16073.2 45.0 -36.5) (3686.6 1465.2  
16073.2 45.0 -36.5) (3686.6 1621.1 16073.2 45.0 -36.5) (3518.4 1621.1 16073.2  
45.0 -36.5)  
SpatialAreaDesc: 1  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 2  
XrayPower: 1.25 W  
XrayBeamDiameter: 5.0 um  
XrayBeamVoltage: 15000.0 V  
XrayCondenserLensVoltage: 11300.0 V  
XrayObjectiveCoilCurrent: 0.725 A  
XrayBlankingVoltage: 280.0 V  
XrayFilamentCurrent: 1.520 A  
XrayStigmator: 0.0 0.0  
XrayHighPower: no  
XrayScanIncXY: 0.632378 0.632378 um  
EgunNeutMode: Standby  
NeutralizerCurrent: 20.0 uA  
NeutralizerEnergy: 1.00 V  
EgunNeutExtractor: 30.0 V  
EgunNeutXSteering: 34.8  
EgunNeutYSteering: -36.8  
EgunNeutFilament: 0.00 A  
EgunNeutPulseLength: 10.0 msec  
SxiPersistence: 1 V  
SxiSecPerDisplay: 1.0  
SxiAutoContrast: yes  
SxiAutoContrastLow: 0.30  
SxiAutoContrastHigh: 0.30  
SxiBindingEnergy: 1458.6 eV  
SxiPassEnergy: 376 eV  
SxiLens2: 476 V  
SxiLens3: 406 V  
SxiLensBias: 0 V  
SxiShutterBias: yes  
SxiShutterBiasVoltage: 409.9 V  
SxiDisplayMode: 2  
Detector Acq Time: 20.0 (min)  
Number Of Channels: 16  
Channel Info: 1 1 1.569  
Channel Info: 2 1 1.232  
Channel Info: 3 1 1.265  
Channel Info: 4 1 1.217  
Channel Info: 5 1 1.162  
Channel Info: 6 1 1.078  
Channel Info: 7 1 1.056

```

Channel Info: 8 1 0.979
Channel Info: 9 1 0.965
Channel Info: 10 1 0.909
Channel Info: 11 1 0.855
Channel Info: 12 1 0.804
Channel Info: 13 1 0.762
Channel Info: 14 1 0.726
Channel Info: 15 1 0.765
Channel Info: 16 1 1.574
StagePosition: 1.9860 -3.2796 16.0732 45.0125 -36.5000
StageCurrentRotationSpeed: 1.0000
DefectPosID: 2
DefectPosComment:
DefectPosU: 3.5478
DefectPosV: -1.4558
DefectPosX: 1.9860
DefectPosY: -3.2806
DefectPosZ: 16.0732
DefectPosTilt: 45.0125
DefectPosRotation: -36.5000
DefectPosAligment: None
DefectPosReferenceImage: ASKim150122-1.13.sxi
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 10u1.25W15KV
EOFH
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...

```

### Software Version 13: SS 2.5.0.9

- Example. snap shot mapping of 256x256 points of one region
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\19-PHI-Mapping(.MAP)\PHI-Mapping-256x256-V13-SS 2.5.0.9.MAP

```

SOFH
Platform: PC
Technique: XPS
FileType: MAP
FileDesc:
SoftwareVersion: SS 2.5.0.9
InstrumentModel: PHI VersaProbe II
AcqFilename: C:\ZCH\140438\140438.15.KWe 140320 2 Map_1.map
FileDate: 2014 4 1
AcqFileDate: 2014 4 1
Institution: PHI
Operator:
ExperimentID: 140438
EnergyReference: none 0.0
AnalyserWorkFcn: 4.132 eV
AnalyserRetardGain: 1.000186
PlatenID:
PhotoFilename: 140438.1.Low Mag.pho
SXIFilename:
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
IntensityRecal: no
IntensityCalCoeff: 100.000 0.330
EnergyRecal: no
ScanDeflectionSpan: 50 70
ScanDeflectionOffset: 0 2
SCAMultiplierVoltage: 1700.0 V
NarrowAcceptanceAngle: no
PeakToNoiseRatioState: no
DelayBeforeAcquire: 5 seconds
C60IonGun: None

```

BiasBoxMode: 0  
SemFieldOfView: 1000.000000  
EBeamCurrent: -2.2 nA  
ImageSizeXY: 1000.0000 1000.0000  
IonGunMode: Off  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 0.000 A/min  
SputterEnergy: 0.100 kV  
FloatVolt: 0.0 V  
FloatEnable: no  
GridVolt: 150.0  
CondensorVolt: 71.00  
ObjectiveVolt: 68.50  
BendVolt: 1.50  
SputterRaster: 3.00 3.00 mm  
SputterRasterOffset: 0.000 0.000 mm  
TargetSputterTime: 10.0 min  
SputterEmission: 0.00 mA  
DeflectionBias: 0.0 V  
XpsScanMode: unscanned  
AnalyserMode: FAT  
SurvNumCycles: 1  
SurvTimePerStep: 1000.000000  
NoMapPixelsXY: 256 256  
MapFramesPerFCC: 1  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 2197 3136  
PhotoOffsetInPixel: 1519 200  
PhotoSizeInMm: 35.000 50.000  
PhotoOffsetInMm: -38.354 -50.000  
NoSpectralRegFull: 2  
SpectralRegDefFull: 1 1 Al2p 13 16 -1.0000 81.5000 66.5000 80.0000 68.0000  
0.000000 117.40 AREA  
SpectralRegDef2Full: 1 15.0 5 0 1 1  
SpectralRegBackgroundFull: 1 0.0 74.0 0.0  
SpectralRegHeroFull: 1 74.0 0.0 0.0 0.0  
SpectralRegIRFull: 1 0 0.000 0.000 0.0  
SpectralRegDefFull: 2 0 Mn2p3 25 16 -1.0000 648.5000 633.5000 647.0000 635.0000  
0.000000 117.40 AREA  
SpectralRegDef2Full: 2 15.0 10 0 1 1  
SpectralRegBackgroundFull: 2 0.0 641.0 0.0  
SpectralRegHeroFull: 2 641.0 0.0 0.0 0.0  
SpectralRegIRFull: 2 0 0.000 0.000 0.0  
NoSpectralReg: 1  
SpectralRegDef: 1 1 Al2p 13 16 -1.0000 81.5000 66.5000 80.0000 68.0000 0.200000  
117.40 AREA  
SpectralRegDef2: 1 15.0 5 0 1 1  
SpectralRegBackground: 1 0.0 74.0 0.0  
SpectralRegHero: 1 74.0 0.0 0.0 0.0  
SpectralRegIR: 1 0 0.000 0.000 0.0  
NoSpatialArea: 1  
SpatialAreaDef: 1 10 4 (9787.3 7171.0 11701.4 46.0 -90.1) (10787.3 7171.0  
11701.4 46.0 -90.1) (10787.3 8171.0 11701.4 46.0 -90.1) (9787.3 8171.0 11701.4  
46.0 -90.1)  
SpatialAreaDesc: 1  
SpatialHRPhotoCor: 1 (0.0 0.0)  
XraySource: Al 1486.6 mono  
XrayAnodePosition: 3  
XrayPower: 0.98 W  
XrayBeamDiameter: 5.0 um  
XrayBeamVoltage: 15000.0 V  
XrayCondenserLensVoltage: 11850.0 V  
XrayObjectiveCoilCurrent: 0.723 A  
XrayBlankingVoltage: 325.0 V  
XrayFilamentCurrent: 1.577 A  
XrayStigmator: 0.0 0.0

```

XRayHighPower: no
XrayScanIncXY: 3.906250 3.906250 um
EgunNeutMode: Off
NeutralizerCurrent: 1.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 30.0 V
EgunNeutXSteering: 0.0
EgunNeutYSteering: 0.0
EgunNeutFilament: 1.11 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 1458.6 eV
SxiPassEnergy: 376 eV
SxiLens2: 476 V
SxiLens3: 406 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 342.0 V
SxiDisplayMode: 2
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.661
Channel Info: 2 1 1.490
Channel Info: 3 1 1.499
Channel Info: 4 1 1.268
Channel Info: 5 1 1.149
Channel Info: 6 1 1.100
Channel Info: 7 1 1.148
Channel Info: 8 1 1.079
Channel Info: 9 1 1.118
Channel Info: 10 1 1.021
Channel Info: 11 1 0.942
Channel Info: 12 1 0.803
Channel Info: 13 1 0.730
Channel Info: 14 1 0.627
Channel Info: 15 1 0.634
Channel Info: 16 1 1.028
StagePosition: -7.5750 -9.9215 11.7014 46.0000 -90.1000
StageCurrentRotationSpeed: 0.6700
DefectPosID: 10
DefectPosComment:
DefectPosU: 10.2873
DefectPosV: -7.6710
DefectPosX: -7.5750
DefectPosY: -9.9215
DefectPosZ: 11.7014
DefectPosTilt: 46.0000
DefectPosRotation: -90.1000
DefectPosAligment: None
DefectPosReferenceImage: 140438.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 9u1.0W15KV
EOFH
□ □ À □ □ □ □ □ □ □ □ pnt pnt <Û¼ `ä@ c/s
□ f4 □ Ð □ □ □ □ □ □ □ □ □ □ chn pnt
...

```

### 3.1.21 Focus CSA (\*.dat)

Comment:

- the header includes the acquisition parameters

- data: 1. column: energy, 2. column: intensities, 3.-5. column: data for normalization
- after [DATA] intensities of the sum spectrum
- from [DATA 1] to [DATA 20] intensities of the single scans
- Example. valence band, 20 scans
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\20-Focus  
CSA(.DAT)\FocusCSA-SingleReg-VB.DAT

```
[REGION_CONFIG]
TIMESTAMP="9/11/2009 / 10:17:40 AM"
USE=TRUE
E_START=10000.000000000000
E_STOP=10070.000000000000
E_STEP=0.318437500000
E_SCAN=1
EPASS=100.000000000000
N_SCAN=20
N_IMAGE=1000
PE=10050.000000
T_DWELL=5000.000000
SLIT=9
COMMENT=""
PATH_LENS_TAB=/C/Program Files/FOCUS ProCSA/lens tables/Mode2/M06_Mo2.lens
PATH_DATA_FILE=/C/Data/090910/STO10KeV/VBdef.dat
[DETECTOR]
CAMRES_X=1280
CAMRES_Y=1024
CAMRANGE_XMIN=100
CAMRANGE_XMAX=599
CAMRANGE_YMIN=115
CAMRANGE_YMAX=350
T_EXPOSURE=5.000000
K_DET=0.101900
WA=4.500000
NX0=337
BINNING=1
K_SPEC=0.859900
CHANNELS=25
U_MCP=2400.000000
U_SCR=4500.000000
IP=127.0.0.1
PORT=5555
[DATA_CONFIG]
TIMESTAMP="9/11/2009 / 3:20:44 AM"
T_EXPOSURE=5.000000
N_SCAN=20
N_Image=1000
PE=10050.000000
WA=4.500000
[DATA]
10000.00000 1537 41 0 0
10000.31844 1553 41 0 0
10000.63688 1538 41 0 0
...
10069.73781 702 43 0 0
10070.05625 688 42 0 0
[DATA_1]
10000.00000 77 2 0 0
10000.31844 96 2 0 0
...
10069.73781 26 3 0 0
10070.05625 45 2 0 0
[DATA_2]
10000.00000 90 2 0 0
10000.31844 85 2 0 0
```

```

...
10069.73781 46    2    0    0
10070.05625 31    2    0    0
[DATA_3]
10000.00000 79    2    0    0
10000.31844 65    2    0    0
...
10069.73781 33    2    0    0
10070.05625 38    2    0    0
[DATA_4]
10000.00000 81    2    0    0
10000.31844 84    2    0    0
...
10069.73781 38    2    0    0
10070.05625 39    2    0    0
[DATA_5]
10000.00000 78    2    0    0
10000.31844 83    2    0    0
...
10069.73781 39    2    0    0
10070.05625 26    2    0    0
...
[DATA_19]
10000.00000 63    2    0    0
10000.31844 78    2    0    0
...
10069.73781 31    2    0    0
10070.05625 28    2    0    0
[DATA_20]
10000.00000 81    2    0    0
10000.31844 60    2    0    0
...
10069.73781 20    2    0    0
10070.05625 33    2    0    0

```

### 3.1.22 Croissant (\*.pesp)

Comment:

- Measurement data format of the University of Basel
- the header includes all important recording parameters
- Data: 1. column: BE, 2. column: kinetic energy, 3. column: Sum of all intensities, 4.-8. column: Intensities of each channeltron
- after [DATA] the intensities are saved
- Example of one region (O 1s), 20 Scans
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\21-Croissant(.PESP)\Croissant-SingleReg-O1s.PESP

```

[Info]
FileFormat=1.2
MeasurementSoftware=croissant experiments
SoftwareVersion=1.3.1.11
Instrument=VG210 Uni Basel
Location=University of Basel
User=lm
Sample=none
OriginalScriptFile=mxps_O1s_C1s_Sils.cexp
ScriptFile=E3-110222N004.cexp
SampleTemperature=300
SamplePressure=1.0E-9
ThetaManipulatorNormal=0.0
PhiManipulatorReference=0.0
CalculatedInitialManipulatorAngles=No
ThetaManipulatorInitial=0.0

```

```

PhiManipulatorInitial=0.0
PhotonSource=MXPS Al Ka
PhotonEnergy=1486.600
RegionName=O1s_20
EnergyScale=Binding
AnalyserMode=FAT/CAE
PassEnergy=20.000
DwellTime=0.1
AutoSupplyRange=Yes
EnergyHigh=524.235
EnergyLow=540.785
WorkFunction=4.200
EnergyFirst=525.000
EnergyLast=540.000
NumberOfEnergies=301
EnergyStep=-0.050
NumberOfSweeps=15
LensMode=Mono Range
KIris=19.0
RIris=10.0
MeasurementType=Energy spectrum
StartDate=22.02.2011
StartTime=17:37:42
EndDate=22.02.2011
EndTime=17:47:25
InternalDimensions=EnergySetpoint

```

[Detector]

```

NumberOfGroups=1
Group1Name=All Channeltrons
Group1Active=yes
NumberOfChannels=5
Channel1Name=Channeltron 1
Channel2Name=Channeltron 2
Channel3Name=Channeltron 3
Channel4Name=Channeltron 4
Channel5Name=Channeltron 5
Channel1Active=yes
Channel2Active=yes
Channel3Active=yes
Channel4Active=yes
Channel5Active=yes

```

[Data]

```

Energy KineticEnergy SpectrumGroup1 SpectrumChannel1 SpectrumChannel2
SpectrumChannel3 SpectrumChannel4 SpectrumChannel5
525.000 961.600 3930 888 711 775 822 734
525.050 961.550 3961 827 697 822 849 766
...
539.900 946.700 3906 916 721 768 775 726
539.950 946.650 3962 837 784 770 847 724
540.000 946.600 3956 917 724 769 831 715

```

### 3.1.23 SSI-XPS (\*.mrs)

Comment:

- Measurement data format of the University Stanford
- In the data file is saved one region only
- The header includes all important recording parameters
- UNIFIT reads only the first block of data (after array\_size=201 and !)
- Example: single region (Ru 3d), 5 Scans
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\22-SSI-XPS(.MRS)\SSI-XPS-SingleReg-Ru3d.MRS

```
file_version=2
type=0 (node)
head_count=1
data=Multiple RegionS
regions=1
file_path=C:\ESC\NID\2DMPD35R
file_name=2DMPD35R
file_type=MRS
pause_flag=0
oper=nid
aperture=0
fgeV=0.
lo_be=275.
up_be=295.
res=2.
spot=2
time_limit=251.
pump_extra_min=0
time_stamp=Thu Sep 29 16:34:24 2011
desc=4-10-2-20 1500cycles 185C
desc2=Ru3d
!
type=0 (node)
data=Region node
head_count=0
!
sub_data_file=1.REG
file_version=2
type=0 (node)
head_count=2
data=Spectrum
region=1
scan_limit=5
tech=scanned
count_limit=0.
time_limit=251.
det_ms=100
fgeV=0.
spot=2
spot_type=3
res=2
res_ev=20.41
aperture=0
sensitivity_exponent=0.5
xrays=0
xrays_ev=0.
start=Thu Sep 29 16:31:24 2011
scan_total=5
delta_ev=0.
detw_ev=8.3
pass_ev=67.38
ref_ev=1486.6
finis=Thu Sep 29 16:34:24 2011
time_total=142.
!
type=0 (node)
head_count=3
data=Data node
!
type=12 (int array)
data=Data Array
lo_be=275.
up_be=295.
array_size=201
!
403
```

```

371
...
75
73
!
type=12 (int array)
array_size=201
data=Peak Fit
lo_be=275.
up_be=295.
display_extra=2
!
403
371
...
75
73
!
type=12 (int array)
array_size=201
data=Peak Fit
lo_be=275.
up_be=295.
display_extra=2
!
403
371
...
75
73
!
type=0 (node)
data=Peak Fit Params
head_count=8
!
type=9 (text)
data=Fit Constants
back_type=1
num_iters=50
peak_type=100
asymmetry=0
min_xx=0.001
low_fit_be=276.4
mid_fit_be=289.8
up_fit_be=289.8
evpch=0.1
ioffset=52
low_fit_chan=186
mid_fit_chan=52
up_fit_chan=52
fit_area=54550.152
!
type=9 (text)
data=Peak Params
title=Peak parameters
subtitle=PEAK ENERGY          WIDTH          HEIGHT          AREA          % GAUSS          % ASYMM
line_count=4
max_line_length=92
!
  1   279.86  0.86   1184.51   10753.27  100   0       1.06   10.510955
42.198685  19.427094
  2   284.13  1.91   1008.48   20379.63  100   0       1.06   34.685749
35.923389   8.611172
  3   280.59  1.87    896.25   17804.85  100   0       1.06   46.851093
37.153889  24.871016
  4   285.83  2.80    174.57    5185.41  100   0       1.06    4.316279
56.311642  11.909515

```

```
type=9 (text)
data=Peak Constr
title=Peak constraints
subtitle=PEAK ENERGY WIDTH HEIGHT
line_count=4
max_line_length=21
!
  1      0      0      0
  2      0      0      0
  3      0      0      0
  4      0      0      0
type=14 (float array)
array_size=135
data=Baseline
lo_be=276.4
up_be=289.8
display_extra=2
long_desc=Baseline: 289.80 to 276.40 eV
displayed=1
!
442.260
442.158
...
78.956
78.965
!
type=0 (node)
data=Models
head_count=4
!
type=14 (float array)
array_size=102
data=Model
model_num=1
peak_type=100
model_limit=50
up_be=51.
lo_be=-50.
model_area=1.064
fwhm=23.554
!
0.000
0.000
...
0.000
0.000
!
type=14 (float array)
array_size=102
data=Model
model_num=2
peak_type=100
model_limit=50
up_be=51.
lo_be=-50.
model_area=1.064
fwhm=23.554
!
0.000
0.000
...
0.000
0.000
!
type=14 (float array)
array_size=102
data=Model
```

```
model_num=3
peak_type=100
model_limit=50
up_be=51.
lo_be=-50.
model_area=1.064
fwhm=23.554
!
0.000
0.000
...
0.000
0.000
!
type=14 (float array)
array_size=102
data=Model
model_num=4
peak_type=100
model_limit=50
up_be=51.
lo_be=-50.
model_area=1.064
fwhm=23.554
!
0.000
0.000
...
0.000
0.000
!
type=0 (node)
data=Peaks
head_count=4
!
type=14 (float array)
array_size=37
data=Peak
peak_num=1
long_desc=# 1: 279.86 eV    0.86 eV    10838.74 cts    19.94%
area_fit=10838.74
up_be=281.6
lo_be=278.
displayed=1
!
256.358
253.726
...
79.117
79.100
!
type=14 (float array)
array_size=83
data=Peak
peak_num=2
long_desc=# 2: 284.13 eV    1.91 eV    20494.73 cts    37.70%
area_fit=20494.732
up_be=288.2
lo_be=280.
displayed=1
!
440.793
440.311
...
167.432
156.168
!
```

```
type=14 (float array)
array_size=81
data=Peak
peak_num=3
long_desc=# 3: 280.59 eV   1.87 eV   17832.51 cts   32.80%
area_fit=17832.508
up_be=284.5
lo_be=276.5
displayed=1
!
371.833
365.134
...
78.979
78.957
!
type=14 (float array)
array_size=101
data=Peak
peak_num=4
long_desc=# 4: 285.83 eV   2.80 eV   5200.79 cts   9.57%
area_fit=5200.79
up_be=289.8
lo_be=279.8
displayed=1
!
442.838
442.918
...
144.408
132.410
!
type=14 (float array)
array_size=135
data=Composite Fit
lo_be=276.4
up_be=289.8
display_extra=2
long_desc=48 iterations, chi square = 2.4591
displayed=1
!
442.838
442.918
...
78.957
78.965
!
type=14 (float array)
array_size=201
data=Peak Error
lo_be=275.
up_be=295.
display_extra=2
long_desc=PEAK ERROR
!
0.000
0.000
...
0.000
0.000
73.000
!
```

### 3.1.24 SPECS Phoibos225/Prodigy (\*.xy)

Comment:

- Measurement data format generated via converter using the SPECSLab Software
- Example (version 2.60) has six regions:
  1. Survey, Scans 1, Pass 40 eV
  2. VB, Scans 5, Pass 20
  3. Sb2p3/2 Sb2p1/2, Scans 2, Pass 40
  4. Survey, Scans 1, Pass 40
  5. VB, Scans 5, Pass 20
  6. Sb3/2 Sb1/2, Scans 1, Pass 40
- the header of the region includes all important recording parameters
- Data: KE, two space characters, intensities (cps)
- the intensities are saved after the two lines: # ColumnLabels and #
- Example: multi region high energy measurement, excitation energy: 5900 eV, 6 regions: survey, VB, Sb 2p, survey 1, VB 1, Sb 2p
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\23-SPECS-Phoibos-Prodigy(.XY)\SPECS-Phoibos-MultiReg-HEXPS-Separatescans-V2.60.XY
- File can have external data: a) Ring current, b) Mirror current c) TYR data

```

# Created by:          SpecsLab2, Version 2.60-r21162
#
# XY-Serializer Export Settings: as follows
# Comment Prefix:      #
# Counts Per Second:   yes
# Kinetic Energy Axis: yes
# Separate Scan Data:  yes
# Separate Channel Data: no
# External Channel Data: no
# Transmission Function: no
# Asymmetry Recalculation: no
# ErrorBar:            no
#
# Group:               MS24
#
# values in kinetic energy
# Region:              Survey
# Analysis Method:     UPS
# Analyzer:             PHOIBOS HSA15000 DLD 225 R6-HV[HWTtype 31:60, 32:63, 33:64,
                       542:511] DLD
# Analyzer Lens:       SmallArea:3.5kV
# Analyzer Slit:       4:3x20\2:open
# Scan Mode:           FixedAnalyzerTransmission
# Number of Scans:     1
# Curves/Scan:         1
# Values/Curve:        2008
# Dwell Time:          0.3
# Excitation Energy:   5900
# Kinetic Energy:      4900
# Pass Energy:         40
# Bias Voltage:        50
# Detector Voltage:    2650
# Eff. Workfunction:   4.658
# Source:              UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
4900 1090
4900.5 1063.3333

```

```
...
5903 0
5903.5 0

# values in kinetic energy
# Region: VB
# Analysis Method: UPS
# Analyzer: PHOIBOS HSA15000 DLD 225 R6-HV[HWType 31:60, 32:63, 33:64,
542:511] DLD
# Analyzer Lens: SmallArea:1.5kV
# Analyzer Slit: 4:3x20\2:open
# Scan Mode: FixedAnalyzerTransmission
# Number of Scans: 5
# Curves/Scan: 1
# Values/Curve: 281
# Dwell Time: 2
# Excitation Energy: 5900
# Kinetic Energy: 5890
# Pass Energy: 20
# Bias Voltage: 50
# Detector Voltage: 2650
# Eff. Workfunction: 4.658
# Source: UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
5890 17.5
5890.05 25.5
...
5903.95 1.5
5904 0

# Cycle: 0, Curve: 0, Scan: 1
#
# ColumnLabels: energy counts/s
#
5890 28
5890.05 24
...
5903.95 0.5
5904 1

# Cycle: 0, Curve: 0, Scan: 2
#
# ColumnLabels: energy counts/s
#
5890 28
5890.05 27
...
5903.95 0
5904 0.5

# Cycle: 0, Curve: 0, Scan: 3
#
# ColumnLabels: energy counts/s
#
5890 24.5
5890.05 23
...
5903.95 0.5
5904 1.5
```

```
# Cycle: 0, Curve: 0, Scan: 4
#
# ColumnLabels: energy counts/s
#
5890 25
5890.05 26
...
5903.95 2
5904 2.5

# values in kinetic energy
# Region: Sb2p3/2 Sn2p1/2
# Analysis Method: UPS
# Analyzer: PHOIBOS HSA15000 DLD 225 R6-HV[HWTtype 31:60, 32:63, 33:64,
542:511] DLD
# Analyzer Lens: SmallArea:3.5kV
# Analyzer Slit: 4:3x20\2:open
# Scan Mode: FixedAnalyzerTransmission
# Number of Scans: 2
# Curves/Scan: 1
# Values/Curve: 501
# Dwell Time: 1
# Excitation Energy: 5900
# Kinetic Energy: 1701.4
# Pass Energy: 40
# Bias Voltage: 50
# Detector Voltage: 2650
# Eff. Workfunction: 4.658
# Source: UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
1701.4 6975
1701.6 7051
...
1801 4745
1801.2 4769
1801.4 4931

# Cycle: 0, Curve: 0, Scan: 1
#
# ColumnLabels: energy counts/s
#
1701.4 7078
1701.6 7064
...
1801.2 4598
1801.4 4338

# Group: MS16
#
# values in kinetic energy
# Region: Survey
# Analysis Method: UPS
# Analyzer: PHOIBOS HSA15000 DLD 225 R6-HV[HWTtype 31:60, 32:63, 33:64,
542:511] DLD
# Analyzer Lens: SmallArea:3.5kV
# Analyzer Slit: 4:3x20\2:open
# Scan Mode: FixedAnalyzerTransmission
# Number of Scans: 1
# Curves/Scan: 1
# Values/Curve: 2008
```

```
# Dwell Time:      0.3
# Excitation Energy: 5900
# Kinetic Energy:  4900
# Pass Energy:     40
# Bias Voltage:    50
# Detector Voltage: 2650
# Eff. Workfunction: 4.658
# Source:          UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
4900 28060
4900.5 26963.333
...
5902.5 6.6666667
5903 3.3333333
5903.5 0

# values in kinetic energy
# Region:          VB
# Analysis Method: UPS
# Analyzer:         PHOIBOS HSA15000 DLD 225 R6-HV[HWTtype 31:60, 32:63, 33:64,
542:511] DLD
# Analyzer Lens:   SmallArea:1.5kV
# Analyzer Slit:   4:3x20\2:open
# Scan Mode:       FixedAnalyzerTransmission
# Number of Scans: 5
# Curves/Scan:    1
# Values/Curve:   281
# Dwell Time:     2
# Excitation Energy: 5900
# Kinetic Energy:  5890
# Pass Energy:     20
# Bias Voltage:    50
# Detector Voltage: 2650
# Eff. Workfunction: 4.658
# Source:          UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
5890 264
5890.05 261.5
...
5903.95 1.5
5904 2

# Cycle: 0, Curve: 0, Scan: 1
#
# ColumnLabels: energy counts/s
#
5890 285
5890.05 302
...
5903.95 0.5
5904 2

# Cycle: 0, Curve: 0, Scan: 2
```

```
#
# ColumnLabels: energy counts/s
#
5890 293
5890.05 304.5
...
5903.95 1
5904 2

# Cycle: 0, Curve: 0, Scan: 3
#
# ColumnLabels: energy counts/s
#
5890 315
5890.05 309.5
...
5903.95 0.5
5904 1

# Cycle: 0, Curve: 0, Scan: 4
#
# ColumnLabels: energy counts/s
#
5890 294
5890.05 298.5
...
5903.95 3
5904 1

# values in kinetic energy
# Region: Sb2p3/2 Sn2p1/2
# Analysis Method: UPS
# Analyzer: PHOIBOS HSA15000 DLD 225 R6-HV[HWTtype 31:60, 32:63, 33:64,
542:511] DLD
# Analyzer Lens: SmallArea:3.5kV
# Analyzer Slit: 4:3x20\2:open
# Scan Mode: FixedAnalyzerTransmission
# Number of Scans: 1
# Curves/Scan: 1
# Values/Curve: 501
# Dwell Time: 1
# Excitation Energy: 5900
# Kinetic Energy: 1701.4
# Pass Energy: 40
# Bias Voltage: 50
# Detector Voltage: 2650
# Eff. Workfunction: 4.658
# Source: UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
1701.4 76318
1701.6 76244
...
1801 60272
1801.2 60102
1801.4 60105
```

### 3.1.25 Energy-Intensity (\*.dat)

Comment:

- Simplest form of a measurement data format, 1. column: energies, 2. - n. column: intensities
- Scan direction: increasing or decreasing energies
- Energy form: binding or kinetic energies
- Only one region saved in the data file
- The reading of the spectrum starts from the first line with numbers
- Lines with characters are ignored
- Peak name, comment, excitation energy, dwell time, number of scans, analyser energy, analyser mode has to be defined manually

#### Version 1: BE decreasing

- Example: single region
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\24-EnergyIntensity(.DAT)\EnergyIntensity-SingleReg-BE-decreasing.DAT

```
Spectrum BE decreasing
27.990    583
27.960    595
27.930    598
...
21.060    240
21.030    252
21.000    217
```

#### Version 2: BE increasing

- Example: single region
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\24-EnergyIntensity(.DAT)\EnergyIntensity-SingleReg-BE-increasing.DAT

```
BE      Int
21      217
21.03   252
21.06   240
...
27.93   598
27.96   595
27.99   583
```

#### Version 3: KE decreasing

- Example: single region
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\24-EnergyIntensity(.DAT)\EnergyIntensity-SingleReg-KE-decreasing.DAT

```
KE      Int
1465.6   217
1465.57  252
...
1458.67  598
1458.64  595
1458.61  583
```

#### Version 4: KE increasing

- Example: single region
- Folder: Install-Memory Card:\XPS\_Measurement\_Reference\_Data\24-EnergyIntensity(.DAT)\EnergyIntensity-SingleReg-KE-increasing.DAT

```
BE      Int
1458.61  583
1458.64  595
```

```

1458.67      598
...
1465.54      240
1465.57      252
1465.6       217

```

### 3.1.26 HTW-Berlin (\*.dat)

#### Comment:

- Data format of the HTW Berlin
- Header includes excitation energy, pass energy, dwell time, comment, step width
- Decimal delimiter: comma
- Columns: 1. kinetic energies, 2. binding energies, 3. sum of scans, 4. - n. intensities of the scans
- Scan direction: increasing kinetic energies
- Only one region saved in the data file
- Peak name, number of scans, analyser mode, x position, y position has to be defined manually

#### XPS

```

Mg - Anode / 1253,60 eV
Austrittsarbeit: 4,50 eV
Messzeit (dwell): 3,00 s
Passenergie: 30,00 eV
Conversion Voltage: 50,00 eV
Multiplierspannung: 2800 V
Tubus: Ground intern
Karte Sweep: NI-6052E
Karte Analysator: SPCI721F
Nullverschiebung Analysatorenergie: 0,000 eV
Korrekturfaktor Analysatorenergie: 1,000 eV
Probenspannung: 0,00 V
Wartezeit Energie: 100,00 ms
Schrittweite: 0,05 eV
Datum der Messung: Donnerstag, 29. Januar 2015 14:55
Gesamtmesszeit: 25min 59s
ausgewählter X-Wert: Bindungsenergie

```

#### Kommentar:

Probe auf altem Halter

#### Messwerte:

kin. Energie	Bindungsenergie	Scan	Summe	Scans	(Counts pro Sekunde)
Scan 1	Scan 2	Scan 1	(Counts pro Sekunde)	Scan 2	(Counts pro Sekunde)
[eV]	[eV]	[1/eV]	[1/(s*eV)]	[1/eV]	[1/(s*eV)]
1,139099E+3	-1,100009E+2	9,510000E+2	1,585000E+2	4,750000E+2	4,760000E+2
1,583333E+2	1,586667E+2				
1,139160E+3	-1,099398E+2	9,620000E+2	1,603333E+2	4,610000E+2	5,010000E+2
1,536667E+2	1,670000E+2				
1,139191E+3	-1,099093E+2	9,540000E+2	1,590000E+2	4,990000E+2	4,550000E+2
1,663333E+2	1,516667E+2				
1,139252E+3	-1,098483E+2	9,620000E+2	1,603333E+2	4,680000E+2	4,940000E+2
1,560000E+2	1,646667E+2				
1,139313E+3	-1,097873E+2	9,040000E+2	1,506667E+2	4,530000E+2	4,510000E+2
1,510000E+2	1,503333E+2				
1,139343E+3	-1,097567E+2	9,360000E+2	1,560000E+2	4,700000E+2	4,660000E+2
1,566667E+2	1,553333E+2				
1,139404E+3	-1,096957E+2	9,380000E+2	1,563333E+2	4,600000E+2	4,780000E+2
1,533333E+2	1,593333E+2				
1,139435E+3	-1,096652E+2	8,590000E+2	1,431667E+2	4,460000E+2	4,130000E+2
1,486667E+2	1,376667E+2				
1,139496E+3	-1,096042E+2	8,770000E+2	1,461667E+2	4,540000E+2	4,230000E+2
1,513333E+2	1,410000E+2				

```
1,139557E+3 -1,095431E+2      8,780000E+2 1,463333E+2 4,200000E+2 4,580000E+2
      1,400000E+2 1,526667E+2
...
```

## 3.2 XAS Data

### 3.2.1 NEXAFS (\*.dat)

Comment:

- Data format of a NEXAFS measurement with non-equidistant steps
- no header, only one region saved
- Data: 1. column: increasing Photon energy, 2. column: Intensity
- Example: single region, C K-edge
- Folder: Install-Memory Card:\XAS\_Measurement\_Reference\_Data\01-NEXAFS(.DAT)\NEXAFS-SingleReg-C-k-edge.DAT

```
2.4950000e+002 2.1793560e-002
2.5000000e+002 2.4780615e-002
2.5050000e+002 2.2961416e-002
2.5100000e+002 1.2672400e-002
2.5150000e+002 4.9331094e-003
...
3.2850000e+002 9.8077209e-001
3.2900000e+002 9.7172535e-001
3.2950000e+002 9.5216975e-001
```

### 3.2.2 BESSY-EMP/2 (\*.\*)

Comment:

- Data format of a BESSY-EMP/2 measurement with non-equidistant steps
- Energy axis is not monotonous
- Header includes number of scans, number of points
- The intensities and reference data are saved after the line BEGIN, 1. columns: Photon energy, next columns intensities and reference data
- Example: single region, Ti L-edge
- Folder: Install-Memory Card:\XAS\_Measurement\_Reference\_Data\02-BESSY-EMP2\BESSY-EMP2-SingleReg-Ti L-edge.008

```
Comment :
Probe :
CfgTyp : $627
Fileform : $BF
Date : 89.6545.14 22:11:26
Program : EMP/2-M
Version : 00.4A0
MeasTyp : CFS
Analys. : 1
Scans : 1
Points : 181
MonSta : 4.540000000E+02
MonEnd : 4.900000000E+02
AnaSta : 2.000000000E+02
AnaEnd : 6.000000000E+02
AnaRange : 9.000000000E+03
AnaMin : 0.000000000E+00
DacSta : 0.000000000E+00
DacEnd : 1.000000000E+01
```

```

DeltaE      : 0.000000000E+00
MonName     : UE56/2-PGM-1
MonType     : 1
MonUnit     : Step/S
MonSpeed    : 5.000000000E+02
MonRewind   : 0.000000000E+00
MonSweep    : 2.000000000E+00
IdPos      : 2.760960000E+01
IdMode     : 0
LiveTime    : 1.000000000E+00
DeadTime    : 8.000000000E-03
MeasTime    : 3.282360000E+02
ScanTime    : 3.281739490E+02
ScanCtrl    : ENERGY
DelayVal    : 0.000000000E+00
SecMeas    : FALSE
XMonFile    :
XAnaFile    :
P_TakeUp   : TRUE
ChanOrder  : 1,2,3
Devices     : NAME=KEITHLEY@4, TIME=
1.00000E+00, MODE=1, RANGE=1, AVERAGE=0, TRIGGER=1, OPEN=256, UNIT=Ampere
             NAME=KEITHLEY@14, TIME=
1.00000E+00, MODE=1, RANGE=1, AVERAGE=0, TRIGGER=1, OPEN=256, UNIT=Ampere
             NAME=Ringstrom EXP, TIME=
1.00000E+00, MODE=1, RANGE=0, AVERAGE=0, TRIGGER=1, OPEN=0, UNIT=mA
Display     : COLOR=$FF0000, TYPE=19, LINE=0, POINT=0, WINNR=1, NAME=
             COLOR=$008200, TYPE=19, LINE=0, POINT=0, WINNR=2, NAME=
             COLOR=$00007B, TYPE=19, LINE=0, POINT=0, WINNR=3, NAME=
Arithm.    : OFFS= 0.000000000E+00, OFFS2=
0.000000000E+00, FUNC=$0, FINR=$10, VAL1=$0, VAL2=$2, OPER=$4, BITS=$0, NAME=STDMATH
             OFFS= 0.000000000E+00, OFFS2=
0.000000000E+00, FUNC=$0, FINR=$0, VAL1=$2, VAL2=$0, OPER=$0, BITS=$0, NAME=STDMATH
             OFFS= 0.000000000E+00, OFFS2=
0.000000000E+00, FUNC=$0, FINR=$0, VAL1=$3, VAL2=$0, OPER=$0, BITS=$0, NAME=STDMATH
DATAVALUE:
BEGIN
4.5400000E+02  6.904326E-10  5.028900E-08  1.900910E+02
4.5420000E+02  8.018045E-10  4.961500E-08  1.900850E+02
...
4.8960000E+02  1.087048E-09  4.486000E-08  1.891690E+02
4.8980000E+02  1.088562E-09  4.480700E-08  1.891660E+02
4.9000000E+02  1.091602E-09  4.494400E-08  1.891600E+02
END

```

### 3.2.3 MAXlab Scan Zeiss (\*.sp7)

#### Comment:

- Data format of a MAXlab Scan Zeiss measurement with non-equidistant and non-monotone steps (Lund)
- Header includes number of start and end energy, number of scans, dwell time, number of points
- The intensities and reference data are saved in 12 columns with 11 characters after the line: start spectrum data, 1. columns: Photon energy, next columns intensities and reference data
- Example: 2 ML Co on BTO,
- Folder: Install-Memory Card:\XAS\_Measurement\_Reference\_Data\03-MAXlabScanZeiss(.SP7)\MaxLabScanZeiss-SingleReg-Ba M-edge.SX7

```

maxlab scan zeiss program
version = 5
comment = 2ML Co on BTO
date and time = 2011-10-28 22:28:00
ring current MAX1 = 4.76
ring current MAX2 = 264.18

```

```

ring current MAX3 = 64.26
undulator gap = 24.966
minimum energy = 770.020
maximum energy = 809.885
scale factor = 1.000e+000
scans = 1
dwell = 500
number of datapoints = 323
start spectrum data
770.019630 0.000000 0.000000 0.000000 0 9647 56
4023 0 23.952000 264.150000 18.700000
770.200133 0.000000 0.000000 0.000000 0 9629 55
3995 0 23.956000 264.150000 18.700000
...
809.604399 0.000000 0.000000 0.000000 0 7952 59
7085 0 24.809000 260.440000 19.630000
809.885143 0.000000 0.000000 0.000000 0 7941 58
6996 0 24.815000 260.440000 19.630000
end spectrum data

```

### 3.2.4 Lausanne-NanoLab (\*.txt)

Comment:

- Data format of a Lausanne NanoLab measurement with non-equidistant and non-monotone steps
- Header includes number of scans
- The intensities and reference data are saved in 20 columns sparated by the Tab character
- Folder: Install-Memory Card:\XAS\_Measurement\_Reference\_Data\04-Lausanne-NanoLab (\*.txt)\ Lausanne-NanoLab-Ex1.txt

```

From File
Mono Energy
C:\Data\ALS_raw_data\BL7_2012\20120249-Deyoreo\Ca L XAS.txt
: -3.00000000
: 0.00000000
: 1.00000000
Delay After Move (s): 0.00000000
Count Time (s): 2.00000000
Scan Number: 1
Bi-directional: No
Stay at End: 0
Description Length: 0

```

Time of Day	Time (s)	Mono Energy	Beam Current	Shutter Status	Izero		
		Counter 0	Counter 1	Counter 2	Counter 3	Counter 4	Counter 5
		Counter 6	Gate 7 Out	Temp A	Temp B	Temp C	Temp D
		Cold Cathode Gauge	SR Energy				
19:44:21	4.61600000	334.98152024	246.03768190	1.00000000			
	0.32811574	0.00000000	217188.00000000	286835.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	3000000000.00000000	1.89397613			
19:44:25	8.60500000	335.19988286	245.99861015	1.00000000			
	0.32949393	0.00000000	218752.00000000	287115.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	3000000000.00000000	1.89397613			
19:44:31	14.83600000	335.39017042	245.93341351	1.00000000			
	0.32907136	0.00000000	218862.00000000	286896.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	3000000000.00000000	1.89397613			
19:44:37	20.77400000	335.59284063	245.87931416	1.00000000			
	0.32790579	0.00000000	217813.00000000	287333.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
	0.00000000	0.00000000	3000000000.00000000	1.89397613			
19:44:41	25.01000000	335.80387690	245.84602226	1.00000000			
	0.32838429	0.00000000	218156.00000000	285864.00000000	0.00000000	0.00000000	0.00000000

```

0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:44:45 29.03500000 336.00704614 245.81550468 1.00000000
0.32809361 0.00000000 218028.00000000 287125.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:44:49 33.17500000 336.20638998 245.77666413 1.00000000
0.32724433 0.00000000 216735.00000000 286256.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:44:55 39.18400000 336.38151877 245.72117112 1.00000000
0.32616590 0.00000000 216126.00000000 283649.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:44:59 42.89200000 336.60170582 245.67399892 1.00000000
0.32634440 0.00000000 215912.00000000 285105.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:04 48.39900000 336.78541472 245.62405239 1.00000000
0.32659269 0.00000000 216056.00000000 284616.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:11 54.60200000 336.98568085 245.56301724 1.00000000
0.32621503 0.00000000 215852.00000000 285602.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:15 58.73700000 337.20665757 245.53249966 1.00000000
0.32609984 0.00000000 215193.00000000 283313.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:18 62.43700000 337.40332407 245.49088478 1.00000000
0.32591437 0.00000000 215181.00000000 281131.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:22 66.38500000 337.60842840 245.46036720 1.00000000
0.32477547 0.00000000 214457.00000000 281865.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
...
20:05:45 1289.45100000 364.52621530 234.35718363 1.00000000
0.34323552 0.00000000 226474.00000000 289185.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:05:50 1293.59700000 364.65540722 234.29892280 1.00000000
0.34345527 0.00000000 225931.00000000 287053.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:05:53 1297.19900000 364.80385136 234.26008224 1.00000000
0.34483647 0.00000000 226430.00000000 290068.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:05:57 1301.47800000 364.95241610 234.22956467 1.00000000
0.34543259 0.00000000 227133.00000000 289884.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:06:01 1305.26500000 365.10110157 234.19072411 1.00000000
0.34546582 0.00000000 227048.00000000 289365.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613

```

### 3.2.5 SPECS Prodigy (\*.xy)

Comment:

- Data format of a SPECS Prodigy, y non-equidistant and non-monotone steps
- Header general options and all acquisition parameters

- Example includes four external data sets: a) Excitation Energy, b) Ring Current, c) TEY data d) Mirror Current
- Folder: Install-Memory Card:\XAS\_Measurement\_Reference\_Data\06-SPECS-Prodigy(.XY)\NEXAFS-V4.54-withExternalData.xy
- # Created by: SpecsLab Prodigy, Version 4.54.2-r81990
- #
- # XY-Serializer Export Settings:
- # Comment Prefix: #
- # Output meta data: yes
- # Energy Axis: Kinetic Energy
- # Count Rate: Counts per Second
- # Separate Scan Data: no
- # Separate Channel Data: no
- # External Channel Data: yes
- # Transmission Function: no
- # ErrorBar: no
- # Operation Results: no
- # Time Zone Format: UTC
- #
- # Group: Ti Cylinder
- #
- # Region: O K 12
- # Acquisition Date: 03/09/16 10:58:09 UTC
- # Analysis Method: XPS
- # Analyzer Lens: MediumMagnification:3.5kV
- # Analyzer Slit: 5:7x20\3:Mesh
- # Scan Mode: ConstantFinalState
- # Curves/Scan: 1
- # Values/Curve: 761
- # Dwell Time: 0.1
- # Excitation Energy: 522
- # Kinetic Energy: 385
- # Pass Energy: 50
- # Bias Voltage: 100
- # Detector Voltage: 1850
- # Eff. Workfunction: 4.27
- # Source: ISISS PGM
- # Comment:
- # OrdinateRange: [-20.166667, 20.166667]
- #
- # Cycle: 0
- # Number of Scans: 1
- #
- # Cycle: 0, Curve: 0
- # Acquisition Date: 03/09/16 10:58:09 UTC
- #
- # ColumnLabels: energy counts/s
- #
- 522 266343.13
- 522.05 293671.56
- 522.1 290481.25
- 522.15 289146.32
- 522.2 291741.02
- 522.25 293941.32

```
• ...
• 559.8 442045.44
• 559.85 440262.91
• 559.9 443258.65
• 559.95 445191.17
• 560 438124.18
•
• # External Channel Data Cycle: 0, Excitation Energy [eV] (ISISS PGM)
• #
• # ColumnLabels: energy Excitation Energy [eV] (ISISS PGM)
• #
• 522 522.01298630215422
• 522.05 522.10904959445077
• 522.1 522.14620941060718
• 522.15 522.194591061251
•
• ...
• 559.95 559.95709460954743
• 560 560.00059620542345
• # External Channel Data Cycle: 0, Ring Current [mA] (ISISS PGM)
• #
• # ColumnLabels: energy Ring Current [mA] (ISISS PGM)
• #
• 522 298.710733
• 522.05 298.710733
• 522.1 298.710733
• 522.15 298.710733
•
• ...
• 559.9 298.28434800000002
• 559.95 298.272899999999999
• 560 298.272899999999999
• # External Channel Data Cycle: 0, TEY [V] (ARMIN-10)
• #
• # ColumnLabels: energy TEY [V] (ARMIN-10)
• #
• 522 1.5191882200350957
• 522.05 1.5190356298161287
•
• ...
• 559.9 2.2957198443579765
• 559.95 2.2989242389562827
• 560 2.2999923704890515
• # External Channel Data Cycle: 0, I_mirror [V] (ARMIN-10)
• #
• # ColumnLabels: energy I_mirror [V] (ARMIN-10)
• #
• 522 1.1810482948043031
• 522.05 1.18120088502327
•
• ...
• 559.8 1.3424887464713511
• 559.85 1.342793926909285
• 559.9 1.342946517128252
• 559.95 1.3432516975661859
• 560 1.3432516975661859
• # Region: Ti L 13
• # Acquisition Date: 03/09/16 11:02:04 UTC
• # Analysis Method: XPS
• # Analyzer Lens: MediumMagnification:3.5kV
```

```

• # Analyzer Slit:      5:7x20\3:Mesh
• # Scan Mode:         ConstantFinalState
• # Curves/Scan:       1
• # Values/Curve:      901
• # Dwell Time:        0.1
• # Excitation Energy: 440
• # Kinetic Energy:    390
• # Pass Energy:       50
• # Bias Voltage:      100
• # Detector Voltage:  1850
• # Eff. Workfunction: 4.27
• # Source:            ISISS PGM
• # Comment:
• # OrdinateRange:     [-20.166667, 20.166667]
• #
• # Cycle: 0
• # Number of Scans:  1
• #
• # Cycle: 0, Curve:  0
• # Acquisition Date: 03/09/16 11:02:04 UTC
• #
• # ColumnLabels:      energy counts/s
• #
• 440  106039.6
• 440.05  116171.64
• 440.1  114897.57
• 440.15  116211.84
• 440.2  115499.73
• 961242085
• 484.95  1.0984969863431755
• 485  1.0986495765621425
...

```

### 3.2.6 Photon Energy/Intensity (\*.dat)

Comment:

- Data format with non-equidistant steps
- no header, only one region saved
- Data: 1. column: increasing Photon energy, 2. column: Intensity

#### Version 1: PE decreasing

- Photon energy direction: decreasing
- Example: single region, C K-edge
- Folder: Install-Memory Card:\XAS\_Measurement\_Reference\_Data\05-PhotonEnergyIntensity(.DAT)\PE-decreasing-SingleReg-C K-edge.DAT

```

329.5 0.95216975
329   0.97172535
328.5 0.98077209
...
250   0.024780615
249.5 0.02179356

```

#### Version 2: PE increasing

- Photon energy direction: increasing

- Example: single region, C K-edge
- Folder: Install-Memory Card:\XAS\_Measurement\_Reference\_Data\05-PhotonEnergyIntensity(.DAT)\PE-increasing-SingleReg-C K-edge.DAT

```
2.4950000e+002  2.1793560e-002
2.5000000e+002  2.4780615e-002
...
3.2900000e+002  9.7172535e-001
3.2950000e+002  9.5216975e-001
```

### 3.3 AES Data

#### 3.3.1 VAMAS (\*.vms)

Comment:

- ‚NORM‘ in 7. row means ‚Multiregion Measurement‘
- Acquisition parameters saved in header of each region
- Energie axis: KE
- Example: multiregion measurement with 6 regions (C,, O, Pb, Mg, Al, Si)
- Folder: Install-Memory Card:\AES\_Measurement\_Reference\_Data\02-Vamas (.VMS)\VAMAS-MultiReg-C-O-Mg-Al-Si.VMS

VAMAS Surface Chemical Analysis standard Data Transfer Format

9500F

```
0
NORM
REGULAR
6
1
Sur1
d
0
0
0
0
6
1st block id
1st sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
```

```
0.0
0.0
0.000000
0.000000
55.0
270.0
C

-1
kinetic energy
eV
245.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.0
1110704128.0
270
0.0
0
48
88991
92272
89655
89357
...
91940
92057
92272
2nd block id
2nd sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
O

-1
kinetic energy
eV
454.000000
```

```
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.000000
1.10625e+009
270
0
0
86
110295
123403
110295
110499
...
114918
114537
3rd block id
3rd sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
Mg

-1
kinetic energy
eV
1139.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.000000
1.10625e+009
270
0
0
64
```

```
154883
160094
154958
...
157743
157784
4th block id
4th sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
Al

-1
kinetic energy
eV
1347.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.000000
1.10625e+009
270
0
0
61
169114
172551
169114
...
171943
172261
5th block id
5th sample id
2011
8
15
12
0
45
```

```
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
Si

-1
kinetic energy
eV
1570.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
6
0.000000
1.10625e+009
270
0
0
75
185302
190447
185302
185576
...
189879
189924
6th block id
6th sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
```

```
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
Pb

-1
kinetic energy
eV
2145.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.000000
1.10625e+009
270
0
0
68
224162
239857
23302
...
224719
225152
end of experiment
```

### 3.3.2 PHI Spectrometer

Comment:

- Header in ASCII from SOFH to EOFH
- Different software versions define the line numbers of acquisition information as well as the format of the saved intensities
- Intensities saved in cps
- Intensities saved on the end of the file as single float or double float numbers (number of bytes: 4x or 8x number of channels of all regions)

#### 3.3.2.1 Multiregion Measurements (\*.spe)

##### Software Version 1: Without software specification

- Example PHI 700. multiregion measurement, 4 regions (C, O, Fe, Ni)
- Folder: Install-USB-Memory-Card:\AES\_Measurement\_Reference\_Data\03-PHI-NORM(.SPE)\PHI-MultiReg-V1-without\_software\_specification-PHI-700-C-O-Fe-Ni.SPE

```
SOFH
Platform: PC
Technique: AES
FileType: SPECTRUM
FileDesc: Stainless Steel
AcqFilename: C:\Datafiles\StainlessSteel\Stahl.101.spe
FileDate: 2011 5 2
AcqFileDate: 2011 5 2
Institution: PHI
Operator: phiuser
```

ExperimentID: IntroPhoto  
EnergyReference: none 0.0  
RegisterImage: no  
RegImageInterval: 1  
RegImageMode: 1  
NegativeData: yes  
PlatenID: apr26a  
PhotoFilename:  
SXIFilename:  
HERO Mode: no  
EBeamScanIncXY: 1.73007813 1.29755860 um  
SemFieldOfView: 885.8000040  
ImageShift: 0.000 0.000  
Focus: 50.000 V  
Stigmation: -0.3 -6.9  
Rotation: 0.0  
Tilt: 0.0  
Detector: 1  
BseEnergy: 0.0  
AesMultiplier: 2150.0 V  
Contrast: 15.0  
Brightness: 50.0  
Gamma: 0.0  
DcOffset: 50.0  
InverseVideo: no  
HoldImage: no  
VideoCalibrate: no  
PseudoColor: no  
EBeamEnergy: 10.0 kV  
EBeamCurrent: (null)  
ExtractorSteering: -1.2 2.9  
FocusSteering: -4.4 -16.7  
GunLensVoltage: 0.510  
ImageSizeXY: 100.0000 75.0000  
IonGunMode: Blank  
SputterIon: Ar+  
SputterCurrent: 0.000 uA  
SputterRate: 150.000 A/min  
SputterEnergy: 2.000 kV  
FloatVolt: 0.0 V  
FloatEnable: no  
GridVolt: 150.0  
CondensorVolt: 1518.00  
ObjectiveVolt: 1475.00  
BendVolt: 75.00  
SputterRaster: 1.00 1.00 mm  
SputterRasterOffset: 0.050 -0.510 mm  
TargetSputterTime: 0.5 min  
SputterEmission: 15.00 mA  
DeflectionBias: 0.0 V  
ScanMode: scan  
AnalyserMode: FRR  
MultNumCycles: 30  
MultTimePerStep: 20.000000  
NumSpatialLines: 3  
SpatialLine: 1 1 1 251.0 251.0  
SpatialLine: 2 1 1 68.0 68.0  
SpatialLine: 3 1 1 318.0 318.0  
PhotoZoomMode: Low Magnification  
PhotoSizeInPixel: 2570 2660  
PhotoOffsetInPixel: 778 56  
PhotoSizeInMm: 57.702 59.690  
PhotoOffsetInMm: -50.000 -50.000  
NoSpectralRegFull: 4  
SpectralRegDefFull: 1 1 C1 6 0 1.0000 231.0 311.0 249.0 283.0 0.000000 0.00 none  
SpectralRegDef2Full: 1 80.0 5 8 1 1  
SpectralRegBackgroundFull: 1 243.0 266.0 287.0

```

SpectralRegHeroFull: 1 266.0 266.0 0.0 0.50
SpectralRegDefFull: 2 1 O1 8 0 1.0000 472.0 552.0 490.0 524.0 0.000000 0.00 none
SpectralRegDef2Full: 2 80.0 5 8 1 1
SpectralRegBackgroundFull: 2 496.0 507.0 525.0
SpectralRegHeroFull: 2 507.0 507.0 0.0 0.50
SpectralRegDefFull: 3 1 Fe2 26 0 1.0000 612.5 672.5 630.5 664.5 0.000000 0.00
none
SpectralRegDef2Full: 3 60.0 10 8 1 1
SpectralRegBackgroundFull: 3 616.0 647.0 669.0
SpectralRegHeroFull: 3 647.0 266.0 0.0 0.50
SpectralRegDefFull: 4 1 Ni1 28 0 1.0000 811.0 871.0 829.0 863.0 0.000000 0.00
none
SpectralRegDef2Full: 4 60.0 20 8 1 1
SpectralRegBackgroundFull: 4 827.0 846.0 873.0
SpectralRegHeroFull: 4 846.0 266.0 0.0 0.50
NoSpectralReg: 4
SpectralRegDef: 1 1 C1 6 81 1.0000 231.0 311.0 249.0 283.0 0.300000 0.00 none
SpectralRegDef2: 1 80.0 5 8 0 0 0.00
SpectralRegBackground: 1 243.0 266.0 287.0
SpectralRegHero: 1 266.0 266.0 0.0 0.50
SpectralRegDef: 2 2 O1 8 81 1.0000 472.0 552.0 490.0 524.0 0.300000 0.00 none
SpectralRegDef2: 2 80.0 5 8 0 0 0.00
SpectralRegBackground: 2 496.0 507.0 525.0
SpectralRegHero: 2 507.0 507.0 0.0 0.50
SpectralRegDef: 3 3 Fe2 26 61 1.0000 612.5 672.5 630.5 664.5 0.600000 0.00 none
SpectralRegDef2: 3 60.0 10 8 0 0 0.00
SpectralRegBackground: 3 616.0 647.0 669.0
SpectralRegHero: 3 647.0 266.0 0.0 0.50
SpectralRegDef: 4 4 Ni1 28 61 1.0000 811.0 871.0 829.0 863.0 1.200000 0.00 none
SpectralRegDef2: 4 60.0 20 8 0 0 0.00
SpectralRegBackground: 4 827.0 846.0 873.0
SpectralRegHero: 4 846.0 266.0 0.0 0.50
NumRefImages: 2
ImageReference: 1 1 1.0 0.0 0.0 0.0 0.0 0.0
ImageReference: 2 0 1.0 0.0 0.0 0.0 0.0 0.0
NumSpatialAreas: 1
SpatialArea: 1 1 1 257.9 261.6 467.9 444.6
DefectPosID: 0
DefectPosComment:
DefectPosU: -11.9814
DefectPosV: -0.2549
DefectPosX: -10.7949
DefectPosY: 0.2203
DefectPosZ: 15.0001
DefectPosTilt: 14.9875
DefectPosRotation: 1.0000
DefectPosRotationSpeed: 1.0000
DefectPosAligment:
DefectPosReferenceImage:
EOFH
□ □ €□ □ □ □ □ □ □ □ pnt sar O^f.Ûã@c/s àñ;
f4 D□ •
...□

```

### 3.3.2.2 PHI Spectrometer/Profile (\*.pro)

Comment:

- With respect to the multiregion files (\*.spe) the header contains additional profile information (e.g. number of parameter steps, sputter time)
- Example PHI 680. multiregion measurement, 4 regions (C, O, Fe, Ni)
- Folder: Install-USB-Memory-Card:\AES\_Measurement\_Reference\_Data\05-PHI-Profile(.PRO)\PHI-Profile-V1-without\_software\_specification-PHI680-SiO2

SOFH

```

Platform: PC
Technique: AES
FileType: DEPTHPRO
FileDesc: 55 nm SiO2 0.5kV 0,5 uA 1x1
FileDate: 113 11 22
AcqFileDate: 113 11 22
AcqFilename: SiO2104.pro
ScanMode: scan
EBeamEnergy: 10.0 keV
EBeamCurrent: 0.000000e+00 A
EBeamDiameter: 0.00 nm
SourceAnalyserAngle: 0.0 d
AnalyserMode: FRR
AnalyserWorkFcn: 4.5 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon:
SputterEnergy: 2.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 1 s
PreAcqSputterRate: 1.0 A/s
NoSpectralReg: 4
SpectralRegDef: 1 1 Si4 14 41 1.0000 1590.0 1630.0 1590.0 1620.0 0.100000 0.00
none
SpectralRegDef: 2 2 O1 8 41 1.0000 487.0 527.0 490.0 524.0 0.100000 0.00 none
SpectralRegDef: 3 3 Si1 14 41 1.0000 73.0 113.0 76.0 110.0 0.100000 0.00 none
SpectralRegDef: 4 4 Cl 6 41 1.0000 246.0 286.0 249.0 283.0 0.100000 0.00 none
NoDPDataCyc: 60
NoPreSputterCyc: 2
SputterInterval: 0.500 s
SputterMode: alt
SampleRotation: off
DepthRecal: no
EBeamScanIncXY: 6.3826 4.8189 um
Magnification: 122.4
NoSpatialArea: 1
SpatialAreaDef: 1 Full 1 (0.0 0.0 0.0 0.0 0.0)
EOFH
  @  ) < pnt øéý•cyc @  ú 1
ñwc/s @  Äú Ôú f4 p& P
...

```

### 3.3.2.3 PHI Spectrometer/Mapping (\*.map)

#### Comment:

- With respect to the multi region files (\*.spe) the header contains additional profile and mapping information (e.g. angle values, number and position of mapping points)

#### Software Version 1: Without software specification

- Example. PHI 700 spectrometer, AES mapping of 256x256 points, one region
- Folder: USB-memory card:\AES\_Measurement\_Reference\_Data\04-PHI-Mapping(.MAP)\PHI-Mapping-256x256-Spectra-PHI700.map

```

SOFH
Platform: PC
Technique: AES
FileType: MAP
FileDesc: Pad 41
SoftwareVersion:
Institution: PHI
FileDate: 112 9 22
AcqFileDate: 2012 9 22

```

```

ScanMode: scan
AcqFilename: C:\Datafiles\IC.412~2_1.map
Operator:
ExperimentID: Pad_41
StagePosition: 0.0000 0.0000 0.0000 0.0000 0.0000
PhotoFilename:
SXIFilename:
EBeamEnergy: 10.0 kV
EBeamCurrent: 10.00 nA
EBeamDiameter: 0.0
NeutralizerEnergy: 0.0
NeutralizerCurrent: 0.0
SourceAnalyserAngle: 0.0 d
AnalyserSolidAngle: 0.0 sr
AnalyserMode: FRR
AnalyserWorkFcn: 3.8 eV
IntensityCalCoeff: 0.000 0.000
SputterIon: Ar+
SputterEnergy: 2.000 kV
SputterCurrent: 0.0 uA
SputterRaster: 2.0 2.0 mm
PreAcqSputterTime: 0
PreAcqSputterRate: 0.0
NoSpectralReg: 1
SpectralRegDef: 1 1 Si4 14 51 0.5000 1628.00000 1603.00000 1627.00000 1604.00000
0.000000 0.00 PEAK_TO PEAK
ImageParam: 1 1.0000 7465.28 32297.05 7465.28 32297.05
NoMapPixelsXY: 256 256
EBeamScanIncXY: 0.7813 0.7813 um
Magnification: 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 -1 1 (-495.6 -15.3 16854.5 0.0 315.1)
SpatialAreaDesc: 1
NoHistory: 1
History: 1 SPEC 1 -1 ""
EOFH
□ □ €□ □ □ □ □ □ □ □ □ pnt pnt c/s
f4

```

### 3.4 RAMAN Data

#### 3.4.1 S\_I VistaControl (\*.tvf)

Comment:

- Data format of the S&I software S&I VistaControl.
- The format has a typical xml structure.
- All acquisition parameters are available.
- All typical measurements can be saved using this format (multi-region measurements, multipoint, parameter-dependent measurements)
- Examples saved on the USB memory installation card:  
RAMAN\_Measurement\_Referecnce\_Data\03-S-I-VistaCtrl(.TVF)

#### 3.4.2 S\_I VistaControl XY Multipoint/Batch Parameter Measurement (\*.csv)

Comment:

- Data format exported using the software S&I VistaControl
- Multipoint measurements and batch-parameter measurements are saved
- Multipoint measurements has the same number of x and y values
- 1. column: wavenumbers, 2. column: intensities

## 1. Batch-Parameter measurement

- Examples includes 300 spectra (frames)
- Batchparameter: Frame number or timestamp
- Examples saved on the USB memory installation card:  
RAMAN\_Measurement\_Referecnce\_Data\02-S-I-VistaCtrlXYMultipoint-BatchParameterMeasurement(.CSV)\S-I-Batch-Parameter-Measurement.csv

Frame 1

44.475;605.000  
46.007;616.000  
47.540;606.000  
49.072;609.000

...

2225.268;5685.000  
2226.488;5487.000  
2227.711;5630.000  
2228.932;5501.000  
2230.154;5507.000  
2231.374;5726.000  
2232.597;5686.000

Frame 2

44.475;599.000  
46.007;616.000  
47.540;622.000  
49.072;595.000  
50.603;596.000  
52.136;615.000  
53.667;614.000  
55.199;617.000

...

2221.600;5628.000  
2222.823;5677.000  
2224.045;5611.000  
2225.268;5676.000  
2226.488;5669.000  
2227.711;5722.000  
2228.932;5672.000  
2230.154;5733.000  
2231.374;5567.000  
2232.597;5677.000

Frame 3

44.475;614.000  
46.007;615.000  
47.540;611.000  
49.072;613.000  
50.603;611.000  
52.136;602.000  
53.667;612.000  
55.199;624.000

...

2228.932;3034.000  
2230.154;3133.000  
2231.374;2935.000  
2232.597;2943.000

Frame 300

44.475;594.000  
46.007;590.000  
47.540;607.000  
49.072;580.000  
50.603;574.000  
52.136;587.000

...  
2230.154;2996.000  
2231.374;2957.000  
2232.597;2998.000

## 2. XY multipoint measurement

- Examples includes 10201 spectra (101x101 frames)
- Batch parameter: Frame number or x|y values generated from the frame number
- Following acquisition parameters are saved: Laser wavelength, slit entrance
- Examples saved on the USB memory installation card:  
RAMAN\_Measurement\_Referecnce\_Data\ 02-S-I-VistaCtrlXYMultipoint-  
BatchParameterMeasurement(.CSV)\ S-I-XY Mapping\_101x101\_Points\_PolySilicon.csv

Document  
Record Time: 29-10-2015 20:58

Experiment  
Used Setup: Raman\_1800\_Stage3

Spectrometers  
Spectrometer  
Serialnumber: 27580596  
Model: SP-2-750i  
Stage\_Number: 1  
Focallength: 752  
Inclusion\_Angle: 6.5  
Detector\_Angle: 0.68  
Groove\_Density: 1800 g/mm  
Slit\_Entrance-Front: 100  
Slit\_Entrance-Side: 0  
Slit\_Exit-Front: 0  
Slit\_Exit-Side: 0

Detector  
Name: PicamModel\_Pixis256E\_08227915  
Serialnumber:  
Detector\_Size: 1024;256  
Detector\_Temperature: -70  
Exposure\_Time\_(ms): 250  
Exposure\_Mode:  
No\_of\_Accumulations: 1  
Calc\_Average: True  
No\_of\_Frames: 1  
ADC\_Readout\_Port:  
ADC\_Rate\_Resolution: 100 KHz  
ADC\_Gain: High  
Clearing\_Mode:  
Clearing\_No\_of\_Cleans: 1  
Region\_of\_Interests: 1|1;1024;1;120;123;4

Calibration  
Center\_Wavelength: 527.980  
Laser\_Wavelength: 514.400

Frame 1  
205.676;27.000  
206.264;23.000  
206.852;27.000  
207.440;24.000  
208.029;24.000  
208.617;24.000  
...

```
780.507;28.000
781.047;24.000
781.588;24.000
782.128;26.000
782.668;24.000
```

```
Frame 2
205.676;25.000
206.264;24.000
206.852;22.000
207.440;24.000
208.029;24.000
208.617;25.000
...
```

### 3.4.3 RRUFF (\*.txt)

#### Comment:

- Data format of RRUFF reference spectra.
- The format has a typical: 1. column: wavelength, 2. column: intensities:
- Following acquisition parameters are available: Name of the reference sample, chemical informations
- Examples saved on the USB memory installation card:  
 RAMAN\_Measurement\_Referecnce\_Data\04-RRUFF(.TXT)\Magnetite\_\_R060191-3\_Raman\_514\_0\_ccw\_Raman\_Data\_RAW\_29858.txt

```
##NAMES=Magnetite
##RRUFFID=R060191
##IDEAL CHEMISTRY=Fe^2+^Fe^3+^_2_O_4_
##LOCALITY=Merry Widow mine, Vancouver Island, British Columbia, Canada
##OWNER=RRUFF
##SOURCE=Lloyd Twaites
##DESCRIPTION=Grayish-black octahedral crystals
##STATUS=The identification of this mineral has been confirmed by X-ray
diffraction and chemical analysis
##URL=ruff.info/R060191
##MEASURED CHEMISTRY=(Fe^2+^_0.97_Mg_0.03_)(Fe^3+^_0.97_Al_0.03_)_2_O_4_
##PIN_ID=M01451
##ORIENTATION=Laser parallel to -a* (-1 0 0). Fiducial mark perpendicular to
laser is parallel to -c [0 0 -1]
126.5290, 41816.00
127.7630, 41778.00
128.9970, 41848.00
130.2300, 42065.00
131.4640, 41809.00
132.6970, 41542.00
133.9300, 41143.00
135.1630, 41653.00
136.3950, 41657.00
...
1539.354, 41909.00
1540.385, 42024.00
1541.415, 41742.00
1542.445, 42134.00
1543.475, 42336.00
1544.505, 42172.73
1545.534, 42228.40
1546.564, 42107.00
##END=
```

### 3.4.4 EMCCD LabRam HR800 (,txt)

Comment:

- One spectrum saved.
- Typical format: 1. column: wavelength (increasing or decreasing), 2. column: intensities
- No acquisition parameters are available.
- Examples saved on the USB memory installation card:  
RAMAN\_Measurement\_Referecnce\_Data\05-EMCCD LabRam HR800(,txt)\Single-Spectrum-WN-decreasing.txt

```
1257.61      126
1256.94      140
1256.27      137.068
1255.6       116.067
1254.93      125.067
1254.26      127
1253.59      133
1252.91      129.068
1252.24      125
...
95.5744      26
94.7839      24
93.9932      21
93.2025      20
92.4117      18
```

### 3.4.5 EMCCD LabRam HR800 Mapping WN decreasing (,txt)

Comment:

- A large number of a multipoint measurement are saved.
- first line: wave number values, decreasing
- next lines: x position, y position, intensities
- Examples saved on the USB memory installation card:  
RAMAN\_Measurement\_Referecnce\_Data\06-EMCCD LabRam HR800 Mapping WN decreasing(,txt)\Mapping-56x56-Points. txt

### 3.4.6 EMCCD LabRam HR800 Mapping WN increasing (,txt)

Comment:

- A large number of a multipoint measurement are saved.
- first line: wave number values, increasing
- next lines: x position, y position, intensities
- Examples saved on the USB memory installation card:  
RAMAN\_Measurement\_Referecnce\_Data\07-EMCCD LabRam HR800 Mapping WN increasing(,txt)\Raman-mapping-WN-increasing. txt

## 4 Files Created Using UNIFIT

### 4.1 Exported Files

#### 4.1.1 Call: [File – Export] (\*.DAT)

##### 4.1.1.1 Standard Windows

Comment:

- 1. row: column labels separated by delimitation characters (comma, semikolon, TAB, space)
- next rows: corresponding values separated by delimitation characters, decimal characters point or comma (selected in preferences)

```
Binding energy(eV);Modified curve;Component1;Component2;Component3;Sumcurve
Summenkurve
408.3;0;0;0;0;0
408.2;0;0;0;0;0
408.1;0;0;0;0;0
408;0;0;0;0;0
...
```

##### 4.1.1.2 3D-Waterfall 0°

Comment:

- Si 2p-Peaks of test spectra Test07, with 11 parameter steps, step width of exported data: 0.01 eV,
- not available intensity values are interpolated,
- 1. row: energy, series name of spectrum 1, series name of spectrum 2, ...,
- 1. column: energy, 2-13 column: intensities,
- intensities are added with an offset according the ,Plot 3D-Waterfall 0°'

```
Energy      0      1      ...     10
113         2.7121940578234  238.137409387496  ...      2369.76427055808
112.99      2.71427871067289  238.138997568196  ...      2369.77127311703
112.98      2.71636336352237  238.140585748896  ...      949.791521608419
112.97      2.71844801637186  238.142173929596  ...      2369.78527823494
...
93.12      6.30441188107536  239.120121329473  ...      948.552694071613
93.11      6.29712509148887  239.117095953769  ...      710.959579868206
93.1       6.28983830190237  239.114070578065  ...      710.957936790574
93.09      *****          *****          *****          *****          *****          *****
93.08      *****          *****          *****          *****          *****          *****
...
93.01      *****          *****          *****          *****          *****          *****          *****          *****
93         *****          *****          *****          *****          *****          *****          *****          *****
```

##### 4.1.1.3 3D-Waterfall 0° Plus

Comment:

- Example: 3 fitted components of the O 1s-Peaks of the test spectra Test07 with 11 parameter steps (0 – 10), energy step width of the exported vales: 0.01 eV,
- not available intensities are interpolated,

- 1. column: energy, 2. column: fitted component 1 of spectrum 11, 2. column: fitted component 2 of spectrum 11, 4. column: sum curve of spectrum 11, 5. column: background of spectrum 11, 6. column: spectrum 11, 7. column: fitted component 1 of spectrum 10, ...
- all intensities are added with an offset according the ‚Plot 3D-Waterfall 0° Plus’

Energy	Comp.11 1	Comp.11 2	Sum11	Backgr.11	Spec.11	Comp.10 1	...
538	*****	*****	*****	*****	*****	*****	...
537.99	11571.1398994772	11567.3744077714	11571.1458861959	...			
537.98	11571.1432848846	11567.3744146244	11571.1492784564	...			
537.97	11571.146670292	11567.3744214775	11571.1526707168	...			
537.96	11571.1500556993	11567.3744283305	11571.1560629772	...			
...							
518.11	11571.2259122073	11567.3710616776	11571.2285528322	...			
518.1	11571.2224181514	11567.3710597136	11571.2250568124	...			
518.09	11571.2189240956	11567.3710577496	11571.2215607926	...			
...							
518.02	*****	*****	*****	*****	*****	*****	...
518.01	*****	*****	*****	*****	*****	*****	...
518	*****	*****	*****	*****	*****	*****	...

#### 4.1.1.4 3D-Waterfall 45°, 3D-Waterfall -45°, 3D-Colour Profile

Comment:

- Example: C 1s-Peaks of test spectra Test07 with 11 parameter steps, energy step width of exported data: 0.01 eV,
- Not available intensities are interpolated,
- 1. row: energy, series name of spectrum 1, series name spectrum 2, ...,
- 1. column: energy, 2-13 columns: intensities

Energy	0	1	2	3	...	9	10	...
291	0.754295684910685			3.01718273964282		3.01718273964282	...	
290.99	0.754972766387796			3.01989106555126		3.01989106555127	...	
290.98	0.755649847864908			3.02259939145971		3.02259939145971	...	
290.97	0.756326929342019			3.02530771736815		3.02530771736816	...	
290.96	0.75700401081913			3.0280160432766		3.0280160432766	...	
...								
271.04	*****	*****	*****	*****	*****	*****	*****	*****
271.03	*****	*****	*****	*****	*****	*****	*****	*****
271.02	*****	*****	*****	*****	*****	*****	*****	*****
271.01	*****	*****	*****	*****	*****	*****	*****	*****
271	*****	*****	*****	*****	*****	*****	*****	*****

#### 4.1.1.5 Parameter Plot

Comment:

- Example: Parameter plot of the quantification of the test spectra Test07 with 11 parameter steps, C 1s (one fitted component), O 1s (two fitted components), Si 2p (three fitted components),
- 1. row: Name of analysed lines,
- 1. column: Parameter values

Energy	0	1	2	3	...	9	10	...
Parameter	C1s Peak1	O1s Peak1	O1s Peak2	Si2p Peak1	Si2p Peak2	Si2p Peak3		
0	199.999999999994	1.00000000000031	999.999999999999	998.985316335666	...			
1	799.999999999998	99.999999999998	899.999999999997	367.799999999992	...			
2	799.999999999998	199.999999999995	799.999999999996	135.299999999989	...			
...								
8	199.999999999994	799.999999999996	199.999999999998	0	...			
9	799.999999999998	899.999999999996	99.999999999997	0	...			

10 799.999999999998 999.999999999999 0.999999999999153 0 ...

#### 4.1.1.6 Wagner Plot

Comment:

- Example: Ag 3d5 + Ag (M4N45N45)
- 1. column: binding energy photoelectron line, 2. column: kinetic energy Auger line, 3. column: Auger parameter, 4. column: chemical compound

BE	KE	AP	Name
368.8	358.2	727	Mg97Ag3
368.2	357.8	726	Ag
368.1	357.2	725.3	Ag2S
367.8	357.4	725.2	Ag2Se
367.8	356.7	724.5	Ag2O
368	356.1	724.1	AgI
367.4	356.6	724	AgO
367.7	355.3	723	AgF
367.3	355.6	722.9	AgF2
367.8	354.2	722	Ag2SO4

#### 4.1.1.7 XY Plot 45°, XY Plot -45°, XY Colour Profile

Comment:

- Example: 'XY Plot 45°' of the peak area of the Si peak, project: Test34.ufp with 24x24 recording points,
- 1. row: Y-axis
- 1. column: X-axis, 2-13 columns: Min/Max intensities or peak areas of the recorded spectra at the points x|y

X-Axis	1	2	...	24
1	423467.7	423467.4	...	423467.4
2	423467.4	379823	...	423467.4
3	423467.4	379823	...	423467.4
...				
23	423467.4	379823	...	423467.4
24	423467.4	423467.6	...	423467.4

#### 4.1.2 Call: [Batch Processing – Export Spectra all Windows] (\*.DAT)

Comments:

- 1. row: ',Binding energy (eV)', delimitation character (comma, semikolon, TAB, space), parameter values separated by delimitation character
- next rows: 1. column: energy, delimitation character, next columns: intensity, separated by delimitation character

```

Bindung energy (eV);0;1;2;3;4;5;6;7;8;9;10
108;1.82855625;1.18251534;1.28344111;1.78622062;2.88535867;4.52153421;3.65612861
;3.29839373;3.44607641;3.74165134;4.08957439
107.9;1.84222591;1.19310322;1.29656132;1.80507558;2.91515248;4.56703303;3.694857
10;3.33490124;3.48489569;3.78410991;4.13614214
...
88.1;4.19741767;1.83362280;1.16257483;1.24468513;2.06188087;3.47350616;2.3483320
2;1.74795594;1.66703554;1.73710620;1.86062184

```

### 4.1.3 Call: [Batch Processing – Export Fit Parameters] (\*.DAT)

Comment:

1. row: 1. region S 2p, 2 doublets, 21 columns
1. column: window number
2. column: intensity 1. peak 1. doublet,
3. column: intensity 2. peak 1. doublet,
4. column: Lorentzian mixing ratio 1. peak 1. doublet,
5. column: Lorentzian mixing ratio 2. peak 1. doublet
- ...
12. column: intensity 1. peak 2. doublet
- ...
2. row: 2. region C 1s, 2 single lines, 11 columns
1. column: window number
- ...
- 3. rows: 3. region N 1s, 2 single lines, 11 columns
- 4. rows: 4. region O 1s, 2 single lines, 11 columns

Example 1: 4 regions (S 2p: 2 doublets; C1s, N1s and O1s: 2 single peaks)

decimal character - comma, delimiter - Tab

Product function, absolute parameters; all parameters exported

1	9180	4590	0,513	0,513	163,88	165,08	1,914	1,914	0	0
	1241	620,83	0	0	168,04	169,24	2,632	2,632	0	0
2	37329	0,449	285,01	2,166	0	2392	0,969	287,66	5	0
3	5005	0,826	399,86	2,465	0	2586	0	401,61	2,516	0
4	14249	0,341	531,79	2,223	0	4381	0,909	533,4	2,028	0

Example 2: Parameter dependent measurement (angle dependent) 18 steps: Si2p, 2 doublets

decimal character - dot, delimiter - semicolon

Product function, absolute parameters; all parameters exported

69.44;328.43;164.21;0.771;0.771;99.36;99.96;0.968;0.968;0;0;182.85;91.42;0.8;0.8  
 ;103.13;103.73;1.868;1.868;0;0  
 65.29;350.12;175.06;0.792;0.792;99.35;99.95;1.052;1.052;0;0;173.49;86.74;0.752;0  
 .752;103.14;103.74;1.853;1.853;0;0  
 61.14;493.58;246.79;0.845;0.845;99.31;99.91;0.888;0.888;0;0;176.81;88.4;0.926;0.  
 926;103.14;103.74;1.733;1.733;0;0  
 56.99;500.5;250.25;0.796;0.796;99.31;99.91;0.956;0.956;0;0;163.92;81.96;0.788;0.  
 788;103.11;103.71;1.81;1.81;0;0  
 52.84;605.71;302.85;0.826;0.826;99.3;99.9;0.897;0.897;0;0;169.89;84.94;0.978;0.9  
 78;103.11;103.71;1.604;1.604;0;0  
 ...  
 7.19;1008;504.41;0.826;0.826;99.34;99.94;0.877;0.877;0;0;130;65;0.999;0.999;103.  
 14;103.74;1.736;1.736;0;0  
 3.04;1228;614.01;0.841;0.841;99.35;99.95;0.854;0.854;0;0;115.04;57.51;0.999;0.99  
 9;103.17;103.77;1.833;1.833;0;0

### 4.1.4 Call: [Concentration - Concentration] and Save 1 (\*.KON)

Comment:

- first row: directory and name of the experimental file
- second row: column annotation
- from third row: data





0.1  
10  
1486.6  
3  
0.3  
FAT  
  
3-5-2004  
LAXL  
23295.2  
23118.5  
23312.2  
23248.2  
23248.7  
23117.2  
23163.2  
23192.3  
23189.6  
23266.4  
23005.6  
23149.6  
23308.6  
23062.1  
23132.7  
23313.4  
23224.6  
23148.4  
23299.8  
23196.4  
23320.4  
23257.7  
23245.1  
23085.6  
22983.8  
22991.1  
23133  
23289.4  
22981  
23021.3  
23436  
23574.4  
23281.3  
23008  
23165.2  
23235.9  
23274.1  
23239.7  
23035.9  
23117.4  
23382.1  
23295.1  
23317.4  
23107  
23131.4  
23378.1  
23157.3  
23291  
23342.7  
23496.7  
23283.8  
23293.5  
23202.3  
23407.7  
23197.6  
23488.6  
23543.2  
23404.1

23467.4  
23524.9  
23547.2  
23637.8  
23658.7  
23696.1  
23820.7  
23963.7  
23885.2  
23954.7  
23766.4  
23897  
23861.9  
24046.7  
24224.2  
24388.4  
24151.8  
24394.1  
24360.3  
24674.3  
24769.5  
25155.8  
25233  
25275  
25615.9  
25914.5  
25779.3  
26122.9  
26406.9  
27010.9  
27557.3  
27907  
28325.1  
29123  
29725.3  
30550.9  
31617.5  
32442.9  
33900.1  
35115.9  
36240.81  
37541.56  
39214.8  
40514.53  
41926.83  
42850.79  
43348.7  
43499.78  
43151.8  
42549.82  
41377.66  
40165.61  
38949.07  
37109.99  
35305.93  
33991.7  
32672.62  
31341.24  
29783.09  
28875.94  
28069.84  
27470.46  
26884.02  
26251.74  
25656.53  
25260.46  
24901.9

24810.52  
24324.52  
24001.17  
23689.34  
23505.6  
23353.8  
23218.05  
22950.42  
22825.78  
22745.92  
22581.12  
22449.29  
22657.66  
22204.4  
22173.21  
22065.13  
21914.06  
21942.75  
22095.5  
21742.55  
21706.65  
21628.56  
21695.16  
21646.55  
21643.82  
21615.08  
21506.93  
21495.3  
21495.96  
21719.95  
21569.77  
21335.37  
21319.21  
21531.32  
21398.7  
21481.54  
21566.87  
21480.9  
21318.7  
21282.54  
21229.77  
21515.82  
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Cu3p_0 Doublet 11
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### 4.3 Fit-Parameter File (\*.PAR)

Comment:

- first row: single peak or doublet
- second row:
  - a) number with three digits: background was fitted, second and third digit = number of peaks
  - b) number with two digits: background subtracted, number = number of peaks
- Parameters
- XPS: for fitted background: last six rows = background parameters: constante parameter, linear parameter, square parameter, cubic parameter, Shirley parameter, Tougaard parameter

- XAS: for fitted background: next five rows = background parameters: constante parameter, linear parameter, square parameter, cubic parameter, Shirley parameter, number of steps, per step: hight, E-A mixing, position, FWHM

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0.956521739130435  
0.866583541147132  
As 3d  
0.939393939393939  
0.822942643391521  
As (L3M45M45)  
0.792322215229704  
0.594219653179191  
C 1s  
0.769433465085639  
0.713216957605985  
Ga (L3M45M45)  
0.679043423536816  
0.530635838150289  
O 1s

0.608558842039018  
0.438150289017341  
O (KL23L23)  
0.272087568412823  
0.66383701188455  
Ga 2p3  
0.206851119894598  
0.251870324189526  
Ga 2p1  
0.13965744400527  
0.397755610972569  
As 2p3  
0.0632411067193676  
0.0236907730673317  
As 2p1  
-0.00592885375494071  
0.0511221945137157  
C (KL23L23)  
0.0691699604743083  
0.665835411471322  
|  
0.794210195091252  
0.757225433526012  
1  
GaAs\_Ozone  
0.262429200755192  
0.0751445086705202  
1  
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Messkurve  
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Curve 299  
Curve 300

1  
1  
0

Binding Energy / eV

```
Intensity / kCounts
Batch parameter
  Intensity / kcps
1936
1031
```

## 4.5 Inelastic Electron Scattering Cross-Section File (\*.CRO)

Remark:

- saved in Unifit\_2024\_User\_Files\cross section\\*.cro
- example: estimated inelastic electron scattering cross section of SiO<sub>2</sub>

```
SiO2-Hesse.cro
Cross Section
1000
1386.6
1486.6
0.1
0
1486.6
1
1
FAT
Cross
24.08.2010
-
630.551
739.378
-1.345
611.651
1
1
1
1
1
1
```

## 4.6 Calculation Transmission Function Synchrotron Radiation (\*.DAT)

Remark:

- saved in Unifit\_2024\_User\_Files\XPS-transfct\\*.dat
- example: ten peak pairs of a IL compound
- first column: energy, second column: intensity ratios, third column: atomic ratio

```
Energy-Intensity-Ratio Estimation T(E)
1195 49.19 7
798 50.81 6
1195 72.38 7
1085 27.63 3
1195 62.2 7
954 37.8 4
954 63.72 4
1318 36.68 2
1085 52.02 3
1318 47.98 2
964 46.27 7
565 53.72 6
864 69.61 7
852 30.39 3
964 61.27 7
721 38.73 4
721 61.52 4
1085 38.48 2
```

```
852 52.47 3
1085 47.53 2
```

## 4.7 Project Processing Steps/Design (\*.PPD)

Remark:

- saved in Unifit\_2024\_User\_Files\ My Unifit Project Processing Steps\\*.ppd
- all processing steps and the design features can be saved in one file without spectra
- all peak-names of the processing steps have to be different
- the number of regions is not limited
- example: sample: analysis and design of the As 2p3 peak of GaAs

```
1
As2p3
0 2024
0
As2p3
1
1
-1
-1
-1
0
0
2866
1643
1
0
0
0 0 0 0 0
0

0
0
0
5
0
0
1595
668
1
As 2p3
0.200831
0.4063205
1
Probe 1
0.1066482
0.1783296
0
4
1
84328.36
17.30417
0.05804748
0
0.000755178
0
0
0
0
0
0
0
```

0  
2  
1  
1  
Wahr  
0  
Peak  
0  
188357.2  
30  
370  
1333.01  
1316.01  
NORM  
Peak  
405  
GaAs  
Dublett 1  
1  
0  
5000000  
36188.75  
0  
0  
1  
0  
1  
0.55  
1  
0.6423534  
0  
0  
1  
0  
1  
1322.9  
1323.3  
1322.907  
0  
0  
1  
1322.907  
1  
0.1  
10  
1.757303  
0  
0  
1  
0  
1  
0  
1  
0  
1  
0  
1  
0  
1  
0  
1  
As  
Dublett 2  
1  
0  
163743400000  
4520.299  
0

0  
1  
0  
1  
0.6002151  
0.9177305  
0.6423534  
1  
0  
1  
0  
1  
1323.707  
1324.107  
1324.107  
0  
0  
1  
1324.107  
1  
0.1676468  
16.76661  
1.757303  
1  
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1  
0  
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1  
AsO  
Dublett 3  
1  
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163743400000  
12283.88  
0  
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1  
0.6002151  
0.9177305  
0.6423534  
1  
0  
1  
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1  
1325.107  
1325.507  
1325.475  
0  
0  
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1325.475  
1  
0.1676468  
16.76661  
1.757303  
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As203  
Dublett 4  
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163743400000  
25805.46  
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0.6002151  
0.9177305  
0.6423534  
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1325.807  
1326.207  
1326.207  
0  
0  
1  
1326.207  
1  
0.1676468  
16.76661  
1.757303  
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As205  
Dublett 5  
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163743400000  
2414.963  
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0.6002151



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16711935  
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16711680  
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65280  
0  
1  
64  
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8421504  
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12615680  
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16744448  
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8454016  
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12615680  
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4259584  
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12615935  
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12615808  
20  
4194432  
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10485760  
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8388736  
23  
16711935  
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8388863  
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16711680  
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4227072  
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RegionEnd

## 5 Data Banks Integrated in UNIFIT

### 5.1 Auger Parameter (\*.AUP)

Comment:

- Saved in Unifit\_2024\_User\_Files\auger parameters
- Example of Ag 3d5 and Ag (M4N45N45)
- Data structure: ,space',Auger parameter',='',position photoelectron peak as BE',+',,position Auger line as KE',',space',,space',,name of the Auger parameter'

```
727.0=368.8+358.2 Mg97Ag3
726.0=368.2+357.8 Ag
725.3=368.1+357.2 Ag2S
725.2=367.8+357.4 Ag2Se
724.5=367.8+356.7 Ag2O
724.1=368.0+356.1 AgI
724.0=367.4+356.6 AgO
723.0=367.7+355.3 AgF
722.9=367.3+355.6 AgF2
722.0=367.8+354.2 Ag2SO4
```

### 5.2 Peaks Positions of Photoelectron Lines (\*.POS)

Comment:

- Saved in Unifit\_2012\_User\_Files\lines
- Example of the Ag 3d5 peak
- Data structure: ,space',position as BE',',space',,space',,name of compound'

```
368.1 Ag2S
367.3 AgF2
367.4 AgO
367.5 Ag2CO3
367.7 AgF
367.8 CuAgSe
367.8 Ag2Se
367.8 Ag2SO4
367.8 Ag2O
368.0 AgI
368.2 Ag
368.4 Ag (OAc)
368.8 AgOCCF3
368.8 Mg97Ag3
368.8 Ag2Yb
```

### 5.3 Sensitivity Factors (\*.SEN)

Comment:

- 1. row ,Sensitivity Factors'
- from row 2: line, comma, sensitivity factor, line...
- number of data pairs as many as you needed
- saved in Unifit\_2024\_User\_Files\sensifivity factors
- Example: Wagner factors
- If the file name starts with WAG, than the values are empirical data and the mean free path and transmission function in the quantification are setted to one.

## Sensitivity Factors

Ag3p3, 1.52, Ag3d3, 2.10, Ag3d5, 3.10, Ag3d, 5.20, Al2s, 0.23, Al2p, 0.185, Ar2s, 0.4, Ar2p, 0.96, As3p1, 0.97, As3d, 0.53, As2p3, 6.8  
 Au4d5, 2.05, Au4f5, 2.15, Au4f7, 2.8, Au4f, 4.95, B1s, 0.13, Ba3d5, 7.9, Ba4d, 2.35, Be1s, 0.059, Bi4d5, 2.5, Bi4f5, 3.15, Bi4f7, 4.25  
 Bi4f, 7.4, Bi5d, 1.1, Br3p, 0.14, Br3d, 0.83, Cl1s, 0.25, Ca2s, 0.47, Ca2p1, 0.53, Ca2p3, 1.05, Ca2p, 1.58, Cd3p3, 1.6, Cd3d5, 3.5, Ce3d, 10.0  
 Ce4d, 2.0, Cl2s, 0.37, Cl2p, 0.73, Co2p1, 1.3, Co2p3, 2.5, Co2p, 3.8, Co3p, 0.35, Cr2p1, 0.8, Cr2p3, 1.5, Cr2p, 2.3, Cr3p, 0.21, Cs3d5, 7.2  
 Cs4d, 2.0, Cu2p1, 2.1, Cu2p3, 4.2, Cu2p, 6.3, Cu3p, 0.65, Dy4d, 2.0, Dy4p3, 0.6, Er4p3, 0.6, Er4d, 2.0, Eu3d, 5.0, Eu4d, 2.0, F1s, 1.0, F2s, 0.04  
 Fe2p1, 1.0, Fe2p3, 2.0, Fe2p, 3.0, Fe3p, 0.26, Ga2p3, 5.4, Ga3p, 0.84, Ga3d, 0.31, Gd3d5, 3.0, Gd4d, 2.0, Ge2p3, 6.1, Ge3p, 0.92, Ge3d, 0.38  
 Hf4d3, 0.93, Hf4d5, 1.42, Hf4d, 2.35, Hf4f, 2.05, Hg4d5, 2.15, Hg4f5, 3.15, Hg4f7, 2.35, Hg4f, 5.5, Ho4d, 2.0, Ho4p3, 0.6, I3d5, 6.0, I4d, 1.44  
 In3p3, 1.68, In3d5, 3.9, Ir4d5, 1.84, Ir4f5, 1.7, Ir4f7, 2.25, Ir4f, 3.95, K2s, 0.43, K2p1, 0.41, K2p3, 0.83, K2p, 1.24, Kr3p1, 0.39, Kr3p3, 0.82  
 Kr3p, 1.23, La3d, 10.0, La4d, 2.0, Li1s, 0.02, Lu4p3, 0.6, Lu4d, 2.0, Mg1s, 3.5, Mg2s, 0.2, Mg2p, 0.12, Mn2p1, 0.9, Mn2p3, 1.7, Mn2p, 2.6, Mn3p, 0.22  
 Mo3p3, 1.17, Mo3d3, 1.09, Mo3d5, 1.66, Mo3d, 2.75, N1s, 0.42, Na1s, 2.3, Na2s, 0.13, Nb3p3, 1.1, Nb3d3, 0.96, Nb3d5, 1.44, Nb3d, 2.4  
 Nd3d, 7.0, Nd4d, 2.0, Ne1s, 1.5, Ne2s, 0.07, Ni2p1, 1.5, Ni2p3, 3.0, Ni2p, 4.5, Ni3p, 0.5, O1s, 0.66, O2s, 0.25, Os4d3, 0.85, Os4d5, 1.75, Os4d, 2.9  
 Os4f, 3.5, P2s, 0.29, P2p, 0.39, Pb4d5, 2.35, Pb4f5, 2.95, Pb4f7, 3.85, Pb4f, 6.7, Pb5d, 1.0, Pd3p3, 1.43, Pd3d3, 1.9, Pd3d5, 2.7, Pd3d, 4.6  
 Pm3d, 6.0, Pm4d, 2.0, Pr3d, 9.0, Pr4d, 2.0, Pt4d5, 1.92, Pt4f5, 1.85, Pt4f7, 2.55, Pt4f, 4.4, Rb3p1, 0.43, Rb3p3, 0.87, Rb3p, 1.3, Rb3d, 1.23  
 Re4d3, 1.09, Re4d5, 1.66, Re4d, 2.75, Re4f5, 3.1, Rh3p3, 1.38, Rh3d3, 1.7, Rh3d5, 2.4, Rh3d, 4.1, Ru3p3, 1.3, Ru3d3, 1.45, Ru3d5, 2.15  
 Ru3d, 3.6, S2s, 0.33, S2p, 0.54, Sb3d5, 4.8, Sb4d, 1.0, Sc2s, 0.5, Sc2p1, 0.55, Sc2p3, 1.1, Sc2p, 1.65, Se3p, 1.05, Se3d, 0.67, Si2s, 0.26, Si2p, 0.27  
 Sm3d3, 5.0, Sm4p1, 2.0, Sn3p3, 1.77, Sn3d5, 4.3, Sr3p1, 0.46, Sr3p3, 0.92, Sr3p, 1.38, Sr3d, 1.48, Ta4d3, 1.0, Ta4d5, 1.5, Ta4d, 2.5, Ta4f, 2.4  
 Tb3d5, 3.0, Tb4d, 2.0, Tc3p3, 1.24, Tc3d3, 1.26, Tc3d5, 1.89, Tc3d, 3.15, Te3d5, 5.4, Te4d, 1.23, Th4d5, 3.5, Th4f7, 7.8, Th5d3, 0.6, Th5d5, 0.9  
 Th5d, 1.5, Ti2s, 0.54, Ti2p1, 0.6, Ti2p3, 1.2, Ti2p, 1.8, Ti3p, 0.21, Tl4f5, 2.65, Tl4f7, 3.5, Tl4f, 6.15, Tl5d, 0.9, Tm4p3, 0.6, Tm4d, 2.0, U4d5, 3.85  
 U4f7, 9.0, U5d3, 0.6, U5d5, 1.0, U5d, 1.6, V2p1, 0.65, V2p3, 1.3, V2p, 1.95, V3p, 0.21, W4d3, 1.03, W4d5, 1.57, W4d, 2.6, W4f, 2.75, Xe3d5, 6.6  
 Xe4d, 1.72, Y3p1, 0.59, Y3p3, 0.98, Y3p, 1.47, Y3d, 1.76, Yb3p3, 0.6, Y4d3, 2.0, Zn2p3, 4.8, Zn3p, 0.75, Zr3p1, 0.53, Zr3p3, 1.04, Zr3p, 1.56, Zr3d3, 2.1

**5.4 Satellite File (satellit.set)**

This file includes the rel. heights and energy-positions of the excitation satellites.

Comment:

- 1<sup>st</sup> row: name of satellite linie (1 =  $\alpha_3$ , 2 =  $\alpha_4$ , 3 =  $\alpha_5$ , 4 =  $\alpha_6$ , 5 =  $\beta$ )
- 2<sup>nd</sup> row: energy position of satellite 1. set
- 3<sup>rd</sup> row: rel. height of the satellite 1. set
- 4<sup>th</sup> row: energy position of the satellite 2. set
- 5<sup>th</sup> row: rel. height of the satellite 2. set etc.

Aluminiumsatelliten 1

9.8  
 0.064  
 0  
 0  
 0  
 0  
 0  
 0  
 0

```

0
Magnesiumsatelliten 1
8.4
0.08
0
0
0
0
0
0
0
...
0
0
Aluminiumsatelliten 5
69.7
0.0055
0
0
0
0
0
0
0
0
0
0
Magnesiumsatelliten 5
48.5
0.005
0
0
0
0
0
0
0
0

```

## 5.5 Doublet File (doublet.dda)

This file contains the relative heights and energy separations of the doublet peaks.

Comment:

- 1. value: name of the peaks
- 2. value: relative intensity
- 3. value: separation of the two peaks

Dublett Werte

```

Ag3p, 0.5, 30.8, Ag3d, 0.666, 6.00, Al2p, 0.5, 0.4, Ar2p, 0.5, 2.2, As3d, 0.5, 0.7, Au4d, 0.666,
18.1, Au4f, 0.75, 3.65
Ba3d, 0.666, 15.4, Ba4d, 0.666, 2.6, Bi4d, 0.666, 23.9, Bi4f, 0.75, 5.39, Bi5d, 0.666, 3.1, Br3
p, 0.5, 7.0, Br3d, 0.66, 1.0
Ca2p, 0.5, 3.5, Cd3p, 0.5, 34.1, Cd3d, 0.666, 6.76, Cd4d, 0.666, 0.6, Ce3d, 0.666, 18.3, Ce4d, 0
.666, 4.0, Cl2p, 0.5, 1.6, Co2p, 0.5, 15.05
Co3p, 0.5, 2.0, Cr2p, 0.5, 9.3, Cr3p, 0.5, 1.0, Cs3d, 0.666, 13.9, Cs4d, 0.666, 2.3
Cu2p, 0.5, 19.8, Cu3p, 0.5, 2.4, Dy4d, 0.666, 0.0, Dy4p, 0.5, 40.3, Er4p, 0.5, 45.8, Er4d, 0.666
, 0.0, Eu3d, 0.666, 31.1
Eu4d, 0.666, 0.0, Fe2p, 0.5, 13.2, Fe3p, 0.5, 1.0, Ga2p, 0.5, 26.8, Ga3p, 0.5, 3.0, Ga3d, 0.666,
0.4, Gd4d, 0.666, 0.0
Ge2p, 0.5, 31.1, Ge3p, 0.5, 4.1, Hf4d, 0.666, 8.5, Hf4f, 0.75, 1.55, Hg4d, 0.666, 19.4, Hg4f, 0.
75, 4.1, Ho4d, 0.666, 0.0
Ho4p, 0.5, 36.8, I3d, 0.666, 11.52, I4d, 0.666, 2.0, In3p, 0.5, 37.9, In3d, 0.666, 7.6, In4d, 0.
666, 0.9, Ir4d, 0.666, 15.6, Ir4f, 0.75, 2.95
K2p, 0.5, 2.8, Kr3p, 0.5, 7.8, La3d, 0.666, 16.8, La4d, 0.666, 2.8, Lu4p, 0.5, 53.2, Lu4d, 0.666
, 9.8, Mg2p, 0.5, 0.4

```

Mn2p, 0.5, 11.25, Mn3p, 0.5, 1.0, Mo3p, 0.5, 16.6, Mo3d, 0.666, 3.15, Nb3p, 0.5, 15.5, Nb3d, 0.666, 2.8, Nd4d, 0.666, 0.0  
 Ni2p, 0.5, 17.4, Ni3p, 0.5, 1.5, Os4d, 0.666, 14.6, Os4f, 0.75, 1.7, P2p, 0.5, 0.87, Pb4d, 0.666, 22.1, Pb4f, 0.75, 4.94, Pb5d, 0.666, 2.6  
 Pd3p, 0.5, 27.7, Pd3d, 0.666, 5.25, Pm3d, 0.666, 25.0, Pm4d, 0.666, 0.0, Pr3d, 0.666, 19.5, Pr4d, 0.666, 0.0, Pt4d, 0.666, 17.0  
 Pt4f, 0.75, 3.35, Rb3p, 0.5, 9.6, Rb3d, 0.666, 1.0, Re4d, 0.666, 13.4, Re4f, 0.75, 2.4, Rh3p, 0.5, 24.8, Rh3d, 0.666, 4.75  
 Ru3p, 0.5, 22.2, Ru3d, 0.666, 4.1, S2p, 0.5, 1.2, Sb3d, 0.666, 9.35, Sb4d, 0.666, 1.3, Sc2p, 0.5, 4.9, Se3p, 0.5, 5.8  
 Se3d, 0.666, 0.9, Si2p, 0.5, 0.60, Sm3d, 0.666, 27.2, Sm4p, 0.5, 18.0, Sn3p, 0.5, 41.9, Sn3d, 0.666, 8.5, Sr3p, 0.5, 9.9  
 Sr3d, 0.666, 1.8, Ta4d, 0.666, 11.5, Ta4f, 0.75, 1.8, Tb3d, 0.666, 35.6, Tb4d, 0.666, 0.0, Tc3p, 0.5, 20.0, Tc3d, 0.666, 3.8  
 Te3d, 0.666, 10.34, Te4d, 0.666, 1.5, Th4d, 0.666, 37.0, Th4f, 0.75, 9.2, Th5d, 0.666, 7.1, Ti2p, 0.5, 6.15, Ti3p, 0.5, 0.0  
 Tl4f, 0.75, 4.45, Tl5d, 0.666, 2.2, Tm4p, 0.5, 48.4, Tm4d, 0.666, 0.0, U4d, 0.666, 42.1, U4f, 0.75, 10.85, U5d, 0.666, 9.0  
 V2p, 0.5, 7.7, V3p, 0.5, 0.0, W4d, 0.666, 12.6, W4f, 0.75, 2.15, Xe3d, 0.666, 12.6, Xe4d, 0.666, 2.0  
 Y3p, 0.5, 11.8, Y3d, 0.666, 1.75, Zn2p, 0.5, 23.1, Zn3p, 0.5, 2.9, Zr3p, 0.5, 13.7, Zr3d, 0.666, 2.4

## 5.6 Energies of AES Target Atom Subshells (\*.apo)

This file contains the energies of the target atom subshells of the Auger electron peaks.

Comment:

- 1. name of the element
- 2. name of the subshell
- 3. value of the binding energy of the subshell

Ag M4:374  
 Ag M5:368  
 Al K:1560  
 Al L23:73  
 Ar L3:248  
 As L2:1359  
 As L3:1324  
 Au M4:2291  
 Au M5:2206  
 Au N7:84  
 Au N67:86  
 Ba M4:796  
 Ba N45:91  
 Bi N6:162  
 Bi N7:157  
 Br L3:1550  
 C K:284  
 Ca L2:350  
 Cd M4:412  
 Cd M5:405  
 Ce M4:902  
 Ce M5:884  
 Cl K:2822  
 Cl L23:201  
 Co L3:778  
 Co M23:59  
 Cr L3:574  
 Cs M4:740  
 Cs N5:78  
 Cs N45:78  
 Cu L2:952  
 Cu L3:932  
 Cu M23:76

Dy M4:1333  
Dy M5:1293  
Dy M45:1323  
Er M4:1453  
Er M5:1409  
Dy M45:1431  
Eu M4:1159  
Eu M5:1127  
Eu M45:1143  
F K:697  
Fe L3:707  
Fe M23:52  
Ga L2:1143  
Ga L3:1116  
Ga M23:102  
Dg M4:412  
Gd M5:405  
Gd M45:409  
Ge L3:1217  
Hf M4:1716  
Hf M5:1662  
Hf M45:1689  
Hg M4:2385  
Ho M4:1392  
Ho M5:1352  
Ho M45:1367  
I M4:631  
I M5:619  
In M4:451  
In M5:444  
Ir M4:2116  
Ir M5:2040  
Ir N4:312  
K L2:297  
K L3:295  
Kr L3:1678  
La M4:853  
La M5:836  
La N45:104  
Li K:55  
Lu M4:1639  
Lu M5:1589  
Mg K:1303  
Mg L23:50  
Mn L3:639  
Mo L2:2625  
Mo L3:2520  
N K:410  
Na K:1071  
Na L23:31  
Nb M45:204  
Nd M5:980  
Nd M45:990  
Ne K:870  
Ni L2:870  
Ni L3:853  
O K:543  
Os M4:2031  
P K:2145  
Pb N6:142  
Pd M4:341  
Pd M45:337  
Pm M5:1027  
Pm M45:1049  
Pr M5:929  
Pr M45:938  
Pt M4:2202

Pt M5:2122  
S K:2472  
Sb M4:537  
Sc L3:399  
Se L3:1434  
Si K:1839  
Sm M4:1111  
Sm M5:1083  
Sm M45:1098  
Sn M4:493  
Sr L3:1940  
Ta M5:1735  
Tb M4:1277  
Tb M5:1241  
Tb M45:1257  
Te M4:583  
Th N67:338  
Ti K:4966  
Ti L3:354  
Tl N7:118  
Tm M4:1515  
Tm M5:1468  
Tm M45:1491  
U N67:383  
V L3:512  
W M5:1809  
Xe M4:689  
Y M45:156  
Yb M4:1576  
Yb M5:1528  
Yb M45:1547  
Zn L3:1022  
Zr M45:180

## 5.7 Conversion of PHI Peak Names

### 5.7.1 Data Set 1: XPS and AES

This file contains the peak name conversion of typical PHI-peak names to the correct scientific names. The data set 1 is for XPS instruments and some AES machines.

Comment:

- 1. column: PHI name of the line
- 2. column: correct scientific line name
- Folder: C:\Program Files (x86)\Unifit2024\phi-names\Phi\_names.ele

Ag1, Ag3d  
Ag2, Ag3p3  
Ag3, AgMNN  
Ag4, Ag3d5  
Ag5, Ag3d3  
Ag6, Ag3p1  
Ag7, Ag (MNN)  
Al1, Al2p  
Al2, Al2s  
Al3, Al (KLL)  
Ar1, Ar2p  
Ar2, Ar2s  
Ar3, ArLMM  
As1, As3d  
As2, As3p  
As3, As2p3  
As4, AsLMM

As5,As2p1  
As6,As (LMM)  
Au1,Au4f  
Au2,Au4d5  
Au3,Au4f7  
Au4,Au (MNN)  
Au5,Au (NVV)  
Au6,Au4p1  
Au7,Au4p3  
Au8,Au4d3  
Au9,Au4f5  
B1,B1s  
B2,BKVV  
Ba1,Ba3d5  
Ba2,Ba4d  
Ba3,Ba (MNN)  
Ba4,Ba3d3  
Ba5,Ba (MNN)  
Ba6,Ba4p3  
Be1,Bels  
Bi1,Bi4f  
Bi2,Bi4d5  
Bi3,Bi5d  
Bi4,Bi4f7  
Bi5,Bi4p3  
Bi6,Bi4d3  
Bi7,Bi4f5  
Br1,Br3d  
Br2,Br3p  
Br3,Br (LMM)  
Br4,Br3s  
Br5,Br3p1  
Br6,Br3p3  
C1,C1s  
C2,C (KLL)  
C3,C1s  
Ca1,Ca2p  
Ca2,Ca2s  
Ca3,Ca (LMM)  
Ca4,Ca2p3  
Ca5,Ca2p1  
Cd1,Cd3d5  
Cd2,Cd3p3  
Cd3,CdMNN  
Cd4,Cd4d  
Cd5,CdMNN  
Cd6,Cd3p1  
Cd7,Cd3d3  
Ce1,Ce3d  
Ce2,Ce4d  
Ce3,Ce3d3  
Ce4,Ce3d5  
Ce5,Ce (MNN)  
Cl1,Cl2p  
Cl2,Cl2s  
Cl3,Cl (LMM)  
Co1,Co2p  
Co2,Co2p3  
Co3,Co3p  
Co4,Co (LMM)  
Co5,Co2p1  
Co6,Co (LMM)  
Co7,Co (LMM)  
Co8,Co3s  
Cr1,Cr2p  
Cr2,Cr2p3  
Cr3,Cr3p

Cr4,Cr (LMM)  
Cr5,Cr (LMM)  
Cr6,Cr (LMM)  
Cr7,Cr2s  
Cr8,Cr2p1  
Cr9,Cr3s  
Cs1,Cs3d5  
Cs2,Cs4d  
Cs3,Cs (MNN)  
Cs4,Cs3p3  
Cs5,Cs3d3  
Cs6,Cs4p3  
Cs7,Cs (MNN)  
Cu1,Cu2p  
Cu2,Cu2p3  
Cu3,Cu3p  
Cu4,Cu (LMM)  
Cu5,Cu2p3  
Cu6,Cu2p1  
Cu7,Cu (LMM)  
Cu8,Cu (LMM)  
Cu9,Cu (LMM)  
Dy1,Dy4d  
Dy2,Dy4p3  
Dy3,Dy3d5  
Er1,Er4d  
Er2,Er4p  
Eu1,Eu3d  
Eu2,Eu4d  
F1,F1s  
F2,F2s  
F3,F (KLL)  
F4,F (KLL)  
F5,F (KLL)  
F6,F (KLL)  
Fe1,Fe2p  
Fe2,Fe2p3  
Fe3,Fe3p  
Fe4,Fe (LMM)  
Fe5,Fe2p1  
Fe6,Fe (LMM)  
Fe7,FeLMM  
Ga1,Ga2p3  
Ga2,Ga3p  
Ga3,Ga (LMM)  
Ga4,Ga3d  
Ga5,Ga2p1  
Ga6,Ga (LMM)  
Ga7,Ga (LMM)  
Ga8,Ga (LMM)  
Ga9,Ga (LMM)  
Gd1,Gd4d  
Gd2,Gd3d  
Ge1,Ge2p3  
Ge2,Ge3p  
Ge3,Ge3d  
Ge4,Ge (LMM)  
Ge5,Ge2p1  
Ge6,Ge (LMM)  
Ge7,Ge (LMM)  
Ge8,Ge (LMM)  
Ge9,Ge (LMM)  
Hf1,Hf4f  
Hf2,Hf4d  
Hf3,Hf4d5  
Hf4,Hf4p1  
Hf5,Hf4p3

Hf6, Hf4d3  
Hg1, Hg4f  
Hg2, Hg4d5  
Hg3, Hg4f7  
Hg4, Hg4p3  
Hg5, Hg4d3  
H6, Hg4f5  
Ho1, Ho4d  
Ho2, Ho4p  
I1, I3d5  
I2, I4d  
I3, I (MNN)  
I4, I3p1  
I5, I3p3  
I6, I (MNN)  
I7, I3d3  
In1, In3d5  
In2, In3p3  
In3, In (MNN)  
In4, In (MNN)  
In5, In3p1  
In6, In3d3  
Ir1, Ir4f  
Ir2, Ir4d5  
Ir3, Ir4f7  
Ir4, Ir4p1  
Ir5, Ir4p3  
Ir6, Ir4d3  
Ir7, Ir4f5  
K1, K2p  
K2, K2s  
K3, K (LMM)  
K4, K2p3  
K5, K2p1  
Kr1, Kr3d  
Kr2, Kr3p  
Kr3, Kr3p3  
La1, La3d  
La2, La4d  
La3, La (MNN)  
La4, La3d3  
La5, La3d5  
La6, La4p3  
Li1, Li1s  
Lu1, Lu4d  
Lu2, Lu4p  
Mg1, Mg2s  
Mg2, Mg2p  
Mg3, Mg1s  
Mg4, Mg (KLL)  
Mn1, Mn2p  
Mn2, Mn2p3  
Mn3, Mn3p  
Mn4, Mn (LMM)  
Mn5, Mn2p1  
Mn6, Mn (LMM)  
Mn7, Mn (LMM)  
Mo1, Mo3d  
Mo2, Mo3p3  
Mo3, Mo3d5  
Mo4, Mo3s  
Mo5, Mo3p1  
Mo6, Mo3d3  
N1, N1s  
N2, N (KVV)  
Na1, Na1s  
Na2, Na2s

Na3, Na (KLL)  
Na4, Na2p  
Na5, Na (KLL)  
Nb1, Nb3d  
Nb2, Nb3p3  
Nb3, Nb3d5  
Nb4, Nb3s  
Nb5, Nb3p1  
Nb6, Nb3d3  
Nd1, Nd3d  
Nd2, Nd4d  
Ne1, Ne1s  
Ne2, Ne2s  
Ne3, Ne (KLL)  
Ni1, Ni2p  
Ni2, Ni2p3  
Ni3, Ni3p  
Ni4, Ni (LMM)  
Ni5, Ni2p1  
Ni6, Ni3s  
Ni7, Ni (LMM)  
Ni8, Ni (LMM)  
O1, O1s  
O2, O2s  
O3, O (KVV)  
Os1, Os4f  
Os2, Os4d  
Os3, Os4d5  
Os4, Os4d3  
Os5, Os4p3  
Os6, Os4p1  
P1, P2p  
P2, P2s  
Pb1, Pb4f  
Pb2, Pb4d5  
Pb3, Pb5d  
Pb4, Pb4f7  
Pb5, Pb4p3  
Pb6, Pb4d3  
Pb7, Pb4f5  
Pd1, Pd3d  
Pd2, Pd3p3  
Pd3, Pd (MNN)  
Pd4, Pd3d5  
Pd5, Pd3p1  
Pd6, Pd3d3  
Pm1, Pm3d  
Pm2, Pm4d  
Pr1, Pr3d  
Pr2, Pr4d  
Pt1, Pt4f  
Pt2, Pt4d5  
Pt3, Pt4f7  
Pt4, Pt (MNN)  
Pt5, Pt4p3  
Pt6, Pt4d3  
Pt7, Pt4f5  
Rb1, Rb3d  
Rb2, Rb3p  
Rb3, Rb3p3  
Rb4, Rb3p1  
Rb5, Rb3s  
Re1, Re4f  
Re2, Re4d  
Re3, Re4d5  
Re4, Re4d3  
Re5, Re4p3

Re6, Re4p1  
Re7, Re4s  
Rh1, Rh3d  
Rh2, Rh3p3  
Rh3, RhMNN  
Rh4, Rh3d5  
Rh5, Rh3p1  
Rh6, Rh3d3  
Ru1, Ru3d  
Ru2, Ru3p3  
Ru3, RuMNN  
Ru4, Ru3d5  
Ru5, Ru3p1  
Ru6, Ru3d3  
S1, S2p  
S2, S2s  
S3, S (LMM)  
S4, S (KLL)  
Sb1, Sb3d5  
Sb2, Sb4d  
Sb3, Sb (MNN)  
Sb4, Sb3d3  
Sb5, Sb (MNN)  
Sb6, Sb3p1  
Sb7, Sb3p3  
Sc1, Sc2p  
Sc2, Sc2s  
Sc3, ScLMM  
Sc4, Sc2p3  
Sc5, Sc2p1  
Sc6, Sc (LMM)  
Se1, Se3d  
Se2, Se (LMM)  
Se3, Se (LMM)  
Se4, Se3s  
Se5, Se3p1  
Se6, Se3p3  
Se7, Se (LMM)  
Se8, Se (LMM)  
Se9, Se (LMM)  
Si1, Si2p  
Si2, Si2s  
Si3, Si (KLL)  
Sm1, Sm3d5  
Sm2, Sm4d  
Sn1, Sn3d5  
Sn2, Sn3p3  
Sn3, Sn (MNN)  
Sn4, Sn4d  
Sn5, Sn3d3  
Sn6, Sn3p1  
Sn7, Sn (MNN)  
Sr1, Sr3d  
Sr2, Sr3p  
Sr3, Sr3p3  
Sr4, Sr3p1  
Sr5, Sr3s  
Ta1, Ta4f  
Ta2, Ta4d  
Ta3, Ta4d5  
Ta4, Ta (MNN)  
Ta5, Ta (MNN)  
Ta6, Ta4d3  
Ta7, Ta4s  
Ta8, Ta4p1  
Ta9, Ta4p3  
Tb1, Tb4d

Tb2, Tb3d  
Tc1, Tc3d  
Tc2, Tc3p3  
Tc3, Tc3d5  
Tc4, Tc (MNN)  
Tc5, Tc3p1  
Tc6, Tc3d3  
Te1, Te3d5  
Te2, Te4d  
Te3, Te (MNN)  
Te4, Te3p1  
Te5, Te3p3  
Te6, Te (MNN)  
Te7, Te3d3  
Th1, Th4f7  
Th2, Th4d5  
Th3, Th5d  
Th4, Th5d5  
Th5, Th4d3  
Th6, Th4f5  
Th7, Th5d3  
Ti1, Ti2p  
Ti2, Ti3p  
Ti3, Ti (LMM)  
Ti4, Ti2p3  
Ti5, Ti2s  
Ti6, Ti2p1  
Ti7, Ti (LMM)  
Tl1, Tl4f  
Tl2, Tl4d5  
Tl3, Tl5d  
Tl4, Tl4f7  
Tl5, Tl4p3  
Tl6, Tl4d3  
Tl7, Tl4f5  
Tm1, Tm4d  
Tm2, Tm4p  
U1, U4f7  
U2, U4d5  
U3, U5d  
U4, U5d5  
U5, U4d3  
U6, U4f5  
U7, U5d3  
V1, V2p  
V2, V3p  
V3, V (LMM)  
V4, V2p3  
V5, V (LMM)  
V6, V (LMM)  
V7, V2s  
V8, V2p1  
W1, W4f  
W2, W4d  
W3, W4d5  
W4, W4s  
W5, W4p1  
W6, W4p3  
W7, W4d3  
Xe1, Xe3d5  
Xe2, Xe4d  
Xe3, Xe (MNN)  
Xe4, Xe3d3  
Y1, Y3d  
Y2, Y3p  
Y3, Y3p3  
Y4, Y3s

Y5, Y3p1  
 Yb1, Yb4d  
 Yb2, Yb4p  
 Zn1, Zn2p3  
 Zn2, Zn3p  
 Zn3, ZnLMM  
 Zn4, Zn2p1  
 Zn5, Zn (LMM)  
 Zn6, Zn (LMM)  
 Zn7, Zn (LMM)  
 Zr1, Zr3d  
 Zr2, Zr3p  
 Zr3, Zr3p3  
 Zr4, Zr3p1  
 Zr5, Zr3s

### 5.7.2 Data Set 2: AES

This file contains the peak name conversion of typical PHI-peak names to the correct scientific names. The data set 2 is for AES instruments (e.g. PHI700).

Comment:

- 1. column: PHI name of the line
- 2. column: correct scientific line name
- Folder: C:\Program Files (x86)\Unifit2024\phi-names\Phi\_names1.ele

Zr5, Zr3s  
 Al1, Al (L23VV)  
 Al3, Al (L23VV)  
 Al2, Al (KL23L23)  
 Al4, Al (KL23L23)  
 Sb1, Sb (M4N45N45)  
 Sb2, Sb (M5N45N45)  
 As4, As (M23M45V)  
 As3, As (L3M23M45)  
 As1, As (L3M45M45)  
 As2, As (L2M45M45)  
 Ba1, Ba (N45O23O23)  
 Ba2, Ba (N45O23V)  
 Ba3, Ba (M4N45N45)  
 Ba4, Ba (M5N45N67)  
 Be1, Be (KL1L1)  
 Bi1, Bi (N6O45O45)  
 Bi2, Bi (N5N67O45)  
 Bi5, Bi (M4N23N23)  
 Bi3, Bi (M5N67N67)  
 Bi4, Bi (M4N67N67)  
 B1, B (KL23L23)  
 Br5, Br (M4N23N23)  
 Br4, Br (M2N45N23)  
 Br3, Br (L3M23M45)  
 Br1, Br (L3M45M45)  
 Br2, Br (L2M45M45)  
 Cd1, Cd (M5N45N45)  
 Cd2, Cd (L3M5M5)  
 Ca1, Ca (L2M23M23)  
 C1, C (KL23L23)  
 Ce1, Ce (N45N67O23)  
 Ce2, Ce (M45N45N45)  
 Ce3, Ce (M4N45N67)  
 Cs1, Cs (M4N45N45)  
 Cs2, Cs (M5N45N67)  
 Cr1, Cr (L3M23M23)  
 Cr2, Cr (L3M23M45)  
 Co4, Co (M23VV)

Co3, Co (L3M23M23)  
Co2, Co (L3M23M45)  
Co1, Co (L3M45M45)  
Cu4, Cu (M23VV)  
Cu3, Cu (L2M23M23)  
Cu2, Cu (L3M23M45)  
Cu1, Cu (L3M45M45)  
Dy1, Dy (N45N67N67)  
Dy3, Dy (M5N45N45)  
Dy2, Dy (M45N45N67)  
Dy4, Dy (M5N67N67)  
Er1, Er (N4N67N67)  
Er3, Er (M5N45N45)  
Er2, Er (M45N45N67)  
Er4, Er (M5N67N67)  
Eu1, Eu (NNO)  
Eu3, Eu (NNN)  
Eu2, Eu (M5N45N45)  
Eu4, Eu (M45N45N67)  
F1, F (KL23L23)  
Gd1, Gd (M45N67O23)  
Gd3, Gd (M45N67N67)  
Gd4, Gd (M5N45N45)  
Gd2, Gd (M5N45N67)  
Ga4, Ga (M23VV)  
Ga3, Ga (L3M23M45)  
Ga1, Ga (L3M45M45)  
Ga2, Ga (L2M45M45)  
Ge4, Ge (M3M45M45)  
Ge3, Ge (L3M23M45)  
Ge1, Ge (L3M45M45)  
Ge2, Ge (L2M45M45)  
Au1, Au (N7VV)  
Au2, Au (N5N67O45)  
Au6, Au (M5N5N5)  
Au5, Au (M5N5N7)  
Au3, Au (M5N67N67)  
Au4, Au (M4N67N67)  
Hf1, Hf (NNO)  
Hf4, Hf (MNO)  
Hf3, Hf (M45N45N67)  
Hf2, Hf (M5N67N67)  
Ho1, Ho (M45N67N67)  
Ho3, Ho (M5N45N45)  
Ho2, Ho (M45N45N67)  
Ho4, Ho (M5N67N67)  
In1, In (M4N45N45)  
In2, In (L3M5M5)  
I1, I (M5N45N45)  
I2, I (M4N45N45)  
I3, I (M5N45O23)  
Ir1, Ir (N4N67N67)  
Ir4, Ir (N5N7O45)  
Ir6, Ir (M5N5N5)  
Ir5, Ir (M5N5N7)  
Ir2, Ir (M5N67N67)  
Ir3, Ir (M4N67N67)  
Fe4, Fe (M23VV)  
Fe1, Fe (L3M23M23)  
Fe2, Fe (L3M23M45)  
Fe3, Fe (L3M45M45)  
La1, La (N45O23O23)  
La2, La (M4N45N45)  
La3, La (M4N45N67)  
Pb1, Pb (N6O45O45)  
Pb2, Pb (M5N7O5)  
Pb6, Pb (M5N5N5)

Pb5, Pb (M5N5N7)  
Pb3, Pb (M5N67N67)  
Pb4, Pb (M4N67N67)  
Li1, Li (KVV)  
Lu1, Lu (N4N67N67)  
Lu4, Lu (M5N5N5)  
Lu3, Lu (M5N45N67)  
Lu2, Lu (M5N67N67)  
Mg1, Mg (L23VV)  
Mg2, Mg (KL23L23)  
Mn4, Mn (M23M45M45)  
Mn1, Mn (L3M23M23)  
Mn2, Mn (L3M23M45)  
Mn3, Mn (L3M45M45)  
Hg1, Hg (N6O45O45)  
Hg2, Hg (N5N7O45)  
Hg5, Hg (M5N5N7)  
Hg3, Hg (M5N67N67)  
Hg4, Hg (M4N67N67)  
Mo1, Mo (M45N23V)  
Mo3, Mo (M45N45N45)  
Mo5, Mo (L3M3M5)  
Mo2, Mo (L3M45M45)  
Mo4, Mo (L2M45M45)  
Nd1, Nd (N45N67O23)  
Nd2, Nd (M5N45N45)  
Nd3, Nd (M4N45O23)  
Ni4, Ni (M23M45M45)  
Ni3, Ni (L2M23M23)  
Ni2, Ni (L3M23M45)  
Ni1, Ni (L3M45M45)  
Nb1, Nb (M45N23V)  
Nb3, Nb (M45N45N45)  
Nb5, Nb (L3M3M45)  
Nb2, Nb (L3M45M45)  
Nb4, Nb (L2M45M45)  
N1, N (KVV)  
Os1, Os (N4N7N7)  
Os4, Os (N5N7O45)  
Os6, Os (M5N5N5)  
Os5, Os (M5N5N7)  
Os2, Os (M5N7N7)  
Os3, Os (M4N67N67)  
O1, O (KL23L23)  
O2, O (KL23L23)  
Pd2, Pd (M45N23V)  
Pd1, Pd (M4N45N45)  
Pd5, Pd (L3M3M45)  
Pd3, Pd (L3M45M45)  
Pd4, Pd (L3M3M45)  
P1, P (L3M23M23)  
P2, P (KL23L23)  
Pt1, Pt (N67O45O45)  
Pt2, Pt (N4N67N67)  
Pt3, Pt (N5N67O45)  
Pt7, Pt (M5N5N5)  
Pt6, Pt (M5N45N67)  
Pt4, Pt (M5N67N67)  
Pt5, Pt (M4N67N67)  
K1, K (L3M23M23)  
Pr1, Pr (N45N67O23)  
Pr2, Pr (M5N45N45)  
Pr3, Pr (M45N45N67)  
Re1, Re (N4N7N7)  
Re4, Re (N5O23O45)  
Re6, Re (M5N5N5)  
Re5, Re (M5N5N7)

Re2, Re (M5N67N67)  
Re3, Re (M4N67N67)  
Rh2, Rh (M45N23V)  
Rh1, Rh (M5N45N45)  
Rh5, Rh (L3M3M45)  
Rh3, Rh (L3M45M45)  
Rh4, Rh (LM5M5)  
Rb2, Rb (M1M5M5)  
Rb1, Rh (M3M45N23)  
Rb5, Rb (L3M2M3)  
Rb3, Rb (L3M5M5)  
Rb4, Rb (L2M45M45)  
Ru2, Ru (M4N23V)  
Ru1, Ru (M45N45N45)  
Ru5, Ru (L3M3M45)  
Ru3, Ru (L3M45M45)  
Ru4, Ru (L2M45M45)  
Sm1, Sm (N45N67O23)  
Sm3, Sm (N45N67N67)  
Sm2, Sm (M5N45N45)  
Sm4, Sm (M45N45N67)  
Sc1, Sc (L3M23M23)  
Sc2, Sc (L3M23M45)  
Se5, Se (M45N23N23)  
Se4, Se (M1N45N45)  
Se3, Se (L3M2M45)  
Se1, Se (L3M45M45)  
Se2, Se (L2M45M45)  
Si1, Si (L23M23M23)  
Si3, Si (L2M23M23)  
Si2, Si (KL23L23)  
Si4, Si (KL23L23)  
Ag1, Ag (M5N45N45)  
Ag4, Ag (L3M3M45)  
Ag2, Ag (L3M45M45)  
Ag3, Ag (L3M3N45)  
Na1, Na (KL23L23)  
Sr4, Sr (M3M45N23)  
Sr3, Sr (L3M3M5)  
Sr1, Sr (L3M45M45)  
Sr2, Sr (L2M45M45)  
S1, S (L23M23M23)  
S2, S (KL23L23)  
Ta1, Ta (N4N67N67)  
Ta4, Ta (M5N5N5)  
Ta3, Ta (M45N45N67)  
Ta2, Ta (M5N67N67)  
Te1, Te (M5N45N45)  
Tb1, Tb (N45N67O23)  
Tb3, Tb (N45O67O67)  
Tb4, Tb (M5N45N45)  
Tb2, Tb (M45N45N67)  
Tb5, Tb (M5N67N67)  
Tl1, Tl (N6O45O45)  
Tl2, Tl (N5N7O5)  
Tl6, Tl (M5N5N5)  
Tl5, Tl (M5N5N67)  
Tl3, Tl (M5N67N67)  
Tl4, Tl (M4N67N67)  
Th1, Th (N6O3O5)  
Th2, Th (N67O45V)  
Th5, Th (M5N5N7)  
Th3, Th (M5N7N7)  
Th4, Th (M4N7N7)  
Tm1, Tm (N45N67N67)  
Tm4, Tm (M5N45N45)  
Tm3, Tm (M45N45N67)







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