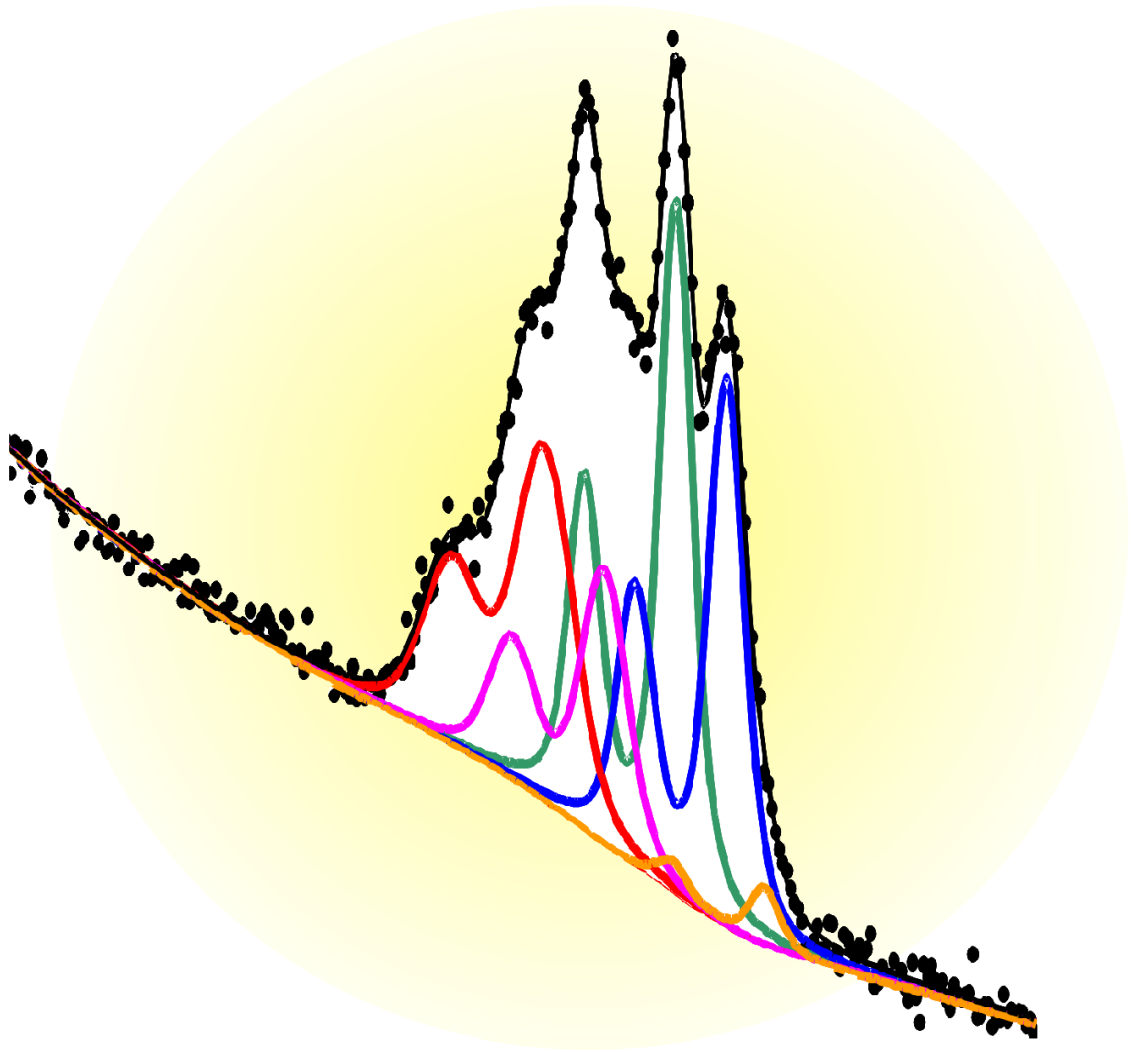


unifit FOR WINDOWS



Line Positions and Data Formats

Version 2021

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Unifit for Windows

Data Formats

Version 2021

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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_2020_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 Ag₂O
 356.6 AgO
 354.2 Ag₂SO₄

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

352.2 Mg₉₇Ag₃
 351.8 Ag
 351.4 Ag₂Se
 351.2 Ag₂S
 350.7 Ag₂O
 350.6 AgO
 350.1 AgI
 349.6 AgF₂
 349.3 AgF

Ag 3d5.pos

367.3 AgF₂
 367.4 AgO
 367.5 Ag₂CO₃
 367.7 AgF

367.8 Ag₂O
 367.8 CuAgSe
 367.8 Ag₂Se
 367.8 Ag₂SO₄
 368.0 AgI
 368.1 Ag₂S
 368.2 Ag
 368.4 Ag(OAc)
 368.8 Ag₂Yb
 368.8 AgOCCF₃
 368.8 Mg₉₇Ag₃

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

1393.1 Al
 1391.2 AlAs
 1389.4 Al₂O₃/Al
 1389.0 AlN
 1388.4 Al₂O₃
 1388.2 Al₂O₃/alpha
 1388.1 Al₂FeO₄
 1387.9 Al₂O₃/sapphire
 1387.8 Al₂O₃/gamma
 1387.7 Al₂O₃/anhydride
 1387.7 Al(OH)₃/bayerite
 1387.6 AlO(OH)/boehmite
 1387.1 KAl₂(AlSi₃O₁₀)₂(OH)₂/muscovite
 1387.1 LiAlSi₂O₆/spodumene
 1386.9 Mol Sieve A
 1386.9 Al₂SiO₅/sillimannite
 1386.9 Al₆Si₂O₁₃/mullite
 1386.8 Al₂SiO₅
 1386.8 Al₂Si₄O₁₀(OH)₂/pyrophyllite
 1386.7 Al₄Si₄O₁₀(OH)₈/kaolinite
 1386.5 Na[AlSi₃O₈]/albite
 1386.5 Na₂Al₂Si₃O₁₀.2H₂O/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 Al₂O₃/Al
 66.4 Al₂O₃/Al

Al 2p.pos

71.0 AlB₂
 72.9 Al

73.4 Fe ₃ Al	1221.1 Ph ₃ As
73.6 AlAs	1219.5 Ph ₃ AsO
73.6 AlGaAs	1218.8 As ₂ O ₃
73.6 CoAl ₂ O ₄	1217.5 As ₂ O ₅
73.7 Mol Sieve A	1213.8 KAsF ₆
73.7 Al ₂ O ₃ /gamma	1218.1 AsBr ₃
73.9 Al ₂ O ₃ /alpha	1222.9 AsI ₃
74.0 AlN	
74.1 Al ₂ O ₃ /sapphire	As 3d.pos
74.2 AlO ₂ H/boehmite	
74.2 Al ₂ (MoO ₄) ₃	40.6 InAs
74.2 NiAl ₂ O ₄	41.0 AlGaAs
74.2 AlO ₂ H	41.0 AlAs
74.2 Al(OH) ₃ /bayerite	41.2 GaAs
74.3 Al ₂ (WO ₄) ₃	41.5 As
74.3 Mica/muskovite	42.8 Ph ₃ As
74.6 Al ₂ S ₃	43.4 As ₂ S ₃
74.6 AlI ₃	43.4 AsI ₃
74.6 Al ₂ SiO ₅ /sillimanite	44.3 Ph ₃ AsO
74.7 AlCl ₃	44.9 As ₂ O ₃
74.7 MgAl ₂ O ₄	45.3 AsBr ₃
74.8 Al ₂ SiO ₅ /mullite	46.2As ₂ O ₅
74.8 H Zeolon	47.8 KAsF ₆
75.2 AlBr ₃	
75.6 LiAlH ₄	As 2p3.pos
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 As₂O₃
 1254.6 NaAsO₂
 1252.9 Na₂HAsO₄

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

1225.1 GaAs
 1224.8 As
 1222.1 As₂S₃

1323.1 GaAs
 1324.3 As
 1325.7 AsO
 1326.4 As₂O₃
 1327.4 As₂O₅

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 AuSn₄
85.3 ClAuPh₃P

B 1s.pos

186.5 B₄C
187.2 NaBH₄
187.3 B
187.5 TiB
187.8 B₁₀H₁₄
188.5 AlB₂
190.5 BN
193.0 H₃BO₃
192.6 Na₂B₄O₇·10H₂O
193.1 B₂O₃
194.9 NaBF₄

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

601.6 Ba
598.0 BaO
596.3 Ba(ClO₃)·H₂O
596.1 BaSO₄
596.1 Ba(NO₃)₂
595.3 Ba(ClO₄)₂
595.2 Ba/Ca/Cd/Sr/in_montmorillonite
594.9 BaF₂
594.9 BaCl₂·2H₂O

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

59.5 BaF₂/Au
56.0 BaCl₂
57.8 BaBr₂
55.4 BaBr₂
55.3 BaTiO₃

Ba (N45O23V).pos

71.4 BaBr₂
71.2 BaCl₂
68.6 BaTiO₃

Ba 3d5.pos

778.9 BaCrO₄
779.1 BaMoO₄
779.8 BaS

779.9 BaO
779.9 BaCO₃
780.6 Ba
780.7 Ba(NO₃)₂
780.8 BaSO₄
781.7 BaF₂

Be 1s.pos

111.8 Be
113.7 BeO
115.3 BeF₂
115.3 NaBeF₃

Bi (N6O45O45).pos, Bi (NOO)

103.7 Bi

Bi (N7O45O45).pos

100.1 Bi

Bi 4f7.pos

156.8 Bi
158.3 Bi₂MoO₆
158.9 Bi₂S₃
159.3 BiI₃
159.8 Bi₂O₃
159.9 BiOCl
160.8 BiF₃
161.2 Bi₂(SO₄)₃·H₂O

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

1390.1 [N(C₁₆H₃₃)(CH₃)₃]Br
1389.2 LiBr
1388.3 NaBr
1388.0 KBr
1384.4 KBrO₃

Br 3d.pos

66.7 Ph₄AsBr
68.3 CsBr
68.4 RbBr
68.7 KBr
68.8 NaBr
68.9 LiBr
68.9 CuBr₂

69.2 K₂PtBr₆
 69.3 K₂PtBr₄
 70.1 Bromanil
 74.8 KBrO₃

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

262.0 Graphite

C 1s.pos

281.6 TiC
 282.8 WC
 283.9 Fe₃C
 283.9 K₃Fe(CN)₆
 284.5 Graphite
 284.6 PhNH₂
 284.7 Benzene
 285.0 -CH₂-
 285.5 C₅H₅N
 285.6 C₆H₅F(C*H)
 285.6 EtNH₂
 285.7 C₆H₅Cl(C*H)
 285.7 (-C*H₂CFH-)n
 285.9 PVC(-C*H₂CHCl-)
 286.1 KCN
 286.3 CH₃C*H₂OH
 286.3 C*H₃CN
 286.4 (-C*H₂CF₂-)
 286.5 (CH₃C*H₂)₂O
 286.5 PVA(-CH₂C*HOH-)n
 286.9 CH₃COOC*H₂CH₃
 287.0 CS₂
 287.0 PVC(-CH₂C*HCl-)
 287.1 C₆H₅Cl(C*Cl)
 287.2 CH₃C*N
 287.8 C₆H₅F(C*F)
 287.9 (-CH₂C*FH-)n
 287.9 CH₃C*OCH₃
 288.0 Fe(CO)₅
 288.0 H₂NCSNH₂
 288.2 CH₃C*OONa
 288.4 CH₃C*ONH₂
 288.7 H₂NCONH₂
 289.3 CH₃C*OOH
 289.4 Na₂CO₃
 289.5 Cl₃C*COONa
 289.6 CaCO₃
 289.6 HCCl₃
 290.0 NaHCO₃

290.9 (-CH₂C*F₂-)n
 291.9 CO₂
 292.2 Teflon(-CF₂CF₂-)n
 292.4 CCl₄
 292.9 C*F₃COOEt
 294.7 HCF₃
 296.7 CF₄

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

298.2 Ca
 292.5 CaO
 291.9 CaCO₃
 291.9 CaCl₂
 288.9 CaF₂

Ca 2p3.pos

345.9 Ca
 346.3 CaCrO₄
 346.5 CaS
 347.0 CaCO₃
 347.0 Ca₃Si₃O₉
 347.3 CaO
 347.9 CaF₂
 348.0 CaSO₄
 348.3 CaCl₂

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

383.6 Cd
 382.5 CdO
 382.4 CdTe
 382.2 CdSe_{0.65}Te_{0.35}
 381.4 Zn_{0.30}Cd_{0.70}Se
 381.5 Zn_{0.50}Cd_{0.50}Se
 381.2 Zn_{0.70}Cd_{0.30}Se
 381.0 Zn_{0.90}Cd_{0.10}Se
 381.3 CdS
 381.0 CdSe
 380.5 CdI₂
 380.0 Cd(OH)₂
 380.0 CdBr₂·4H₂O
 379.8 (CdCl₂)₂·5H₂O
 378.5 CdF₂
 378.3 Ba/Ca/Cd/Sr/in_montmorillonite

Cd (M5N45N45).pos

377.0 Cd

370.5 Cd
 374.4 CdI₂
 375.8 CdTe
 369.5 CdTe
 368.5 CdTe
 375.6 CdO
 374.8 CdSe
 374.5 CdS
 372.2 CdF₂

Cd 3d5.pos

404.2 CdO
 404.6 Hg_{0.8}Cd_{0.2}Te
 405.0 CdSe
 405.1 Cd
 405.1 Cd(OH)₂
 405.1 CdCO₃
 405.2 CdTe
 405.3 CdS
 405.4 CdI₂
 405.9 CdF₂
 406.0 CdBr₂
 406.1 CdCl₂

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

771.0 CeO₂

Ce (M5N45N67).pos

755.0 CeO₂

Ce 3d5.pos

881.9 CeO₂
 883.5 CeAl₂
 883.6 CeCu₂Si₂
 883.9 Ce
 884.3 CePd₃
 884.3 CeSe
 886.0 CeH₃

Cl (K123L23).pos, Cl (KLL).pos

2392.2 CsCl
 2391.3 KCl
 2391.0 RbCl
 2391.4 LiCl
 2390.9 NaCl

Cl (LVV).pos

182.5 GdCl₃.H₂O
 181.0 KCl
 181.0 KClO₃
 180.7 KClO₄

Cl 2p3.pos

196.3 CsCl
 198.3 UOCl₂
 198.4 KCl
 198.5 LiCl
 198.5 ZnCl₂
 198.6 NaCl
 198.6 RhCl₃
 198.8 K₂PdCl₄
 198.8 K₂PtCl₄
 198.9 PdCl₂
 199.4 NiCl₂
 199.6 CuCl₂
 199.7 ZnCl₂
 200.5 Poly(-chlorostyren)
 200.6 PVC
 206.2 KClO₃
 208.7 KClO₄

Co (L3M45M45).pos

773.6 Co₃O₄
 773.2 Co
 769.4 CoO
 766.8 K₃Co(CN)₆
 768.6 Co(NH₃)₆Cl₃
 768.3 CoSiF₆

Co (LMM).pos

770.7 Co((C₆H₅)₃PO)₂(NO₃)₂

Co (M23VV).pos

53.6 Co

Co 2p3.pos

778.1 CoS₂
 778.3 Co
 779.9 Co₃O₄

780.3 CoOOH
 780.4 CoO
 781.3 Co(OH)₂
 781.3 CoAl₂O₄
 781.7 Co(NH₃)₆Cl₃
 781.9 K₃Co(CN)₆
 782.4 CoF₃
 783.0 CoF₂
 783.6 CoSiF₆
 784.0 CoSO₄

Cr (L3M23M45).pos, Cr (LMM).pos

528.8 Cr₂O₃
 527.2 Cr
 525.5 CrF₃

Cr 2p3.pos

574.3 Cr
 576.3 K₃Cr(CN)₆
 576.6 Cr₂O₃
 576.6 Cr(CO)₆
 576.9 Cr(acac)₃
 577.0 CrOOH
 577.3 Cr(OH)₃
 577.4 CrCl₃
 579.4 Na₂Cr₂O₇
 579.9 K₂Cr₂O₇
 580.1 CrO₃
 580.5 Na₂CrO₄

Cs (M4N45N45).pos, Cs (MNN).pos

568.7 CsOH
 568.4 Cs₂SO₄

Cs (N5O23O23).pos

46.3 Cs

Cs (N45O23O23).pos

50.8 CsF/Au
 49.0 CsCl
 51.2 CsCl
 49.2 CsBr
 51.4 CsBr

Cs (N45O23V).pos

61.6 CsBr
 61.4 CsCl

Cs 3d5.pos

723.6 CsF
 723.9 CsI
 723.9 Cs₂SO₄
 724.0 CsBr
 724.0 CsCl
 724.0 CsF
 724.2 CsOH
 726.4 Cs

Cu (L2M45M45).pos

939.0 Cu
 937.80 CuO
 934.10 (GeO₂)_{0.5}(Na₂O)_{0.3}(CuO)_{0.2}/glass
 934.00 (GeO₂)_{0.6}(Na₂O)_{0.3}(CuO)_{0.1}/glass
 933.50
 (GeO₂)_{0.65}(Na₂O)_{0.3}(CuO)_{0.05}/glass

Cu (L2VV).pos

938.3 Cu
 934.7 Cu

Cu (L3M45M45).pos, Cu (LMM).pos

918.6 Cu
 918.6 Cu₆₄Zn₃₆
 918.5 Ag_{28.6}Au_{17.1}Cu_{54.3}
 918.4 CuSe
 918.1 CuS
 918.0 CuCr₂O₄
 917.9 CuO
 917.8 CuFeS₂
 917.7 Cu₂Se
 917.7 AgCuSe
 917.6 CuInSe₂
 917.1 Cu₂S
 917.0 Cu₂CO₃(OH)₂
 917.0 CuIn₃Se₅
 917.0 CuGa₅Se₈
 916.8 Cu(OH)₂
 916.8 Al₂CuO₄
 916.7 Cu₂O
 916.7 CuInS₂

916.6 CuMoO4	Dy (M5N45N45).pos
916.6 Cu3Mo2O9	
916.3 CuCO3	960.0 Dy
916.3 CuBr2	
916.1 CuI	Dy (M5N67N67).pos
916.1 CuSO4	
915.3 CuCl	1280.0 Dy
915.5 CuCl2	
915.3 Cu(NO3)2	Dy (M45N45N67).pos, Dy (MNN).pos
915.2 CuSiO3	
915.1 CuF2	1115.0 Dy
914.6 CuCN	
914.5 [CuC(CN)3]	Dy 3d5.pos
914.4 Cu2S	
	1295.5 Dy
Cu (L3VV).pos	1298.9 Dy2O3
921.2 Cu	Dy 4d.pos
918.4 Cu	
916.0 Cu	152.4 Dy
914.1 Cu	167.7 Dy2O3
911.0 Cu	
Cu (M23VV).pos, Cu (MVV).pos	
62.4 Cu	
63.7 6-8A Fe/Cu	
60.8 6-8A Fe/Cu	
Cu 2p3.pos	
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	Er (M4N67N67).pos
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	Er (M45N45N67).pos, Er (MNN).pos
936.1 CuF2	
Dy (M4N67N67).pos	
1318.0 Dy	1218.0 Er
	1221.0 Er2O3
	Er 4d.pos
	167.3 Er
	168.7 Er2O3
	Eu (M4N67N67).pos
	1150.0 Eu

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

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

Ge 3d.pos

29.3 Ge
 30.5 GeS
 30.7 GeSe
 32.7 GeO₂
 33.3 Na₂GeF₆

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 HfO₂

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

2159.8 Hg

Hg 4f7.pos

99.9 Hg
 100.2 Hg_{0.8}Cd_{0.2}Te
 100.8 Hg₂Cl₂
 100.8 HgO
 101.0 HgS/cinnabar
 101.4 HgCl₂

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 I₂
 518.3 AgI
 517.7 CdI
 517.3 UI₃
 517.0 KI
 517.0 LiI
 516.4 SrI₂
 513.8 KNiIO₆

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

507.3 NiI₂
 507.1 CuI
 507.0 CdI₂
 506.8 AgI
 506.0 ZnI₂
 503.6 KNiIO₆

I 3d5.pos

618.4 NaI
 618.8 KI
 619.2 CdI
 619.4 AgI
 619.7 LiI
 619.9 I₂
 620.3 UI₃
 621.5 ICl
 622.5 ICl₃
 623.3 I₂O₅
 623.5 NaIO₃
 624.0 NaIO₃

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

410.2 In
 409.3 InP
 408.9 In₂Te₃
 408.5 CuInSe₂
 408.0 InP

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

La (M5N45N67).pos711.0 La₂O₃**La (N45O23O23).pos, La (NOO).pos**64.0 LaF₃/Au**La 3d5.pos**834.8 La₂O₃

835.8 La

838.8 LaH₃**La 4d5.pos**101.3 La₂O₃

103.9 La

Li (KVV).pos

52.9 Li

48.4 Li-O/1L O₂43.6 Li-O/1L O₂37.6 Li-O/1L O₂42.3 Li-O/5L O₂36.0 Li-O/5L O₂**Li 1s.pos**

54.8 Li

54.9 LiOH

55.2 Li₂CO₃55.6 Li₂O

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.pos196.5 Lu₂O₃

196.6 Lu

198.5 Lu₂(SO₄)₃**Lu 4f7.pos**

6.3 Lu

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

1185.6 Mg

1180.7 MgBr₂·6H₂O1180.6 (Mg/Fe)₂SiO₄1180.5 KMg₃Si₃AlO₁₀(OH/F)₂1180.5 Mg₃H₂(SiO₃)₄1180.5 (Mg/Fe)SiO₃

1180.4 MgO

1179.0 (Na/Al/Mg)Si₄O₁₀(OH)₂·nH₂O1178.8 MgSO₄·7H₂O1178.5 MgCl₂/Au1178.2 MgF₂**Mg (L23VV).pos**

43.0 Mg/Ru

31.0 O₂/Mg/Ru**Mg 1s.pos**1302.7 Mg(OH)₂

1303.2 Mg

1304.0 MgAl₂O₃1305.0 MgF₂**Mg 2p.pos**49.5 Mg(OH)₂

49.6 Mg

50.4 MgAl₂O₄

50.4 MgO

51.0 MgF₂51.6 MgSO₄·7H₂O**Mn (L3M23M45).pos, Mn (LMM).pos**

586.4 Mn

585.7 MnO₂

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 MoO_x
 2143.6 Mo

Mo (L₃M₄₅M₄₅).pos

2039.0 MoSi₂
 2038.8 Mo
 2032.2 MoO_x

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 MoO_x
 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/Pyrrole
 401.3 (NH₄)₂SO₄
 401.4 Et₄NCl
 401.7 NH₄Cl
 402.2 Bu₄NHSO₄
 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 ₄	733.0 Nd
Na (L23VV).pos	Nd (M45N45N67).pos
23.8 NaI	840.0 Nd
23.1 NaBr	Nd 3d5.pos
21.6 NaCl	980.8 Nd
20.2 NaF	982.0 Nd ₂ O ₃
Na 1s.pos	984.9 Nd ₂ (SO ₄) ₃
1070.8 NaN ₃	Nd 4d.pos
1070.8 Na ₂ C ₂ O ₄	120.8 Nd ₂ O ₃
1071.1 Na ₃ PO ₄	122.5 Nd ₂ (SO ₄) ₃
1071.1 NaOAc	Ne (KL23L23).pos
1071.2 NaF	818.0 Ne in Fe
1071.2 Na ₂ SO ₄	Ne 1s.pos
1071.4 NaNO ₃	861.6 Ne in Au
1071.5 Na ₂ CO ₃	863.1 Ne in graphite
1071.5 Na ₂ HPO ₄	863.4 Ne in Fe
1071.6 NaI	Ni (L2VV).pos
1071.6 NaPO ₃	866.6 NiO
1071.6 NaCl	863.7 Ni(OH) ₂
1071.7 Na ₂ SiF ₆	863.3 ((Ni(OH) ₂) _{0.75} (H ₂ O) _{0.16} (NiCO ₃) _{0.09})
1071.7 NaBr	863.3 ((Ni(OH) ₂) _{3.2} H ₂ O)
1071.8 Na	862.9 NiOOH
1072.0 NaH ₂ PO ₄	862.7 KNiIO ₆
1072.5 Na ₂ O	Ni (L3M45M45).pos, Ni (LMM).pos
1072.7 NaBF ₄	856.0 ((P ₂ O ₅) _{0.40} (V ₂ O ₅) _{0.60}) _{0.95} (NiO) _{0.05}
Nb (M45N23V).pos, Nb (MNV).pos	855.7 ((P ₂ O ₅) _{0.40} (V ₂ O ₅) _{0.60}) _{0.98} (NiO) _{0.02}
167.8 Nb	855.7 ((P ₂ O ₅) _{0.40} (V ₂ O ₅) _{0.60}) _{0.90} (NiO) _{0.10}
165.6 NbH _x	855.3 ((P ₂ O ₅) _{0.40} (V ₂ O ₅) _{0.60}) _{0.85} (NiO) _{0.15}
161.6 Nb ₂ O ₅	849.8 NiO
Nb 3d5.pos	848.1 Ni(OH) ₂
202.4 Nb	848.1 NiOOH
203.2 NbH _x	847.3 ((Ni(OH) ₂) _{0.75} (H ₂ O) _{0.16} (NiCO ₃) _{0.09})
203.7 NbO	846.2 Ni
203.8 NbN	846.0 Ni/Ca _{0.166} Ni _{0.833}
206.5 KNbO ₃	845.2 Al ₇₀ Co ₁₅ Ni ₁₅
207.1 NbBr ₅	844.9 AlNi
207.6 Nb ₂ O ₅	
207.7 NbS ₂	
208.0 NbCl ₅	
Nd (M5N45N45).pos, Nd (MNN).pos	

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 K₂OsI₆
 52.0 OsO₂
 52.2 Os(HSO₃)₂
 52.9 K₂OsBr₆
 53.1 OsCl₃
 53.2 K₂OsCl₆
 53.4 K₂Os(NO)Cl₅
 55.2 K₂OsO₂(OH)₄

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

1907.7 K₂OsCl₆
 1909.8 K₄Os(CN)₆

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

1858.6 Cd₃P₂
 1858.4 InP
 1858.2 Zn₃P₂
 1858.0 Cd(3-x)Zn(x)P₂
 1858.0 CdP₂
 1858.0 Fe₄₀Ni₄₀P₁₄B₈
 1858.0 ZnSiP₂
 1857.5 CdGeP₂
 1857.3 ZnP₂
 1857.3 GaP
 1856.3 P
 1856.1 P/red
 1853.2 P₄S₁₀
 1851.6 Na₃SPO₃
 1850.9 Ca₃(PO₄)₂
 1850.9 Ni₃(PO₄)₂
 1850.8 Mn₃(PO₄)₂
 1850.8 Na₂HPO₄
 1850.6 FePO₄
 1850.5 Na₃PO₄
 1849.9 Na₄P₂O₇
 1849.8 PON
 1849.8 InPO₄
 1849.6 GaPO₄
 1849.0 BPO₄
 1848.6 NaPO₃
 1848.4 Na₂PFO₃
 1848.0 P₄O₁₀
 1845.4 [NH₄]PF₆
 1845.4 [(CH₃)P(N(CH₃)₂)₂]
 1845.2 NH₄PF₆
 1843.8 [PCl₂(C₆H₅)₂]

1843.4 [PCl₂(N(CH₃)₂)₂]
 1842.8 [PCl(CH₃)₂]
 1842.1 [PCl₂(CH₃O)]
 1842.1 [P(O)(CH₃O)(CH₃)₂]
 1841.3 [PSF₂(N(CH₃)₂)₂]
 1841.2 [PF(N(CH₃)₂)₂]
 1841.0 [P(O)Cl₂(CH₃O)]
 1840.4 [PF₂N]₅

P 2p3.pos

128.3 Zn₃P₂
 128.9 InP
 129.4 GaP
 129.8 ZnP₂
 130.7 P/red
 130.9 Ph₃P
 132.5 Ph₃PS
 132.5 Ph₃PO
 132.8 Na₃PO₄
 132.9 AlPO₄
 133.1 Na₂HPO₄
 134.2 NaH₂PO₄
 134.7 NaPO₃
 134.7 (PhO)₃P
 135.2 P₄O₁₀
 137.7 NH₄PF₆
 133.6 Na₄P₂O₇

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

96.3 Pb
 95.5 PbTe
 94.8 PbSe
 94.6 PbS
 93.4 PbI₂
 93.1 PbO₂
 92.9 PbO
 92.8 PbCrO₄
 92.8 Pb₃O₄
 92.6 PbBr₂
 92.6 PbTiO₃
 92.1 PbCl₂
 92.1 PbCO₃
 92.0 Pb(OH)₂
 91.7 Pb(NO₃)₂
 91.7 Pb₃(OH)₂(CO₃)₂
 91.7 PbZrO₃
 91.5 Pb(C₂H₃O₂)₂
 91.1 PbSiO₃

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 NiSO₄
 2110.2 Fe₂(SO₄)₃.nH₂O
 2110.2 MnSO₄
 2109.9 BaSO₄
 2109.7 (NH₄)₂SO₄.FeSO₄.6H₂O
 2109.7 CaSO₄.2H₂O
 2109.6 HgSO₄
 2109.5 (NH₄)₂SO₄
 2109.3 (NH₄)₂(SO₄)₂
 2109.3 SrSO₄
 2109.3 Al(NH₄)(SO₄)₂.12H₂O
 2109.2 KAl(SO₄)₂.12H₂O
 2109.2 MgSO₄.7H₂O
 2109.1 K₂S₂O₇
 2109.1 BeSO₄
 2109.1 Al₂(SO₄)₃.18H₂O
 2109.0 SnSO₄
 2108.9 K₂(SO₄)₂
 2108.8 Li₂SO₄
 2108.5 Na₂SO₄
 2108.2 K₂SO₄
 2107.8 Na₂S₂O₃
 2105.9 CaSO₄
 2103.9 (CH₃)₂S
 2103.7 [PS(CH₃O)₃]
 2103.3 [PSCI₂(CH₃O)]
 2103.2 [PSCI₂(CH₃)]
 2102.9 [PSCI₃]
 2102.5 (CH₃S)₂
 2102.5 (CH₃S)₂
 2100.9 (CF₃S)₂
 2100.7 [PSF₃]
 2100.5 CH₃SH
 2100.4 SF₆
 2099.9 (CH₃)₂SO
 2098.7 SO(CH₃O)₂
 2098.6 H₂S
 2098.1 SOCl₂
 2097.6 (CH₃O)₂SO₂
 2097.0 SO₂Cl₂
 2095.5 SO₂ClF
 2095.5 SO₂
 2094.5 SOF₂
 2094.3 SCIF₅
 2093.9 SF₄
 2093.8 SO₂F₂
 2092.6 SF₆

S 2p.pos

160.8 PbS
 161.6 FeS
 161.7 CdS
 162.1 NH₂CSNH₂
 162.3 ZnS
 162.8 NiS
 162.8 Na₂S*SO₃
 162.8 WS₂
 163.0 FeS₂/Pyrite
 163.2 Ph₂S
 163.2 Cysteine
 163.7 CS₂
 163.8 S
 164.3 Thiophene
 164.4 PhSSPh
 166.3 PhSO₂Na
 166.5 Me₂SO
 167.4 SO₂
 167.6 Na₂SO₃
 168.1 p-NH₂C₆H₄SO₃Na
 168.6 Na₂SS*O₃
 169.0 Me₂SO₂
 169.1 CuSO₄
 169.4 Na₂SO₄
 169.7 CaSO₄
 174.4 SF₆

Sb (M4N45N45).pos, Sb (MNN).pos

464.5 Sb
 462.2 Sb₂S₅
 462.1 Sb₂S₃
 459.7 Sb₂O₃
 454.4 KSbF₆

Sb 3d5.pos

528.1 Bu₃Sb
 528.2 Sb
 528.6 AlSb
 528.9 Ph₃Sb
 529.3 Sb₂S₅
 529.5 Sb₂S₃
 530.0 Sb₂O₃
 530.8 Sb₂O₅
 532.9 KSbF₆

Sc 2p3.pos

398.6 Sc

400.7 ScN	Si (KL23L23).pos, Si (KLL).pos
401.4 ClSc(C5H5)2	
401.8 Sc2O3	1617.2 MoSi2
401.9 Sc2O3	1616.6 Si
	1613.8 SiC
Sc (L3M23M23).pos, Sc (LMM).pos	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
Se (L3M45M45).pos	1609.0 Kaolinite
1307.3 Zn0.30Cd0.70Se	1608.8 SiO2
1307.2 Zn0.42Cd0.58Se	1608.8 Methylsilicone
1307.0 Se	1608.6 Mol Sieve Y
1306.8 CdSe	1608.6 SiO2/Quartz
1306.7 Zn0.50Cd0.50Se	1606.4 Na2SiF6
1306.5 Zn0.70Cd0.30Se	Si 2p.pos
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
Se 3d5.pos	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)	Sm (M4N67N67).pos
59.0 H2SeO3	
61.0 H2SeO4	1094.0 Sm2O3

Sm (M5N45N45).pos	133.8 SrF2
	134.3 SrSO4
808.0 Sm2O3	134.4 Sr
	134.7 Sr(NO3)2
Sm (M5N67N67).pos	135.3 SrO
1068.0 Sm2O3	Ta (M5N67N67).pos, Ta (MNN).pos
Sm (M45N45N67).pos	1674.7 Ta
950.0 Sm2O3	Ta 4f7.pos
Sm 3d5.pos	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
Sn (M4N45N45).pos, Sn (MNN).pos	27.3 TaCl5
	27.8 TaF5
437.3 Sn	29.4 K2TaF7
435.7 SnS	
434.1 SnO	Tb (M4N67N67).pos
432.6 SnO2	
431.7 Na2SnO3	1256.0 Tb
430.8 NaSnF	
Sn 3d5.pos	Tb (M5N45N45).pos
	920.0 Tb
484.9 Sn	
485.6 SnS	Tb (M5N67N67).pos
485.6 Ph3SnOH	
485.7 SnSe	1223.0 Tb
486.6 Ph4Sn	
486.6 SnO2	Tb (M45N45N67).pos, Tb (MNN).pos
486.7 SmCl2	
486.7 (NH4)2SnCl6	1068.0 Tb
486.7 KSnF3	
486.7 Na2SnO3	Tb 3d5.pos
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	Tb 4d.pos
488.2 SnF4	
Sr 3d5.pos	146.0 Tb
	148.7 Tb2O3
133.2 SrCO3	149.2 TbO2

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

492.1 Te
 491.1 CdSe_{0.65}Te_{0.35}
 490.8 CdTe
 488.5 Ph₂Te₂
 487.6 TeI₂(C₂H₅)₂
 487.3 TeBr₄
 487.1 TeO₂
 486.7 [TeBr₂(C₆H₅)₂]
 486.6 [TeI₂(CH₃)₂]
 486.6 [TeBr₂(C₆H₅CH₃)]
 486.4 (NH₄)₂TeCl₆
 486.3 Cl₂TePh₂
 486.3 TeCl₂(C₆H₅)₂
 486.1 TeCl₄
 485.5 Na₂TeO₄
 485.5 TeO₃
 485.1 Te(OH)₆

Te 3d5.pos

572.3 Hg_{0.8}Cd_{0.2}Te
 572.7 CdTe
 572.7 GeTe
 572.9 Te
 573.9 Ph₂Te₂
 575.5 K₂TeO₃
 575.8 TeI₄
 576.1 TeO₂
 576.2 Cl₂TePh₂
 576.7 TeBr₄
 576.8 Na₂TeO₄
 576.9 TeCl₄
 576.9 (NH₄)₂TeCl₆
 577.1 Te(OH)₆
 577.3 TeO₃

Th (N67O45O45).pos

154.0 Th

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

249.0 Th

Th 4d5.pos

675.2 Th
 675.5 ThO₂

Th 4f7.pos

333.1 Th
 334.4 ThO₂
 336.5 ThF₄

Ti (KL23L23).pos

4002.0 TiO₂

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

419.0 Ti
 418.2 TiC
 409.8 Na₂TiF₆

Ti 2p3.pos

454.0 Ti
 454.4 TiB₂
 454.6 TiC
 455.1 TiO
 455.8 TiN
 457.1 Cl₂Ti(C₅H₅)₂
 458.5 TiCl₄
 458.5 BaTiO₃ (cubic/tetra)
 458.7 TiO₂
 459.2 TiO₂ (anatase/rutile)
 462.6 Na₂TiF₆

Tl 4f7.pos

117.5 Tl₂O₃
 117.7 Tl
 118.5 TlI
 118.7 Tl₂S
 118.7 Tl₄S₃
 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
Tm (M5N45N45).pos	381.6 UO2Cl2
	381.6 U(SO4)2
1080.0 Tm	381.9 UCl5
	382.2 UF4
Tm (M5N67N67).pos	382.4 K2UF6
	383.0 UO2F2
1440.0 Tm	384.9 UF6
Tm (M45N45N67).pos, Tm (MNN).pos	V (L3M23M45).pos, V (LMM).pos
1270.0 Tm	472.0 V
	468.0 V2O5
Tm 4d.pos	468.6 VO2
175.4 Tm	V 2p3.pos
176.6 Tm2O3	512.2 V
178.3 Tm2(SO4)3	512.9 V(C5H5)2
U (N67O45N45).pos	513.3 K4V(CN)6
	514.2 V(acac)3
190.0 U	514.4 VN
	515.1 VO(acac)2
U (N67O45V).pos	516.3 VO2
	516.4 VOCl2
284.0 U	517.3 Na3VO4
	517.6 V2O5
U 4f7.pos	W (M5N67N67).pos, W (MNN).pos
377.4 U	1727.8 WS2
378.3 UCl3	1723.9 H2WO4
378.4 UBr3	1723.8 WO3
379.1 USe3	1722.0 Na2WO4
379.4 US3	
379.9 UBr4	W 4f7.pos
380.0 UOCl	31.3 W
380.1 US	31.5 WC
380.1 UF3	32.7 WO2
380.1 UOBr	33.2 WS2
380.2 UCl4	35.1 CaWO4
380.2 UO2	35.7 WO3
380.3 UOCl2	35.9 WBr6
380.3 USe	36.2 H2WO4
380.4 UOBr2	36.3 Na2WO4
380.5 UO2Br	36.3 WBr5
380.5 U2Te3	36.3 Al2(WO4)3
380.7 U3O8	36.9 WCl6
380.7 CaUO4	37.2 WOCl4
381.1 UO2Br2	
381.3 UTe3	

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

184.2 K_2ZrF_6

185.3 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_2020_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(NO₃)₃.5H₂O
 782.1=397.1+385.0 GaN
 777.3=398.1+379.2 BN
 775.4=398.8+376.6 NH₃

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 Na₂O
 2062.3=1071.7+990.6 NaBr
 2061.9=1071.6+990.3 NaCl
 2061.3=1071.5+989.8 Na₂CO₃
 2061.3=1070.8+990.5 Na₂C₂O₄
 2061.3=1071.1+990.2 Na₃PO₄
 2061.2=1071.5+989.7 Na₂HPO₄
 2061.1=1071.6+989.4 NaPO₃
 2061.1=1072.0+989.1 NaH₂PO₄
 2061.0=1071.2+989.8 Na₂SO₄
 2061.0=1071.1+989.9 NaOAc
 2060.8=1071.4+989.4 NaNO₃
 2059.8=1072.7+987.1 NaBF₄
 2059.8=1071.2+988.6 NaF
 2059.4=1071.7+987.7 Na₂SiF₆

Nb 3d₅ + Nb (M45N23V).aup

370.2=202.4+167.8 Nb
 369.7=208.1+161.6 Nb₂O₅
 368.6=203.2+165.6 NbH_x

Ne 1s + Ne (KL23L23).aup

1681.4=863.4+818.0 Ne in Fe

Ni 2p₃ + Ni (L3M45M45).aup

1699.8=857.4+842.4 NiF₂
 1698.9=852.7+846.2 Ni
 1698.1=855.7+842.4 Ni(acac)₂

O 1s + O (KL23L23).aup

1043.8=528.7+515.1 PbO₂
 1042.1=529.0+513.1 PbO
 1041.7=530.9+510.8 ZrO₂
 1041.0=531.3+509.7 CaCO₃
 1040.8=533.1+507.7 H₂O
 1040.7=532.0+508.7 CaSO₄

1040.6=531.3+509.3 CaO
 1040.2=531.4+508.8 CaSiO₃
 1040.1=531.5+508.6 Al(OH)₃
 1039.9=532.0+507.9 NaPO₃
 1039.6=532.8+506.8 SiO₂
 1039.6=531.9+507.7 NaAlSi₃O₈
 1039.1=530.6+508.5 Al₂O₃

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 P₄S₁₀
 1983.8=135.8+1848.0 P₄O₁₀
 1983.5=133.6+1849.9 Na₄P₂O₇
 1983.3=132.8+1850.5 Na₃PO₄
 1983.3=134.7+1848.6 NaPO₃
 1982.9=137.7+1845.2 NH₄PF₆

Pb 4f₇ + 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 PbI₂
 231.4=138.8+92.6 PbBr₂
 231.0=138.9+92.1 PbCl₂
 230.5=137.4+93.1 PbO₂
 230.2=138.5+91.7 Pb(NO₃)₂
 230.1=137.3+92.8 PbO
 230.1=140.0+90.1 PbSO₄
 229.9=138.0+91.9 Pb(OH)₂
 229.1=138.5+90.6 PbF₂

Pd 3d₅ + Pd (M4N45N45).aup

662.9=335.1+327.8 Pd
 661.0=337.9+323.1 K₂PdCl₄

Pt 4f₇ + Pt (M4N67N67).aup

2111.7=71.2+2040.5 Pt
 2108.6=73.4+2035.2 K₂PtCl₄

S 2p + S (KL23L23).aup

2278.9=162.8+2116.1 NiS
 2278.8=163.0+2115.8 FeS₂/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 YH_x
 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 ZnCl₂

2011.2=1022.5+988.7 ZnI₂

2010.7=1023.4+987.3 ZnBr₂

2009.8=1022.1+987.7 ZnO

2009.2=1023.0+986.2 ZnSO₄

2009.1=1021.4+987.7 Zn(acac)₂

2008.0=1021.8+986.2 ZnF₂

Zr 3d₅ + Zr (M45N23V).aup

327.6=179.0+148.6 Zr

325.2=183.3+141.9 ZrO₂

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 Avantage (*.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_{3/2} 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

```

CYCLE                               Registration type
596                                 Register:every Nth cycle,region etc.

```

SEQUENCE CONTROL: acquisition sequence control parameters

```

10                                  Number of cycles
1                                   Number of spatial points
5                                   Number of scans
5                                   Number of regions

```

ELECTRON GUN: electron gun control information

```

1000.000000                        Magnification
80.000000                           Focus voltage
2.000000                             Beam voltage KeV
50.000000                             Condenser
0.000000                              Beam diameter in angstroms
30.000000                             Emission voltage
1.000000                              Frames averaged
5.000000                              Emission current
0.000000                              x_raster
0.000000                              yx_ratio
0                                       abs_bias

```

ION GUN: ion gun control information

```

04-300 ION GUN                      Gun currently in system
3.000000                             Ion gun voltage
0.000000                             Ion gun current
25.000000                             Emission current
10.000000                             x raster range
0.000000                              y raster range
1.000000                              Ratio of y raster to x raster
Ar                                       Ion source gas type
75.000000                             Focus voltage
0.000000                              Condenser setting
190.000000                             Grid voltage
15.000000                             spc charge offset

```

X-RAY: x-ray control settings

```

2                                       Anode id
13.000000                             X_ray voltage (KV)
MCD                                     scd or mcd
Al                                       Anode 1 name
                                         Anode 2 name

```

ANGLES: angle information

```

0                                       Take off angle between sample/analyzer
0                                       Scattering angle
0                                       Number of defined angles

```

SIMS ANALYZER: SIMS analyzer information

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_{3/2}, 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_{3/2}, As 3d, C 1s, Ga 2p_{3/2}, 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
2975.699999999348
3025.55999999944
3080.799999999792
...
3039.599999999812
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
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
113.819999999877
99.2999999998113
103.619999999768
...
43.7999999998772
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:

- SDP⁶ 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
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: "O 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
*

```

```

105890.000000
106290.000000
107775.000000
...
94910.000000
93670.000000
93560.000000
*
72170.000000
74455.000000
75405.000000
...
62980.000000
62970.000000
65290.000000
*
*

```

3.1.17 VGS2000 (*.XPS)

Comment::

- Each region saved in two columns: 1. column: BE, 2. column: intensities in cps (e.g. 2 regions are saved in four columns)
- Columns have 8 characters
- Excitation energy not available, has to be defined manually
- Dwell time has to be calculated in a special manner
- Example: survey
- Folder: Install-Memory Card:\XPS_Measurement_Reference_Data\15-VGS2000(.XPS)\VGS2000-SingleReg-survey.XPS

```

30308IA      1 Bereich
tv30308 interkaliert ungesputtert
24 19,35 158 33,5 Mg
-
1. Bereich: SURV1    BE
10 Scans      100 ms Dwell-Time    50 eV Pass-Energie    4000 Kanäle
Start 1000.00 eV      Step 0.25 eV
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-

```

```
-
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_{5/2}, 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 +@c/s àø'
f4  É  pnt sar
+@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"DUµDU"DU...•D p'DUö'D 0"D δD
...

```

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_{1/2}, Ag 3d, Au 4f, C 1s, Au 3p, Au 4d_{3/2}, Au 4d_{5/2}, 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

```

```

SpectralRegDef: 4 4 Au4f 79 181 -0.100 97.000 79.000 97.000 79.000 1.250 23.50
none
SpectralRegDef: 5 5 C1s 6 201 -0.100 300.000 280.000 300.000 280.000 1.250 23.50
none
SpectralRegDef: 6 6 Cu3p 29 502 -0.100 109.100 59.000 109.100 59.000 1.250 23.50
none
SpectralRegDef: 7 7 Au4d3 79 201 -0.100 364.000 344.000 364.000 344.000 1.250
23.50 none
SpectralRegDef: 8 8 Au4d5 79 201 -0.100 345.000 325.000 345.000 325.000 1.250
23.50 none
SpectralRegDef: 9 9 O1s 8 201 -0.100 543.000 523.000 543.000 523.000 1.250 23.50
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDesc: 1
EOFH
  _      _  _      _  _      _  _      _  _      _  chn      sar          c/s
f8  0
  p      _  _      _  _      _  _      _  _      _  chn      sar          c/s
^@Yø†µ/□^@ ó" /k^@DUtÑ...8^@ÒJž□'f°@ç (Až□^,@z
...
```

Software Version 4: XPS V1.30

- Example of 5 regions: Sc 2p_{3/2}, Ge 3d, Gd 3d, O 1s, C 1s
- Folder: Install-Memory Card:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V4-XPS V1.30.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
Comment: 5min 1KV 3x3 Nr 1
SoftwareVersion: XPS V1.30
InstrumentModel: PHI Model 1600/3057
Institution:
FileDate: 2009 06 29
AcqFileDate: 2009 06 29
AcqFilename: C:\XPS_Data\Besmehn\20180004.pdt
Operator:
ExperimentID:
PlatenID:
PlatenDesc: 5min 1KV 3x3 Nr 1
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: 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@ ・鯨@ `・@ `□袒@ @z□リ@ □@・@ □聡@ □
・レ@ 潦@ ・+レ@ ・@
...

```

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
  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

```



```

FileDate: 2008 10 21
AcqFileDate: 2008 10 21
AcqFilename: MK_102108_001.spe
Operator:
ExperimentID: 102108
PlatenID: MK
PlatenDesc:
PlatenDesc:
StagePosition: 38.7920 29.2560 21.0685 45.0000 0.0000
PhotoFilename: none
ActualPhotoFilename:
SXIFilename: none
ActualSXIFilename:
XraySource: Al 1486.6 mono
XrayPower: 51.40 W
XrayBeamDiameter: 200.0 um
NeutralizerEnergy: 0.0 V
NeutralizerCurrent: 0.0 uA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 3.900 eV
IntensityRecal: no
IntensityCalCoeff: 50.207 0.202
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 3.000 keV
SputterCurrent: 25.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0.2 A/s
NoSpectralReg: 1
SpectralRegDef: 1 1 Su1 111 1101 -1.0000 1100.0 -0.0 1100.0 -0.0
0.200000 280.00 TOTAL
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (39092.0 29656.0 10000.0 45.0 0.0)
SpatialAreaDesc: 1 SC12
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH
  0 0 0 0 0 0 0 M 0 0 0 pnt ° ·o sar 0 *k h
È c/s Té 0 0 îÂr f8 h" p 0" 0 0 0 0 0 0 0 0
  0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
  ...

```

Software Version 10: Without software specification

- Example. multiregion measurement, 4 Ad 3d regions with different pass energies
- Folder: Install-Memory Card:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V10-without_software_specification.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc:
FileDate: 109 8 21
AcqFileDate: 109 8 21
AcqFilename: E1169.spe
StagePosition: 0.0 0.0 0.0 45.0 0.0
XraySource: Mg 1253.6 std
XrayPower: 300.00 W
NeutralizerEnergy: 0.0 eV
NeutralizerCurrent: 0.0 mA

```

```

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
□ □ € □ □ □ □ □ □ 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 V2.6.1.2.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 V2.7.1.22.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 V2.8.9.30.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
□ □ ` □ □ □ □ □ □ □ □ □ □ 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_{5/2}
- 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 01s 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 Fls 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 01s 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 4: 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_{3/2}, Fe 2p_{3/2}, Cr 2p_{3/2}, Mo 3d,
- Folder: Install-Memory Card:\XPS_Measurement_Reference_Data\19-PHI-Profile(.PRO)\PHI-Profile-V4-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 5: 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-V5-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
□ □ □ □ □ □ □ □
□ □ cyc 7777reg 7777 7777777s 77777777777777f8 7□□ □□ □ □ □ □ □

```

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...

Software Version 10: 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-V10-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 11: 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-V11-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 Areal 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 12: SS 2.6.1.2

- Example of 1 regions: survey
- Folder: Install-Memory Card:\XPS_Measurement_Reference_Data\19-PHI-Profile(.PRO)\PHI-Profile-V12-SS2.6.1.2.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: 0.0000000
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: 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
DefectPosAlignment: None
DefectPosReferenceImage: 20kV.1.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 200u50W15KV
EOFH
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ñDNv □ □ f4 1 µ ð □ □ □ □ □ □ □ □ y H □ p
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```

Software Version 13: SS 2.5.0.9

- Example of 1 regions: survey
- Folder: Install-Memory Card:\XPS_Measurement_Reference_Data\19-PHI-Profile(.PRO)\PHI-Profile-V13-SS2.5.0.9.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: 1400.0000000
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
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: -5.8668 -8.6215 19.3127 46.0031 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 13
DefectPosComment:
DefectPosU: 8.9165
DefectPosV: -6.0062
DefectPosX: -5.8668
DefectPosY: -8.6215
DefectPosZ: 19.3127
DefectPosTilt: 46.0031
DefectPosRotation: -90.0500
DefectPosAlignment: None
DefectPosReferenceImage: 140420.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 100u100W20kV_HP
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_{3/2}, 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
XrayObjectiveCoilCurrent: 0.748 A
XrayBlankingVoltage: 325.0 V
XrayFilamentCurrent: 1.575 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: 534.0 eV
SxiPassEnergy: 188 eV
```

```

SxiLens2: -711 V
SxiLens3: -673 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: -7.6122 3.8962 12.7194 45.0062 -0.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 2
DefectPosComment:
DefectPosU: -7.0063
DefectPosV: 3.8434
DefectPosX: -7.6114
DefectPosY: 3.8962
DefectPosZ: 12.7194
DefectPosTilt: 45.0094
DefectPosRotation: -0.0500
DefectPosAlignment: None
DefectPosReferenceImage: 120749.17.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
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Software Version 3: XPS V1.20

- Example. angle resolved measurement with 3 angles and 8 regions: C 1s, O 1s, N 1s, P 2p, Si 2p, Al 2p, Ti 2p_{3/2}, 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)
SpatialAreaDesc: 1
EOFH
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f8 À ☐☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ☐ ang reg
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Software Version 4: XPS V1.30

- Example. angle resolved measurement with 4 angles and 3 regions: O 1s, C 1s, Si 2p
- Folder: Install-Memory Card:\XPS_Measurement_Reference_Data\19-PHI-Profile(.ANG)\PHI-Profile-V4-XPS V1.30.ANG

```

SOFH
Platform: PC
Technique: XPS
FileType: ANGLEPRO
FileDesc: AR Si wafer
SoftwareVersion: XPS V1.30
InstrumentModel: PHI Model 5000

```

```

Institution:
FileDate: 2010 01 21
AcqFileDate: 2010 01 21
AcqFilename: D:\PHI\AGL\Training\2010_01_20_0016.pdt
Operator:
ExperimentID:
PlatenID:
PlatenDesc:
StagePosition: 18.699 5.000 16.189 45.019 154.450
SampleID:
SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Al 1486.6 mono
XrayPower: 100.6W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 1.0 eV
NeutralizerCurrent: 20.0 mA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20 sr
AnalyserMode: FAT
AnalyserWorkFcn: 4.2 eV
IntensityRecal: no
IntensityCalCoeff: 14.342 0.066
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 2.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 2000.0 2000.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 3
SpectralRegDef: 1 1 O1s 8 221 -0.050 538.000 527.000 538.000 527.000 0.050 23.50
AREA
SpectralRegDef: 2 2 C1s 6 421 -0.050 300.000 279.000 300.000 279.000 0.200 23.50
AREA
SpectralRegDef: 3 3 Si2p 14 221 -0.050 107.000 96.000 107.000 96.000 0.100 23.50
AREA
NoPolarAngles: 4
PolarIncrement: 5 d
PolarMode: irreg
NoSpatialArea: 1
SpatialAreaDef: 1 Areal 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDesc: 1
EOFH
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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
  ang  iiiiireg  iiii  iiiiideg  iiii
iiiiiiiiif8 ig  ii  i  i  ang  iiiiireg  iiii
iiiiiiic/s *
...

```

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 Đ
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
□ □ Å □ □ □ □ □ □ ö
...
```

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 0.00
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 0.00
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 0.00
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
□ □ Å □ □ □ □ □ □ □ □ 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/ST010KeV/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 (*.peps)

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_Si1s.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. Sb_{2p3/2} Sb_{2p1/2}, Scans 2, Pass 40
 4. Survey, Scans 1, Pass 40
 5. VB, Scans 5, Pass 20
 6. Sb_{3/2} Sb_{1/2}, 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[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 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[HWType 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[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 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[HWType 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
- Deciaml 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 seved 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	Scan 2	Scan 2
[eV]	[eV]	[1/eV]	[1/eV]	[1/(s*eV)]
1,139099E+3	-1,100009E+2	9,510000E+2	1,585000E+2	4,750000E+2
1,583333E+2	1,586667E+2	1,585000E+2	4,750000E+2	4,760000E+2
1,139160E+3	-1,099398E+2	9,620000E+2	1,603333E+2	4,610000E+2
1,536667E+2	1,670000E+2	1,603333E+2	4,610000E+2	5,010000E+2
1,139191E+3	-1,099093E+2	9,540000E+2	1,590000E+2	4,990000E+2
1,663333E+2	1,516667E+2	1,590000E+2	4,990000E+2	4,550000E+2
1,139252E+3	-1,098483E+2	9,620000E+2	1,603333E+2	4,680000E+2
1,560000E+2	1,646667E+2	1,603333E+2	4,680000E+2	4,940000E+2
1,139313E+3	-1,097873E+2	9,040000E+2	1,506667E+2	4,530000E+2
1,510000E+2	1,503333E+2	1,506667E+2	4,530000E+2	4,510000E+2
1,139343E+3	-1,097567E+2	9,360000E+2	1,560000E+2	4,700000E+2
1,566667E+2	1,553333E+2	1,560000E+2	4,700000E+2	4,660000E+2
1,139404E+3	-1,096957E+2	9,380000E+2	1,563333E+2	4,600000E+2
1,533333E+2	1,593333E+2	1,563333E+2	4,600000E+2	4,780000E+2
1,139435E+3	-1,096652E+2	8,590000E+2	1,431667E+2	4,460000E+2
1,486667E+2	1,376667E+2	1,431667E+2	4,460000E+2	4,130000E+2
1,139496E+3	-1,096042E+2	8,770000E+2	1,461667E+2	4,540000E+2
1,513333E+2	1,410000E+2	1,461667E+2	4,540000E+2	4,230000E+2
1,139557E+3	-1,095431E+2	8,780000E+2	1,463333E+2	4,200000E+2
1,400000E+2	1,526667E+2	1,463333E+2	4,200000E+2	4,580000E+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 : 4.5400000000E+02
MonEnd : 4.9000000000E+02
AnaSta : 2.0000000000E+02
AnaEnd : 6.0000000000E+02
AnaRange : 9.0000000000E+03
AnaMin : 0.0000000000E+00
DacSta : 0.0000000000E+00
DacEnd : 1.0000000000E+01
DeltaE : 0.0000000000E+00
MonName : UE56/2-PGM-1
MonType : 1
MonUnit : Step/S
MonSpeed : 5.0000000000E+02
MonRewind: 0.0000000000E+00
MonSweep : 2.0000000000E+00
IdPos : 2.7609600000E+01
IdMode : 0
LiveTime : 1.0000000000E+00
DeadTime : 8.0000000000E-03
MeasTime : 3.2823600000E+02
ScanTime : 3.281739490E+02
ScanCtrl : ENERGY
DelayVal : 0.0000000000E+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\20120229-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	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	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	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	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	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	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	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	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	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 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 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
0

-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
□ □ €□ □ □ □ □ □ □ Q □ □ 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 C1 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_0_4_
##LOCALITY=Merrry 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=rruff.info/R060191
##MEASURED CHEMISTRY=(Fe^2+^_0.97_Mg_0.03_)(Fe^3+^_0.97_Al_0.03_)_2_0_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, 42022.00
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
0
0
0 0 0 0 0
0
Calibration of intensity scale
Acquisition conditions:
Twin, LAX, 50eV pass
0
0
0
0
0
0
0
0
0
0
0
0
0
0
0
0
512
348
0
0
0
0
0
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0
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0
0
0
0
0
0
0
0
0
1
0
0
4
1
1
0
0
0
0
0
1
0
1
Falsch
1
Peak
0
119857.8
206
411
C:\Users\rhesse\Documents\Unifit_2020_User_Files\examples\Calibration_Intensity_
Cu\CUATLX19.VMS
1
12
Cu2p3_0
Cu2p3_0
0
411
523.6
564.6
```

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  
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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  
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23291  
23342.7  
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23283.8  
23293.5  
23202.3  
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23197.6  
23488.6  
23543.2  
23404.1



23467.4  
23524.9  
23547.2  
23637.8  
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23963.7  
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23954.7  
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22204.4  
22173.21  
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22095.5  
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21695.16  
21646.55  
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21615.08  
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401  
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Falsch

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Wahr
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0 0
1643
Wahr
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Wahr
0
Wahr
0
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76770.7
13536
77000
13000
64000
Intensity / kCounts
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0
7
942.5
922
943
922
21
Binding Energy / eV
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0
0
0
0
0
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1
1
1
0
0
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16777215
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16711680
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16711680  
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16744448  
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32768  
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0  
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8421504  
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3  
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8421440  
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8421504  
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8421440  
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1  
8421504  
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2  
255



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16711680  
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Falsch  
Falsch  
0  
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12  
28  
Arial  
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16777215  
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Arial  
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Arial  
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Arial  
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0  
0



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Kurve 1
Kurve 2
Kurve 3
Kurve 4
Kurve 5
1
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1
1
1
frei
1
0
0 2020
42
2
frei
frei
frei
frei
frei
frei
frei
frei
frei
frei
1
1
-1
-1
-1
100
7
10
1
0
0
0
0 0 0 0 0
0
Calibration of intensity scale
Acquisition conditions:
Twin, LAX, 50eV pass
0
0
0
0
0
0
0
0
0
0
0
0
512
0
512
348
0
0
0
0
0
0
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1
Falsch
1
Doublet
0
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1
401
C:\Users\rhesse\Documents\Unifit_2020_User_Files\examples\Calibration_Intensity_
Cu\CUATLX19.VMS
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Cu3p_0
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401
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10
1486.6
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0.3
FAT

3-5-2004
LAXL
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1127  
1102.84  
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547.6791  
576.3229



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525.2892  
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539.8656  
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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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Ga 3d  
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  
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Binding Energy / eV  
Intensity / kCounts  
Batch parameter  
Intensity / kcps  
1936

1031

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

Remark:

- saved in Unifit\_2020\_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

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

Remark:

- saved in Unifit\_2020\_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\_2020\_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 2020
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As2p3
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-1
-1
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2866
1643
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0 0 0 0 0
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```

```

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

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Peak
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188357.2
30
370
1333.01
1316.01
NORM
Peak
405
GaAs
Dublett 1
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5000000
36188.75
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0.6423534
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1322.9
1323.3
1322.907
0
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1322.907
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10
1.757303
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Dublett 2
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4520.299
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1324.107  
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8388672  
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16777215  
16777215  
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16777215  
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29  
0  
30  
5  
Messkurve  
Untergrund  
Komponenten  
Summenkurve  
Residuum  
0  
0  
0  
0  
0  
1  
0  
RegionEnd

## 5 Data Banks Integrated in UNIFIT

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

Comment:

- Saved in Unifit\_2020\_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\_2020\_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

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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)\Unifit2020\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,BKV  
Ba1,Ba3d5  
Ba2,Ba4d  
Ba3,Ba (MNN)  
Ba4,Ba3d3  
Ba5,Ba (MNN)  
Ba6,Ba4p3  
Be1,Bel  
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)\Unifit2020\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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