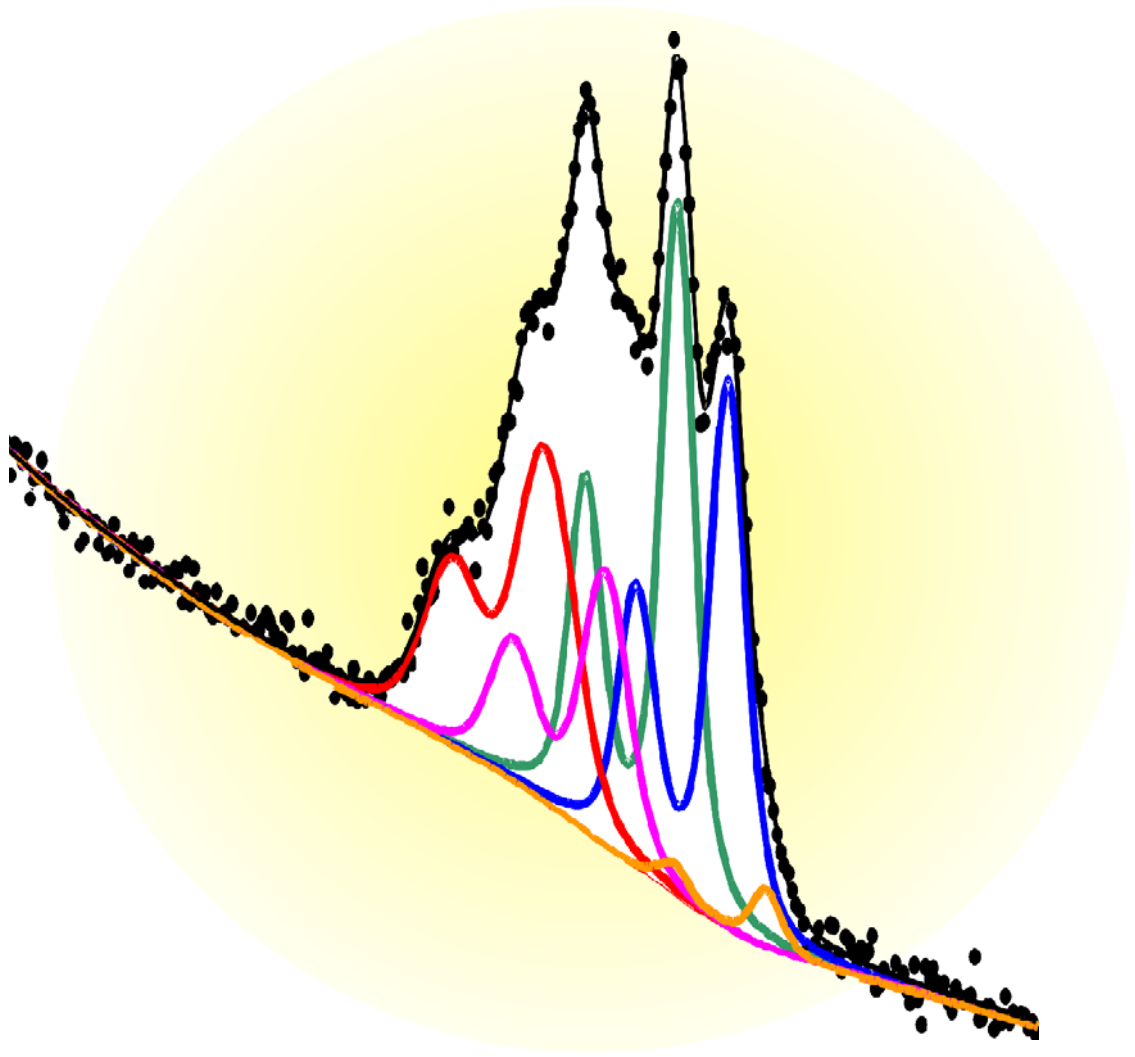


unifit FOR WINDOWS



Line Positions and Data Formats

Version 2019

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Unifit for Windows

Data Formats

Version 2019

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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_2019_User_Files\lines. The second part gives the chemical shifts of some compounds.

line positions.pos

1 Pd 4d	17 K 3p
1 Zr (M45N1N45)	18 Cl 3s
1 Mo (M45N23N23)	18 Pb 5d5
1 In (M45N1N45)	19* Ga 3d
1 Sn (M45N1N45)	19 Xe 5s
2 V 3d	20 Sr 4p
2 Cr 3d	20 Sm 5p
2 Mo 4d	20 Ho 5p
2 Tc 4d	21 Gd 5p
2 Ru 4d	21 Pb 5d3
3 Zr 4d	22 Kr 4s
3 Co 3d	22 Ba 5s
3 Y 4d	22 Pm 5p
3 Cu 3d	22* Ta 4f7
3 Rh 4d	23* O 2s
3 Ag 4d	23* Na (L23VV)
4 Mn 3d	24 Ar 3s
4 Ni 3d	24 Cs 5s
4 Nb 4d	24* Ta 4f5
5 Ca 3d	24 Eu 5p
5 Ti 3d	25 Ca 3p
5 Br 4p	25 Er 5p
6 Fe 3d	25* Sn 4d
6 Se 4p	26 Y 4p
7 Cl 3p	26 Dy 5p
7 Sc 3d	26 Tm 5p3
7* Lu 4f7	26 Yb 5p3
9* Lu 4f5	26 Bi 5d5
9 Cd 4d	27 Br 4s
10 Zn 3d	27 Lu 5p3
11 Kr 4p	29 Rb 4s
12 Ar 3p	29 Zr 4p
13 Tl 5d5	29 Tb 5p
14 P 3s	29 Bi 5d3
14 S 3s	29* Ge 3d
14 Rb 4p	30 Hf 5p3
14 Te 5s	30* F 2s
14* Hf 4f7	31 Na 2p
15 Tl 5d3	31 Sc 3p
16* Hf 4f5	31* W 4f7
16 In 4d	32 Cr (MVV)
16 I 5s	32 Sb 4d
	32 Tm 5p1
	33 K 3s

33 Ti 3p	50* Mg 2p
33 Yb 5p1	50* Cs (M45O23O23)
33 Ta 5p3	51 Ho 5s
33 Re 5p3	51 Po 5d
33* W 4f5	51 Zr 4s
34 Nb 4p	51* I 4d3
34 Eu 5s	51* Os 4f7
34 Lu 5p1	52 Pt 5p3
35 La 5s	53* Co (M23VV)
36 Mo 4p3	53* Co (MVV)
36 Ce 5s	53 Pd 4p
36 Gd 5s	53 Ir 5p3
37 Mo 4p1	53* Fe 3p
37 Sr 4s	53* Li (KV V)
37 Hf 5p1	54* Se 3d
37 W 5p3	54 Tm 5s
37* V 3p	54* Os 4f5
38 Pr 5s	55 Ge (M3M45M45)
38 Pm 5s	55 Ge (MMM)
39 Tc 4p	55* Se 3d5
39 Nd 5s	55 Yb 5s
40 At 5d	54 Br (M4N23N23)
40 V 3p	54 Br (MNN)
40 Te 4d	56 Ag 4p3
40 Ta 5p1	56* Li 1s
40* Re 4f7	56* Ba (N45O23O23)
41 Sm 5s	58* Ba (NOO)
41* As 3d	56* Se 3d
41* Ne 2s	56* Ga (M23VV)
42 Cr 3p3	58 Zn (LVV)
42* Re 4f5	58 Au 5p3
42* As 3d	58 Lu 5s
43* Cr 3p	58 Fr 5d
43* Mg (L23VV)	59 Ti 3s
43* Mg (LVV)	59 Ni (M3VV)
44 Ca 3s	60 Os 5p1
45 Ru 4p	60* Co 3p
45 Mn (M23M45M45)	61 Ni (M23M45M45)
46 Y 4s	61 Ni (MMM)
46 Tb 5s	61 Nb 4s
46* Cs (N5O23O23)	61 Er 5s
47* Se (M45N23N23)	61* Xe 4d5
47* Se (MNN)	61* Ir 4f7
47* Fe (M23VV)	61 Pt (N67O45O45)
47* Fe (MVV)	61 Pt (NOO)
47 W 5p1	61* Cu (M23VV)
48 Os 5p3	61* Cu (MVV)
48 Rn 5d	62* Cs (N45O23V)
48* Mn 3p	62 Ag 4p1
49 Rh 4p	63 Co 3p1
49* I 4d5	63* Xe 4d3

63 Dy 5s	86* Tl (N7O45O45)
64 Mo 4s	87* Ce (N45N67O23)
64* Ir 4f5	87* Ce (NNO)
64* Na 2s	87 Zn 3p3
64 Hf 5s	87* Kr 3d
64* La (N45O23O23)	87 Th 5d5
64* La (NOO)	88* Au 4f5
64* La (NOO)	88* Tl (N6O45O45)
65 Hg 5p3	88* Tl (NOO)
66 V 3s	88 Si (LVV)
67* Ni 3p	88 Si (L23M23M23)
67* Al (L23VV)	88 Si (LMM)
67* Al (LMM)	88 Pd 4s
68 Tc 4s	89* Mg 2s
68 Cd 4p	89* Zn 3p3
68 Ra 5d	90* Ba 4d5
69* Br 3d	91 Sn 4p
69 Ta 5s	91* Zn 3p1
69 Th (N6O3O5)	91 Pr (N45N67O23)
69 Th (NOO)	91 Pr (NNO)
70* Au (N7VV)	92 Fe 3s
70* Au (NVV)	93* Ba 4d3
71 U (OPV)	93 Pb (N7O45O45)
71* Ba (N45O23V)	94 Bi 5p3
71* Au (N67VV)	94 Th 5d3
71* Pt 4f7	94 Zr (M45N1N23)
73* Al 2p	96* Pb (N6O45O45)
74 Cr 3s	96* Pb (NOO)
74* Pt 4f5	96 Nd (N45N67O23)
75* Cu 3p3	96 Nd (NNO)
75* Hg (N7O45O45)	97 As (M23M45V)
75 Cs 4d5	97 As (MMV)
76 Tl 5p3	98 Ag 4s
76 W 5s	98 Ir 5s
77* Cs 4d5	99* Si 2p
77* Cu 3p1	100 Tl 5p1
77 Ru 4s	100* Bi (N7O45O45)
78 Rb (M5N23N23)	101* Hg 4f7
78 Rb (MNN)	102 Br (M2N45N23)
79 In 4p	103* La 4d5
80* Cs 4d3	103 Co 3s
80 Ac 5d	103 Sm (N45N67O23)
81 Hg (N6O45O45)	103 Sm (NNO)
81 Hg (NOO)	104* Bi (N6O45O45)
81 Re 5s	104* Bi (NOO)
83 Mn 3s	104 Pt 5s
83 Rh 4s	104 Po 5p3
83 Pb 5p3	104* Ga 3p3
84 Hg 5p1	104 Se (M1N45N45)
84* Au 4f7	105 Sb 4p
86 Os 5s	105* Hg 4f5

106* La 4d3	136 Nb (M45N23N23)
107* Ga 3p1	137* Pb 4f7
107 Eu (NNO)	135 Sm (N45N67N67)
107 Pb 5p1	137 Sn 4s
107 Rb (M3M45N23)	139 Xe 4p
108 Be (KL1L1)	140 Fr 5p3
108 Be (KLL)	140* Gd 4d
109 Cd 4s	140 Zn 3s
109* Ce 4d5	140 Eu (NNN)
111 Au 5s	141* As 3p3
111 Ni 3s	142* Pb 4f5
111* Rb 3d5	143 Gd (M45N67N67)
112* Ce 4d3	143 Gd (MNN)
112* Rb 3d	145 Nb (M45N1N45)
112* Be 1s	146* Tb 4d
112 Gd (M45N67O23)	146* As 3p1
112 Gd (MNO)	148* Zr (M45N23V)
114 Te 4p	148* Zr (MNV)
114 Nb (M45N1N23)	148 At 5p1
114 Sr (M3M45N23)	150 Pb 5s
115 At 5p3	150 Tb (N45O67O67)
115* Pr 4d	151* S (L23M23M23)
116 Tb (N45N67O23)	151* S (LMM)
116 Tb (NNO)	151* Si 2s
118* Tl 4f7	152* Dy 4d
118* Al 2s	152* Th (N67O45O45)
119 Zr (M45N23N23)	152 Ru (M45N1N23)
120 Bi 5p1	153 Sb 4s
121* Nd 4d	153 Ra 5p3
122* Tl 4f5	154 Dy (N45N67N67)
122* Ge 3p3	154 Dy (NNN)
122 Mo (M45N1N23)	156* Y 3d5
123 Cu 3s	157* Bi 4f7
123 In 4s	158* Y 3d3
123 I 4p	160* Ho 4d
123 P (L3M23M23)	160 Ga 3s
123 P (LMM)	161 Bi 5s
124* Y (M45N23V)	161 Cs 4p3
124* Y (MNV)	162* Bi 4f5
126* Ge 3p1	162 Ho (M45N67N67)
127 Rn 5p3	163* Se 3p3
127 Hg 5s	163 Mo (M45N1N45)
128* Eu 4d	164* S 2p
129* Sm 4d	164 Rn 5p1
129 Pm 4d	167* Er 4d
131* P 2p	167 Ac 5p3
131* P 2p3	168* Nb (M45N23V)
132 Po 5p1	168* Nb (MNV)
133 Tl 5s	168 Er (N4N67N67)
134* Sr 3d5	168 Er (NNN)
136* Sr 3d3	169* Se 3p1

170 Tm (N45N67N67)	202* Nb 3d5
170 Tm (NNN)	205 As 3s
171 Te 4s	205* Nb 3d3
172* Ir (N4N67N67)	206* Lu 4d3
172* Ir (NNN)	207 Ce 4p3
173 Cs 4p1	207 Tc (M45N23V)
173 Pt (N4N67N67)	207 Xe 4s
174 Yb (N5N67N67)	208* Kr 3p3
174 Yb (NNN)	210 At 4f
175* Tm 4d	210 W (N45O23O45)
177 Th 5p3	211* Ar (L3M23M23)
177 Po 5s	211* Hf 4d5
179* Zr 3d5	213* Ar (L3M23M23)
179 Ba 4p3	213 La 4p1
179 Re (N4N7N7)	214 Rn 5s
179 Re (NNN)	215 Ac 5p1
180 Os (N4N7N7)	216* Kr 3p1
181* Zr 3d3	218 Pr 4p3
181 Ge 3s	218 K (L3M1M23)
182 Fr 5p1	218 Re (N5O23O45)
182* B (KL23L23)	218 Re (NOO)
182 W (N4N7N7)	222* Hf 4d3
182 W (NNN)	223 Mo (M45N45N45)
182* B (KLL)	223 Mo (MNN)
182* Yb 4d5	223 Ce 4p1
182* Br 3p3	223 Rh (M45N1N45)
182 Lu (N4N67N67)	226 K (L3M1M23)
182 Lu (NNN)	226 Th 5p1
183* Cl (LVV)	226 Os (N5N7O45)
183 Ta (N4N67N67)	226* Ta 4d5
183 Ta (NNN)	228 Nd 4p3
184 Po 4f	228* Mo 3d5
184 Hf (NNO)	228* S 2s
187 I 4s	231 Ru (M4N23V)
188* P 2s	231 Ru (MNV)
188* Mo (M45N23V)	231* Mo 3d3
188* Mo (MNV)	232 Se 3s
189* B 1s	233 Ir (N5N7O45)
189* Br 3p1	234 Fr 5s
190* U (N67O45N45)	234 Pr 4p1
191* Yb 4d3	234 Cs 4s
193 Ba 4p1	238 Rn 4f
195 At 5s	238* Ta 4d3
196* Lu 4d5	240* Rb 3p3
197 La 4p3	241 Pt (N5N67O45)
199* Cl 2p3	242 Pm 4p3
200 Nb (M45N45N45)	242* Ar 2p3
200 Nb (MNN)	243* W 4d5
200 Ra 5p1	243 Pd (M45N1N45)
201* Cl 2p1	143 Au (N5N67O45)
201 Ru (M45N1N45)	244* Ar 2p1

245 Nd 4p1	293* Os 4d3
246 Hg (N5N7O45)	294 Th 5s
246 Tc (M5N45N45)	294* K 2p3
248* Th (N67O45V)	296 Ag (M45N23V)
248* Th (NOV)	297* Dy 4p3
248* K (L3M23M23)	297* K 2p1
248* K (LMM)	297* Ir 4d5
249* Rb 3p1	297* Ca (L2M23M23)
250 Sm 4p3	297* Ca (LMM)
250* K (L3M23M23)	298 Cs (L3M23M23)
250 Tl (N5N7O5)	299* Y 3p3
251 Pb (M5N7O5)	299 Ra 4f
253 Tc 3d5	301 Gd 4p1
253 Rh (M45N23V)	302* Rh (M5N45N45)
253 Rh (MNV)	302* Rh (MNN)
253 Bi (M5N67O45)	305 Pr 4s
254 Ra 5s	307* Rh 3d5
254 Ba 4s	307 Sc (L3M1M23)
256* W 4d3	309* Ho 4p3
256 Br 3s	311* Y 3p1
257 Tc 3d3	312* Rh 3d3
260* Re 4d5	312* Ir 4d3
261 Eu 4p3	315 Sc (L3M1M23)
262 Ag (M45N1N45)	315* Pt 4d5
264* C (KVV)	316 Cd (M45N23V)
264 Pm 4p1	319 Ac 4f
268 Fr 4f	320* Ar 2s
270 Gd 4p3	320 Nd 4s
270* Sr 3p3	321* Er 4p3
271* Cl 2s	322* Tb 4p1
272 Ac 5s	325 Rb 3s
274* Re 4d3	328* Pd (M4N45N45)
275 La 4s	328* Pd (MNN)
275* C (KL23L23)	330* Zr 3p3
275* C (KLL)	332* Pt 4d3
275* Ru (M45N45N45)	333* Tm 4p3
275* Ru (MNN)	333* Th 4f7
276* Pd (M45N23V)	335* Pd 3d5
279* Os 4d5	335* Au 4d5
280* Ru 3d5	337* Dy 4p1
280 Cd (M45N1N45)	337 Pm 4s
281* Sr 3p1	338* Sc (L3M23M23)
283 Sm 4p1	338* Sc (LMM)
283* U (N67O45V)	340* Pd 3d3
283* U (NOV)	341* Yb 4p3
284* Ru 3d3	342* Th 4f5
285* C 1s	344* Zr 3p1
285* Tb 4p3	346 Ti (L3M1M23)
287 Kr 3s	347* Ca 2p3
289 Eu 4p1	349 Sm 4s
290 Ce 4s	350* Ca 2p1

352* Ag (M5N45N45)	419* Ti (L3M23M45)
352* Ag (MNN)	419* Ti (LMM)
353* Au 4d3	424 W 4p3
353* Ho 4p1	425 Tc 3p3
355 Ti (L3M1M23)	430 Zr 3s
358* Ag (M4N45N45)	431* Sn (M5N45N45)
360 Sr 3s	431* Sn (MNN)
360* Lu 4p3	432 Cr (L3M23M23)
361* Hg 4d5	434* Pb 4d3
361* Nb 3p3	435 Ho 4s
366 Eu 4s	437 Hf 4p1
368* Ag 3d5	438 Sn (M4N45N45)
368* Er 4p1	439* V (L3M23M23)
369 Sc (L3M23M45)	440* Ca 2s
374* Ag 3d3	441* Bi 4d5
376* Nb 3p1	444* In 3d5
377* U 4f7	445 Tc 3p1
377* Cd (M5N45N45)	446 Re 4p3
377* Cd (MNN)	448 Cr (L3M1M23)
378 Gd 4s	451 Er 4s
380 Hf 4p3	451 Ti (L3M45M45)
380* K 2s	452* In 3d3
380* N (KVV)	454* Ti 2p3
381* Hg 4d3	455* Sb (M4N45N45)
383 Ti (L3M23M23)	455* Sb (MNN)
384* Tm 4p1	460* Ti 2p1
384* Cd (M4N45N45)	460 Cr (L3M1M23)
385* Tl 4d5	462* Ru 3p3
388* U 4f5	463 Ta 4p1
389 Ti (L3M23M23)	465* Bi 4d3
389* Yb 4p1	467 Nb 3s
394 Y 3s	470 Tm 4s
394* Mo 3p3	471 Os 4p3
396 Tb 4s	473 Po 4d5
399* Sc 2p3	473* V (L3M23M45)
400* N 1s	475* V (LMM)
400 V (L3M1M23)	474* O (KL1L1)
401 Ta 4p3	482 Yb 4s
403* In (M4N45N45)	482* Te (M5N45N45)
403* In (MNN)	482* Te (MNN)
404* Sc 2p1	484* Ru 3p1
405* Cd 3d5	485* Sn 3d5
405 In (M5N45N45)	488 O (KL1L23)
406* Tl 4d3	490 Cr (L3M23M23)
411* In (M4N45N45)	491 W 4p1
411* Mo 3p1	492* Te (M4N45N45)
411 V (L3M1M23)	493* Sn 3d3
412* Cd 3d3	495 Ir 4p3
412* Pb 4d5	497* Rh 3p3
413* Lu 4p1	499* Sc 2s
417 Dy 4s	500 Po 4d3

500 Mn (L3M1M23)	586 Ru 3s
505* I (M5N45N45)	587* Mn (L3M23M45)
505* I (MNN)	587* Mn (LMM)
506 Mo 3s	587* Ba (M5N45N45)
507 At 4d5	594 W 4s
509 Lu 4s	599 Fe (L3M23M23)
509* O (KL23L23)	601* Ba (M4N45N45)
509* O (KLL)	601* Ba (MNN)
510* V (L3M45M45)	603 Ra 4d5
512* V 2p3	603 Fr 4d3
514 Mn (L3M1M23)	604* Ag 3p1
516* I (M4N45N45)	607 Co (L3M1M23)
518 Re 4p1	609 Pt 4p1
520 Pt 4p3	609* F (KL1L1)
520* V 2p1	610 Tl 4p3
521* Rh 3p1	619* I 3d5
527* Cr (L3M23M45)	619* Cd 3p3
527* Cr (LMM)	620* La (M5N45N45)
528* Sb 3d5	620 Co (L3M1M23)
531* O 1s	625 Re 4s
532* Xe (M5N45N45)	626 V 2s
533 At 4d3	628* F (KL1L23)
533* Pd 3p3	629 Rh 3s
534 Hf 4s	630 Cs (M5N45N67)
536 Xe (M5N45N45)	631* I 3d3
537* Sb 3d3	633* La (M4N45N45)
541 Rn 4d5	633* La (MNN)
543 Mn (L3M23M23)	635 Mn (L3M45M45)
544 Tc 3s	636 Ra 4d3
545* Xe (M4N45N45)	638 F (KL1L23)
547 Au 4p3	639 Ac 4d5
548 Os 4p1	639* Mn 2p3
549 Fe (L3M1M23)	643 Au 4p1
555* Cs (M5N45N45)	643 Cs (M4N45N67)
560* Pd 3p1	644 Pb 4p3
561* Ti 2s	648 Fe (L3M23M45)
562 I (M5N45O23)	649 Co (L3M23M23)
563 Ta 4s	650* Mn 2p1
564 Fe (L3M1M23)	651 Fe (L3M23M45)
567 Rn 4d3	653* Cd 3p1
569* Cs (M4N45N45)	653* F (KL23L23)
569* Cs (MNN)	653* F (KLL)
570 Cr (L3M45M45)	654* Ce (M45N45N45)
573* Ag 3p3	655* F (KL23L23)
573* Te 3d5	656 Co (L3M23M23)
574* Cr 2p3	658 Os 4s
577 Fr 4d5	662 Ni (L3M1M23)
578 Ir 4p1	665* In 3p3
579 Hg 4p3	669 Ba (M5N45N67)
583* Cr 2p1	670* Xe 3d5
583* Te 3d3	671 Pd 3s

675 Ac 4d3	771* Ce (MNN)
675 Ni (L3M1M23)	772 Cd 3s
676* Th 4d5	774* Co (L3M45M45)
679 Bi 4p3	774* Co (LMM)
682 Hg 4p1	775 Ni (L3M23M45)
683* Xe 3d3	775 Cu (L2M23M23)
683 Ba (M4N45N67)	778* Co 2p3
685* F 1s	779* U 4d3
692 Ir 4s	781* Ba 3d5
695* Pr (M5N45N45)	781 Ni (L3M23M45)
695* Pr (MNN)	784 Zn (L3M1M23)
696* Cr 2s	785 Ne (KL1L23)
703* In 3p1	789 Co (L2M45M45)
703* Fe (L3M45M45)	793* Co 2p1
703* Fe (LMM)	795* Pr (M45N45N67)
705 Po 4p3	796* Ba 3d3
707* Fe 2p3	798 Ne (KL1L23)
709 Ni (L3M23M23)	805* Sm (M5N45N45)
710 Co (L3M23M45)	805* Sm (MNN)
711* La (M5N45N67)	805 Hg 4s
713* Th 4d3	806 Bi 4p1
715 Ni (L2M23M23)	810 Fr 4p3
715* Sn 3p3	813* Sb 3p1
715 Fe (L2M45M45)	814 Ne (KL23L23)
716 Co (L3M23M45)	818* Ne (KL23L23)
718 Cu (L3M1M23)	818* Ne (KL23L23)
719 Ag 3s	820* Te 3p3
720 Tl 4p1	827 Zn (L3M23M23)
720* Fe 2p1	828 In 3s
723 Co (L2M23M45)	831 Ga (L3M1M23)
725 Pt 4s	835 Zn (L2M23M23)
726* Cs 3d5	836* La 3d5
728* La (M4N45N67)	839* Cu (L3M23M45)
731 Cu (L3M1M23)	840* Nd (M45N45N67)
733* Nd (M5N45N45)	845 Fe 2s
733* Nd (MNN)	845 Ga (L3M1M23)
736* U 4d5	846* Ni (L3M45M45)
740* Cs 3d3	846* Ni (LMM)
740 At 4p3	846* Eu (M5N45N45)
755* Ce (M5N45N67)	847 Tl 4s
757* Sn 3p1	850* Eu (M45N45N45)
762 Pb 4p1	851 Po 4p1
762 Ne (KL1L1)	853* La 3d3
763 Au 4s	853* Ni 2p3
767* Sb 3p3	859 Cu (L2M23M45)
768 Rn 4p3	861 Nd (M4N45O23)
768 Cu (L3M23M23)	863* Ni (L2VV)
769 Zn (L3M1M23)	863* Ne 1s
769 Mn 2s	870* Ni 2p1
770* Pm (M5N45N45)	871* Te 3p1
771* Ce (M4N45N67)	875 I 3p3

879 Ra 4p3	992* Zn (LMM)
884* Ce 3d5	994* Na (KL23L23)
884* Gd (M5N45N45)	994* Na (KLL)
885 Sn 3s	995 Po 4s
885* Pm (M45N45N67)	996 Xe 3p1
886 At 4p1	998* Ho (M5N45N45)
888 Ga (L3M23M23)	1000 Ga (L2M23M45)
890 Ge (L3M1M23)	1002* Nd 3d3
893 Pb 4s	1002 Cs 3p3
895 Ge (L3M1M23)	1009 Te 3s
898 Ga (L2M23M23)	1009 Ni 2s
900 Ac 4p3	1013 Se (L3M1M23)
902* Ce 3d3	1015 Zn (L2M45M45)
905 Zn (L3M23M45)	1020 As (L3M23M23)
914 Zn (L3M23M45)	1020* Gd (M45N45N67)
919* Cu (L3M45M45)	1022* Zn 2p3
919* Cu (LMM)	1030 As (L2M23M23)
920* Tb (M5N45N45)	1033 Se (L3M1M23)
921* Cu (L3VV)	1034* Pm 3d5
925 Co 2s	1043 Ge (L3M23M45)
926 Na (KL1L1)	1045* Zn 2p1
928 Zn (L2M23M45)	1045 At 4s
929 Rn 4p1	1047* Er (M5N45N45)
930 I 3p1	1058 Ra 4p1
932* Pr 3d5	1060* Pm 3d3
933* Cu 2p3	1064 Ba 3p3
934 Xe 3p3	1068* Sm (M5N67N67)
938* Cu (L2VV)	1068* Tb (M45N45N67)
939* Cu (L2M45M45)	1068* Tb (MNN)
940 Bi 4s	1069* Ga (L3M45M45)
944 Sb 3s	1069* Ga (LMM)
950 As (L3M1M23)	1069 Cs 3p1
950* Sm (M45N45N67)	1071 I 3s
951 Na (KL1L23)	1072* Na 1s
952* Pr 3d3	1075 Ge (L2M23M45)
953 Ge (L3M23M23)	1080 Ac 4p1
953* Cu 2p1	1080* Tm (M5N45N45)
962 Ge (L3M23M23)	1081* Sm 3d5
965 Th 4p3	1086 Se (L3M23M23)
966 As (L3M1M23)	1091 Ga (L2M45M45)
967 Na (KL1L23)	1094* Sm (M4N67N67)
973* Ga (L3M23M45)	1096 Se (L3M23M23)
978* Dy (M5N45N45)	1097 Rn 4s
980 Fr 4p1	1097 Cu 2s
980* Eu (M45N45N67)	1106 Mg (KL1L1)
980* Eu (MNN)	1108* Sm 3d3
981* Nd 3d5	1116 As (L3M23M45)
983 Ga (L3M23M45)	1117* Ga 2p3
989 Na (KL23L23)	1118* As (L3M23M45)
989 Na (KLL)	1119* Dy (M45N45N67)
992* Zn (L3M45M45)	1119* Dy (MNN)

1120* Eu (M5N67N67)	1248* Ge 2p1
1126* Eu 3d5	1253 Br (L3M23M45)
1127 As (L3M23M45)	1256* Tb (M4N67N67)
1127 Se (L3M1M45)	1261* As (L2M45M45)
1128 La 3p3	1264* As (L2M45M45)
1138 Ba 3p1	1267 Br (L3M1M23)
1140 Mg (KL1L23)	1269 Ac 4s
1141 Xe 3s	1270* Tm (M45N45N67)
1141 Yb (M5N5N5)	1270* Tm (MNN)
1143 Br (L3M23M23)	1271 Ta (M5N5N5)
1144* Ga 2p1	1272 Ce 3p1
1145* Ge (L3M45M45)	1276* Tb 3d3
1150* Ge (LMM)	1280* Dy (M5N67N67)
1150* Eu (M4N67N67)	1292 Ba 3s
1151 As (L2M23M45)	1296* Dy 3d5
1153 Fr 4s	1300 Br (L2M23M45)
1155 Mg (KL2L23)	1301 Ga 2s
1155 Br (L3M23M23)	1301 Nd 3p3
1156* Eu 3d3	1302 Al (KL1L1)
1165* Ho (M45N45N67)	1303* Mg 1s
1165* Ho (MNN)	1306* Se (L3M45M45)
1170 Th 4p1	1306* Se (LMM)
1170* Gd (M5N67N67)	1312 W (M5N5N5)
1177 Ge (L2M45M45)	1318* Dy (M4N67N67)
1181* Mg (KL23L23)	1320* Yb (M45N45N67)
1181* Mg (KLL)	1324* As 2p3
1184 Ce 3p3	1327 Kr (L3M23M45)
1186* Mg (KL23L23)	1330 Th 4s
1186* Gd 3d5	1332* Ho (M5N67N67)
1188 Lu (M5N5N5)	1333* Dy 3d3
1188 Se (L3M2M45)	1339 Pr 3p1
1195 Zn 2s	1341 Al (KL1L23)
1200 Se (L3M3M45)	1345 Kr (L3M23M45)
1202* Gd (M4N67N67)	1347 Se (L2M45M45)
1208 La 3p1	1354 Re (M5N5N5)
1208 Ra 4s	1357 Al (KL1L23)
1210 Kr (L3M23M23)	1359* As 2p1
1212 Mg (KL23M)	1370* Ho (M4VV)
1216 Cs 3s	1370* Lu (M5N45N67)
1217* Ge 2p3	1372* Ho (M4N67N67)
1218* Er (M45N45N67)	1380 Kr (L2M23M45)
1218* Er (MNN)	1387* Al (KL23L23)
1218* Gd 3d3	1387* Al (KLL)
1223 Kr (L3M23M23)	1388* Br (L3M45M45)
1225* As (L3M45M45)	1388 Br (LMM)
1225* As (LMM)	1389* Er (M5N67N67)
1227* Tb (M5N67N67)	1393* Al (KL23L23)
1230 Se (L2M23M45)	1396 Os (M5N5N5)
1231 Hf (MNO)	1420* Hf (M45N45N67)
1241* Tb 3d5	1424 Br (L2M45M45)
1242 Pr 3p	1428* Er (M4N67N67)

1433 Rb (L3M3M3)	1737 Y (LMM)
1439 Br (LMM)	1771 Au (M5N5N7)
1439 Ir (M5N5N5)	1787 Nb (L3M3M45)
1440* Tm (M5N67N67)	1790 Re (M5N67N67)
1460 Kr (L3M45M45)	1790 Re (MNN)
1462 Ta (M45N45N67)	1791 W (M4N6N6)
1484 Pt (M5N5N5)	1792 P (KL1L2)
1487* Tm (M4N67N67)	1793 Ta 3d3
1500* Yb (M5N67N67)	1809 W 3d5
1500* Yb (MNN)	1818 Hg (M5N5N7)
1513 Kr (L2M45M45)	1823 Y (L2M45M45)
1514 Si (KL1L1)	1831 Zr (L3M45M45)
1516 Sr (L3M3M5)	1831 Zr (LMM)
1522 Au (M5N5N5)	1837 Os (M5N7N7)
1524 W (M5N5N7)	1839 Si 1s
1549* Yb (M4N67N67)	1850* P (KL23L23)
1559 Si (KL1L23)	1850* P (KLL)
1560 Al 1s	1856 Re (M4N67N67)
1560* Lu (M5N67N67)	1862 P (K1L3L3)
1560* Lu (MNN)	1865 Tl (M5N5N67)
1561 Rb (L3M5M5)	1872 W 3d3
1561 Rb (LMM)	1881 Mo (L3M3M5)
1572 Re (M5N5N7)	1883 Re 3d5
1576 Si (KL1L23)	1901* Ir (M5N67N67)
1589 Lu 3d5	1901* Ir (MNN)
1615* Hf (M5N67N67)	1907* Os (M4N67N67)
1601 Tl (M5N5N5)	1907* Os (MNN)
1606 Y (L3M23M45)	1914 Pb (M5M5N7)
1615* Hf (MNN)	1920* Nb (L3M45M45)
1615* Lu (M4N67N67)	1920* Nb (LMM)
1617* Si (KL23L23)	1929 Zr (L2M45M5)
1617* Si (KLL)	1938 P (KL1M1)
1620 Rb (L2M45M45)	1949 Re 3d3
1622 Os (M5N5N7)	1949 P (KL1M23)
1639 Lu 3d3	1960 Os 3d5
1640* Sr (L3M45M45)	1960 Bi (M5N5N67)
1640* Sr (LMM)	1961* Pt (M5N67N67)
1641 Pb (M5N5N5)	1961* Pt (MNN)
1662 Hf 3d5	1978* Ir (M4N67N67)
1669* Hf (M4N67N67)	1996 P (KL23M1)
1675* Ta (M5N67N67)	2001 P (KL23M23)
1675* Ta (MNN)	2016* Au (M5N67N67)
1695 Zn (L3M3M45)	2016* Au (MNN)
1716 Hf 3d3	2024 Lu 3p3
1718 Sr (L2M45M45)	2026* S (KL1L23)
1725* W (M5N67N67)	2031 Os 3d3
1725* W (MNN)	2039* Mo (L3M45M45)
1725 Pt (M5N45N67)	2039* Mo (LMM)
1733 Ta (M4N67N67)	2039 Nb (L2M45M45)
1735 Ta 3d5	2040 Ir 3d5
1737 Y (L3M45M45)	2040* Pt (M4N67N67)

2070 Hg (M5N67N67)	2491 Lu 3s
2078 Ru (L3M3M45)	2507 Rh (L2M5M5)
2102* Au (M4N67N67)	2508 Ar (KL1L1)
2108 Hf 3p3	2551 Ir 3p3
2116 Ir 3d3	2575 W 3p1
2116* S (KL23L23)	2576 Ar (KL1L23)
2116* S (KLL)	2580 Bi 3d5
2122 Pt 3d5	1583 Ag (L3M45M45)
2128 Tl (M5N67N67)	2586 Pb 3d3
2128 Tl (MNN)	2600 Ar (KL1L23)
2144* Mo (L2M45M45)	2601 Hf 3s
2145 P 1s	2633 Pd (L3M3M45)
2160* Hg (M4N67N67)	2634 Th (M5N7N7)
2160* Hg (MNN)	2645 Pt 3p3
2180 Pb (M5N67N67)	2651 Ar (KL23L23)
2180 Rh (L3M3M45)	2661 Ar (KL23L23)
2180 Pb (MNN)	2682 Re 3p1
2194 Ta 3p3	2683 Po 3d5
2202 Pt 3d3	2688 Bi 3d3
2206 Au 3d5	2694 Cd (L3M5M5)
2223 Tl (M4N67N67)	2694 Cd (LMM)
2235 Bi (M5N67N67)	2708 Ta 3s
2235 Bi (MNN)	2743 Au 3p3
2256 Ru (L3M45M45)	2755 Ag (L3M3N45)
2256 Ru (LMM)	2764 U (M5N7N7)
2264 Lu 3p1	2787 At 3d5
2281 W 3p3	2789 Th (M4N7N7)
2282 Pb (M4N67N67)	2792 Os 3p1
2282 Pd (L3M3M45)	2798 Po 3d3
2291 Au 3d3	2806 In (L3M5M5)
2295 Hg 3d5	2820 W 3s
2296 Th (M5N5N7)	2822 Cl 1s
2343 Bi (M4N67N67)	2847 Hg 3p3
2343 Bi (MNN)	2892 Rn 3d5
2365 Hf 3p1	2909 Ir 3p1
2366 Rh (L3M45M45)	2909 At 3d3
2366 Rh (LMM)	2919 Sn (L3M5M5)
2367 Re 3p3	2932 Re 3s
2370* Cl (KL23L23)	2940 U (M4N6N7)
2370* Cl (KLL)	2957 Tl 3p3
2381 Ag (L3M3M45)	3000 Fr 3d5
2385 Hg 3d3	3004 Rh 2p3
2385 Ru (L2M45M45)	3022 Rn 3d3
2389 Tl 3d5	3027 Pt 3p1
2414 U (M5N5N7)	3035 Sb (M5N45N45)
2457 Os 3p3	3049 Os 3s
2469 Ta 3p1	3066 Pb 3p3
2472 S 1s	3105 Fr 3d5
2476 Pd (L3M45M45)	3136 Fr 3d3
2484 Pb 3d5	3146 Rh 2p1
2485 Tl 3d3	3148 Au 3p1

3173 Pd 2p3	4492 Sc 1s
3174 Ir 3s	4652 Fr 3s
3177 Bi 3p3	4656 Ac 3p1
3206 Ar 1s	4698 Sb 2s
3219 Ac 3d5	4822 Ra 3s
3248 Ra 3d3	4830 Th 3p1
3279 Hg 3p1	4966 Ti 1s
3296 Pt 3s	5001 Pa 3p1
3302 Po 3p3	5002 Ac 3s
3330 Pd 2p1	5182 Th 3s
3332 Th 3d5	5182 U 3p1
3351 Ag 2p3	5367 Pa 3s
3370 Ac 3d3	5465 V 1s
3412 Rh 1s	5548 U 3s
3416 Tl 3p1	5989 Cr 1s
3425 Au 3s	6539 Mn 1s
3426 At 3p3	7112 Fe 1s
3442 Pa 3d5	7709 Co 1s
3491 Th 3d3	8333 Ni 1s
3524 Ag 2p1	8979 Cu 1s
3538 Rn 3p3	9244 Lu 2p3
3552 U 3d5	9561 Hf 2p3
3554 Pb 3p1	9659 Zn 1s
3562 Hg 3s	9881 Ta 2p3
3604 Pd 1s	10207 W 2p3
3608 K 1s	10349 Lu 2p1
3611 Pa 3d3	10367 Ga 1s
3663 Fr 3p3	10535 Re 2p3
3696 Bi 3p1	10739 Hf 2p1
3704 Tl 3s	10870 Lu 2s
3728 U 3d3	10871 Os 2p3
3792 Ra 3p3	11103 Ge 1s
3806 Ag 1s	11136 Ta 2p1
3851 Pb 3s	11215 Ir 2p3
3854 Po 3p1	11271 Hf 2s
3909 Ac 3p3	11544 W 2p1
3999 Bi 3s	11564 Pt 2p3
4002* Ti (KL23L23)	11682 Ta 2s
4008 At 3p1	11867 As 1s
4132 2p3	11919 Au 2p3
4038 Ca 1s	11959 Re 2p1
4046 Th 3p3	12100 W 2s
4149 Po 3s	12284 Hg 2p3
4159 Rn 3p1	12385 Os 2p1
4174 Pa 3p3	12658 Se 1s
4303 U 3p3	12658 Tl 2p3
4317 At 3s	12824 Ir 2p1
4327 Fr 3p1	12968 Os 2s
4380 Sb 2p1	13035 Pb 2p3
4482 Rn 3s	13273 Pt 2p1
4490 Ra 3p1	13419 Ir 2s

13419 Bi 2p3	26711 Cd 1s
13474 Br 1s	27940 In 1s
13734 Au 2p1	29200 Sn 1s
13814 Po 2p3	30491 Sb 1s
13880 Pt 2s	31814 Te 1s
14209 Hg 2p1	33169 I 1s
14214 At 2p3	34561 Xe 1s
14326 Kr 1s	35985 Cs 1s
14353 Au 2s	37441 Ba 1s
14619 Rn 2p3	38925 La 1s
14698 Tl 2p1	40443 Ce 1s
15031 Fr 2p3	41991 Pr 1s
15200 Rb 1s	43569 Nd 1s
15200 Pb 2p1	45184 Pm 1s
15347 Tl 2s	46834 Sm 1s
15444 Ra 2p3	48519 Eu 1s
15711 Bi 2p1	50239 Gd 1s
15861 Pb 2s	51996 Tb 1s
15871 Ac 2p3	53789 Dy 1s
16105 Sr 1s	55618 Ho 1s
16244 Po 2p1	57486 Er 1s
16300 Th 2p3	59390 Tm 1s
16388 Bi 2s	61332 Yb 1s
16733 Pa 2p3	63314 Lu 1s
16785 At 2p1	65351 Hf 1s
16939 Po 2s	67416 Ta 1s
17038 Y 1s	69525 W 1s
17166 U 2p3	71676 Re 1s
17337 Rn 2p1	73871 Os 1s
17493 At 2s	76111 Ir 1s
17907 Fr 2p1	78395 Pt 1s
17998 Zr 1s	80725 Au 1s
18049 Rn 2s	83102 Hg 1s
18484 Ra 2p1	85530 Tl 1s
18639 Fr 2s	88005 Pb 1s
18986 Nb 1s	90524 Bi 1s
19083 Ac 2p1	93105 Po 1s
19237 Ra 2s	95730 At 1s
19693 Th 2p1	98404 Rn 1s
19840 Ac 2s	101137 Fr 1s
20000 Mo 1s	103922 Ra 1s
20314 Pa 2p1	106755 Ac 1s
20472 Th 2s	109651 Th 1s
20948 U 2p1	112601 Pa 1s
21044 Te 1s	115606 U 1s
21105 Pa 2s	
21757 U 2s	
22117 Ru 1s	
23220 Rh 1s	
24350 Pd 1s	
25514 Ag 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 Ag₂Se351.2 Ag₂S350.7 Ag₂O

350.6 AgO

350.1 AgI

349.6 AgF₂

349.3 AgF

Ag 3d5.pos367.3 AgF₂

367.4 AgO

367.5 Ag₂CO₃

367.7 AgF

367.8 Ag₂O

367.8 CuAgSe

367.8 Ag₂Se367.8 Ag₂SO₄

368.0 AgI

368.1 Ag₂S

368.2 Ag

368.4 Ag(OAc)

368.8 Ag₂Yb368.8 AgOOCFF₃368.8 Mg₉₇Ag₃**Al (KL23L23;1D).pos, Al (KLL).pos**

1393.1 Al

1391.2 AlAs

1389.4 Al₂O₃/Al

1389.0 AlN

1388.4 Al₂O₃1388.2 Al₂O₃/alpha1388.1 Al₂FeO₄1387.9 Al₂O₃/sapphire1387.8 Al₂O₃/gamma1387.7 Al₂O₃/anhydride1387.7 Al(OH)₃/bayerite

1387.6 AlO(OH)/boehmite

1387.1 KAl₂(AlSi₃O₁₀)₂(OH)₂/muscovite1387.1 LiAlSi₂O₆/spodumene

1386.9 Mol Sieve A

1386.9 Al₂SiO₅/sillimannite1386.9 Al₆Si₂O₁₃/mullite1386.8 Al₂SiO₅1386.8 Al₂Si₄O₁₀(OH)₂/pyrophyllite1386.7 Al₄Si₄O₁₀(OH)₈/kaolinite1386.5 Na[AlSi₃O₈]/albite1386.5 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/Al66.4 Al₂O₃/Al**Al 2p.pos**71.0 AlB₂

72.9 Al

73.4 Fe₃Al

73.6 AlAs

73.6 AlGaAs

73.6 CoAl₂O₄

73.7 Mol Sieve A

73.7 Al₂O₃/gamma73.9 Al₂O₃/alpha

74.0 AlN

74.1 Al₂O₃/sapphire74.2 AlO₂H/boehmite74.2 Al₂(MoO₄)₃74.2 NiAl₂O₄74.2 AlO₂H74.2 Al(OH)₃/bayerite74.3 Al₂(WO₄)₃

74.3 Mica/muskovite

74.6 Al₂S₃74.6 AlI₃74.6 Al₂SiO₅/sillimanite74.7 AlCl₃74.7 MgAl₂O₄74.8 Al₂SiO₅/mullite

74.8 H Zeolon

75.2 AlBr₃75.6 LiAlH₄

76.3 AlF

Ar (L3M23M23).pos

211.0 Ar

Ar (L3M23M23;3P).pos

212.8 Ar	2101.5 Au
Ar 2p.pos	Au (M5N67N67).pos, Au (MNN).pos
241.5 Ar in graphite	2015.7 Au
As (L2M45M45).pos	Au (N7VV).pos
1254.9 As ₂ O ₃	69.8 Au
1254.6 NaAsO ₂	Au (N67VV).pos, Au (NVV).pos
1252.9 Na ₂ HAsO ₄	
As (L3M45M45).pos, As (LMM).pos	71.2 Au
1225.1 GaAs	Au 4f7.pos
1224.8 As	84.0 Au
1222.1 As ₂ S ₃	84.5 AuSn
1221.1 Ph ₃ As	85.1 AuSn ₄
1219.5 Ph ₃ AsO	85.3 ClAuPh ₃ P
1218.8 As ₂ O ₃	
1217.5 As ₂ O ₅	B 1s.pos
1213.8 KAsF ₆	186.5 B ₄ C
1218.1 AsBr ₃	187.2 NaBH ₄
1222.9 AsI ₃	187.3 B
As 3d.pos	187.5 TiB
40.6 InAs	187.8 B ₁₀ H ₁₄
41.0 AlGaAs	188.5 AlB ₂
41.0 AlAs	190.5 BN
41.2 GaAs	193.0 H ₃ BO ₃
41.5 As	192.6 Na ₂ B ₄ O ₇ ·10H ₂ O
42.8 Ph ₃ As	193.1 B ₂ O ₃
43.4 As ₂ S ₃	194.9 NaBF ₄
43.4 AsI ₃	
44.3 Ph ₃ AsO	Ba (M4N45N45).pos, Ba (MNN).pos
44.9 As ₂ O ₃	601.6 Ba
45.3 AsBr ₃	598.0 BaO
46.2As ₂ O ₅	596.3 Ba(ClO ₃)·H ₂ O
47.8 KAsF ₆	596.1 BaSO ₄
As 2p3.pos	596.1 Ba(NO ₃) ₂
1323.1 GaAs	595.3 Ba(ClO ₄) ₂
1324.3 As	595.2 Ba/Ca/Cd/Sr/in_montmorillonite
1325.7 AsO	594.9 BaF ₂
1326.4 As ₂ O ₃	594.9 BaCl ₂ ·2H ₂ O
1327.4 As ₂ O ₅	Ba (N45O23O23).pos, Ba (NOO).pos
Au (M4N67N67).pos	59.5 BaF ₂ /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	C ₆ H ₅ F(C*F)	381.0	Zn _{0.90} Cd _{0.10} Se
287.9	(-CH ₂ C*FH-)n	381.3	CdS
287.9	CH ₃ C*OCH ₃	381.0	CdSe
288.0	Fe(CO) ₅	380.5	CdI ₂
288.0	H ₂ NCSNH ₂	380.0	Cd(OH) ₂
288.2	CH ₃ C*OONa	380.0	CdBr ₂ ·4H ₂ O
288.4	CH ₃ C*ONH ₂	379.8	(CdCl ₂) ₂ ·5H ₂ O
288.7	H ₂ NCONH ₂	378.5	CdF ₂
289.3	CH ₃ C*OOH	378.3	Ba/Ca/Cd/Sr/in_montmorillonite
289.4	Na ₂ CO ₃		
289.5	Cl ₃ C*COONa		Cd (M5N45N45).pos
289.6	CaCO ₃		
289.6	HCCl ₃	377.0	Cd
290.0	NaHCO ₃	370.5	Cd
290.9	(-CH ₂ C*F ₂ -)n	374.4	CdI ₂
291.9	CO ₂	375.8	CdTe
292.2	Teflon(-CF ₂ CF ₂ -)n	369.5	CdTe
292.4	CCl ₄	368.5	CdTe
292.9	C*F ₃ COOEt	375.6	CdO
294.7	HCF ₃	374.8	CdSe
296.7	CF ₄	374.5	CdS
		372.2	CdF ₂
	Ca (L2M23M23).pos, Ca (LMM).pos		
298.2	Ca		Cd 3d5.pos
292.5	CaO	404.2	CdO
291.9	CaCO ₃	404.6	Hg _{0.8} Cd _{0.2} Te
291.9	CaCl ₂	405.0	CdSe
288.9	CaF ₂	405.1	Cd
		405.1	Cd(OH) ₂
	Ca 2p3.pos	405.1	CdCO ₃
345.9	Ca	405.2	CdTe
346.3	CaCrO ₄	405.3	CdS
346.5	CaS	405.4	CdI ₂
347.0	CaCO ₃	405.9	CdF ₂
347.0	Ca ₃ Si ₃ O ₉	406.0	CdBr ₂
347.3	CaO	406.1	CdCl ₂
347.9	CaF ₂		Ce (M4N45N67).pos, Ce (MNN).pos
348.0	CaSO ₄	771.0	CeO ₂
348.3	CaCl ₂		
	Cd (M4N45N45).pos, Cd (MNN).pos		Ce (M5N45N67).pos
383.6	Cd	755.0	CeO ₂
382.5	CdO		
382.4	CdTe		Ce 3d5.pos
382.2	CdSe _{0.65} Te _{0.35}	881.9	CeO ₂
381.4	Zn _{0.30} Cd _{0.70} Se	883.5	CeAl ₂
381.5	Zn _{0.50} Cd _{0.50} Se	883.6	CeCu ₂ Si ₂
381.2	Zn _{0.70} Cd _{0.30} Se		

883.9 Ce
884.3 CePd3
884.3 CeSe
886.0 CeH3

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

2392.2 CsCl
2391.3 KCl
2391.0 RbCl
2391.4 LiCl
2390.9 NaCl

Cl (LVV).pos

182.5 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	917.6 CuInSe2
50.8 CsF/Au	917.1 Cu2S
49.0 CsCl	917.0 Cu2CO3(OH)2
51.2 CsCl	917.0 CuIn3Se5
49.2 CsBr	917.0 CuGa5Se8
51.4 CsBr	916.8 Cu(OH)2
	916.8 Al2CuO4
Cs (N45O23V).pos	916.7 Cu2O
61.6 CsBr	916.7 CuInS2
61.4 CsCl	916.6 CuMoO4
	916.6 Cu3Mo2O9
Cs 3d5.pos	916.3 CuCO3
723.6 CsF	916.3 CuBr2
723.9 CsI	916.1 CuI
723.9 Cs2SO4	916.1 CuSO4
724.0 CsBr	915.3 CuCl
724.0 CsCl	915.5 CuCl2
724.0 CsF	915.3 Cu(NO3)2
724.2 CsOH	915.2 CuSiO3
726.4 Cs	915.1 CuF2
	914.6 CuCN
	914.5 [CuC(CN)3]
	914.4 Cu2S
Cu (L2M45M45).pos	Cu (L3VV).pos
939.0 Cu	921.2 Cu
937.80 CuO	918.4 Cu
934.10 (GeO2)0.5(Na2O)0.3(CuO)0.2/glass	916.0 Cu
934.00 (GeO2)0.6(Na2O)0.3(CuO)0.1/glass	914.1 Cu
933.50	911.0 Cu
(GeO2)0.65(Na2O)0.3(CuO)0.05/glass	Cu (M23VV).pos, Cu (MVV).pos
Cu (L2VV).pos	62.4 Cu
938.3 Cu	63.7 6-8A Fe/Cu
934.7 Cu	60.8 6-8A Fe/Cu
Cu (L3M45M45).pos, Cu (LMM).pos	Cu 2p3.pos
918.6 Cu	931.9 CuInSe2
918.6 Cu64Zn36	932.3 CuS
918.5 Ag28.6Au17.1Cu54.3	932.5 Cu2O
918.4 CuSe	932.5 Cu2S
918.1 CuS	932.5 CuCl
918.0 CuCr2O4	932.6 Cu64Zn36
917.9 CuO	932.7 Cu
917.8 CuFeS2	933.1 CuCN
917.7 Cu2Se	933.8 CuO
917.7 AgCuSe	935.2 CuCl2
	934.5 Cu(acac)2

934.9 CuSO ₄	
935.1 Cu(OH) ₂	167.3 Er
936.1 CuF ₂	168.7 Er ₂ O ₃
Dy (M4N67N67).pos	Eu (M4N67N67).pos
1318.0 Dy	1150.0 Eu
Dy (M5N45N45).pos	Eu (M5N45N45).pos
960.0 Dy	846.0 Eu
Dy (M5N67N67).pos	Eu (M5N67N67).pos
1280.0 Dy	1120.0 Eu
Dy (M45N45N67).pos, Dy (MNN).pos	Eu (M45N45N67).pos, Eu (MNN).pos
1115.0 Dy	980.0 Eu
Dy 3d5.pos	Eu 3d5.pos
1295.5 Dy	1125.6 Eu
1298.9 Dy ₂ O ₃	
Dy 4d.pos	Eu 4d.pos
152.4 Dy	128.2 Eu
167.7 Dy ₂ O ₃	135.9 Eu ₂ O ₃
Er (M4N67N67).pos	F (KL1L1).pos
1428.0 Er	608.0 LiF
1429.0 Er ₂ O ₃	F (KL1L23).pos
Er (M5N45N45).pos	627.4 LiF
1035.0 Er	F (KL23L23).pos, F (KLL).pos
1037.0 Er ₂ O ₃	
Er (M5N67N67).pos	659.3 AgF
1387.0 Er	658.5 PbF ₂
1386.0 Er ₂ O ₃	658.0 LaF ₃
	657.2 PrF ₃
	657.0 SmF ₃
	657.0 NdF ₃
Er (M45N45N67).pos, Er (MNN).pos	657.0 ThF ₄
1218.0 Er	656.6 CuF ₂
1221.0 Er ₂ O ₃	656.4 InF ₃
	656.3 SrF ₂
	656.2 BaF ₂
Er 4d.pos	656.1 GdF ₃

656.0 CdF ₂	
656.0 K ₃ FeF ₆	703.0 FeS ₂
655.8 YF ₃	702.9 FeB
655.7 K ₂ TiF ₆	702.9 Fe ₂ B
655.6 ZnF ₂	702.7 Fe
655.6 CrF ₃	702.6 CuFeS ₂
655.5 MnF ₂	
655.5 NiF ₂	Fe (M23VV).pos, Fe (MVV).pos
655.4 CaF ₂	
655.3 HfF ₄	48.6 8-9A Fe/Cu
655.2 K ₂ NbF ₇	
655.1 Na ₂ TiF ₆	Fe 2p₃.pos
655.1 Na ₂ ZrF ₆	
655.0 NaF	706.7 Fe
655.0 K ₂ TaF ₇	707.1 K ₄ Fe(CN) ₆
654.7 LiF	707.2 FeS ₂
654.4 MgF ₂	707.4 FeB
654.4 NaSnF ₃	708.1 Fe ₃ C
654.1 Na ₃ AlF ₆	709.6 FeO
654.0 Na ₂ GeF ₆	709.6 K ₃ Fe(CN) ₆
653.9 KSbF ₆	710.6 Fe ₃ O ₄
653.8 CsF	710.9 Fe ₂ O ₃
653.5 SiF ₆ monolayer/Ni	712.1 FeSO ₄
653.0 Na ₂ SiF ₆	
653.0 SiF ₆ monolayer/O ₂ /Ni	Ga (L2M4M4).pos
652.9 [Ni(CF ₃ COO) ₂]	
652.8 NaBF ₄	1091.5 GaN
652.6 Al ₂ .3(OH)0.3.H ₂ O	
652.4 (-CF ₂ -CF ₂ -) _n	Ga (L3M45M45).pos, Ga (LMM).pos
651.7 AlF ₃	
	1068.0 Ga
F 1s.pos	1066.3 GaAs
683.9 KF	1065.6 GaP
684.5 CuF ₂	1065.3 Ga ₂ Se ₃
684.5 NaF	1065.3 CuGa ₅ Se ₈
684.6 CdF ₂	1064.3 GaN
684.8 CaF ₂	1062.3 Ga ₂ O ₃
684.8 UF ₂	
685.0 LiF	Ga (M23VV).pos, Ga (MVV).pos
685.5 MgF ₂	
685.5 Na ₃ AlF ₆	56.1 Ga
685.9 CsF	
686.2 Na ₂ SiF ₆	Ga 2p₃.pos
686.9 (-CHF-CH ₂ -) _n	
687.0 NaBF ₄	1116.7 Ga
688.2 (-CF ₂ -CH ₂ -) _n	1116.8 GaP
689.7 (-CF ₂ -CF ₂ -) _n	1116.9 Ga ₂ O ₃
694.2 NF ₄ BF ₄	
	Ga 3d.pos
Fe (L3M45M45).pos, Fe (LMM).pos	
	18.7 Ga

19.0 AlGaAs	1220.4 GeO ₂
19.3 GaAs	1221.3 Na ₂ GeF ₆
19.3 GaP	
19.5 GaN	Ge 3d.pos
20.5 Ga ₂ O ₃	
Gd (M4N67N67).pos	29.3 Ge
	30.5 GeS
	30.7 GeSe
1202.0 Gd	32.7 GeO ₂
	33.3 Na ₂ GeF ₆
Gd (M5N45N45).pos	Hf (M4N67N67).pos
884.0 Gd	1669.0 Hf
Gd (M5N6N67).pos	Hf (M5N67N67).pos, Hf (MNN).pos
1170.0 Gd	1615.0 Hf
Gd (M45N45N67).pos, Gc (MNN).pos	Hf (M45N45N67).pos
1020.0 Gd	1420.0 Hf
Gd 3d5.pos	Hf 4f7.pos
1187.0 Gd	14.2 Hf
1189.0 Gd ₂ O ₃	16.7 HfO ₂
1190.0 Gd ₂ (SO ₄) ₃	Hg (M4N67N67).pos, Hg (MNN).pos
Gd 4d.pso	
	2159.8 Hg
140.4 Gd	Hg 4f7.pos
143.8 Gd ₂ O ₃	
143.8 Gd ₂ (SO ₄) ₃	99.9 Hg
Ge (L3M45M45).pos, Ge (LMM).pos	100.2 Hg _{0.8} Cd _{0.2} Te
	100.8 Hg ₂ Cl ₂
1145.2 Ge	100.8 HgO
1144.8 GeTe	101.0 HgS/cinnabar
1143.7 GeS	101.4 HgCl ₂
1143.5 GeSe	Ho (M4N67N67).pos
1142.8 Ge ₂ Se ₃	
1141.8 GeSe ₂	1372.0 Ho
1141.7 GeSe ₃	Ho (M5N45N45).pos
1137.8 GeO ₂	
1136.6 Si _{0.4} Ge _{0.9} O _{0.6}	998.0 Ho
1135.7 Na ₂ GeF ₆ 1135.7 Na ₂ GeF ₆	Ho (M5N67N67).pos
Ge 2p3.pos	
1217.2 Ge	
1219.8 GeS ₂	

1332.0 Ho	408.0 InP
Ho (M45N45N67).pos, Ho (MNN).pos	408.1 In ₂ Se ₃
1165.0 Ho	407.4 CuIn ₃ Se ₅
Ho 4d.pos	407.3 In ₂ S ₃
159.6 Ho	407.3 CuInS ₂
I (M4N45N45).pos	406.5 In ₂ O ₃
519.0 I ₂	405.8 InI ₃
518.3 AgI	405.7 In(OH) ₃ .nH ₂ O
517.7 CdI	405.3 In(OH) ₃
517.3 UI ₃	404.8 InBr ₃
517.0 KI	404.7 InPO ₄
517.0 LiI	404.6 InCl ₃
516.4 SrI ₂	404.6 In(PO ₃) ₃
513.8 KNiIO ₆	404.4 In(PO ₃) ₄
I (M5N45N45).pos, I (MNN).pos	404.1 (NH ₄) ₃ [InF ₆]
507.3 NiI ₂	403.7 InF ₃
507.1 CuI	401.6 InSb
507.0 CdI ₂	In (M5N45N45).pos
506.8 AgI	397.5 In
506.0 ZnI ₂	393.0 In
503.6 KNiIO ₆	397.5 InP
I 3d5.pos	396.0 InP
618.4 NaI	In (M5N45N45;1G).pos
618.8 KI	402.6 In
619.2 CdI	In 3d5.pos
619.4 AgI	443.8 In
619.7 LiI	444.1 CuInSe ₂
619.9 I ₂	444.3 InSb
620.3 UI ₃	444.5 InP
621.5 ICl	444.5 In ₂ Te ₃
622.5 ICl ₃	444.8 In ₂ Se ₃
623.3 I ₂ O ₅	444.8 In ₂ O ₃
623.5 NaIO ₃	444.9 In ₂ S ₃
624.0 NaIO ₃	444.9 InCl
In (M4N45N45).pos, In (MNN).pos	445.0 In(OH) ₃
410.2 In	445.4 In(acac) ₃
409.3 InP	445.8 InI ₃
408.9 In ₂ Te ₃	446.0 InBr ₃
408.5 CuInSe ₂	446.0 InCl ₃
	446.2 InF ₃
	Ir (M4N67N67).pos
	1977.8 Ir

Ir (M5N67N67).pos, Ir (MNN).pos

1900.8 Ir

Ir (N4N67N67).pos, Ir (NNN).pos

172.2 Ir

Ir 4f7.pos

60.8 Ir
 62.0 IrO₂
 62.7 IrCl₃
 63.5 K₂IrCl₆

K (L2M23M23;1D).pos

250.7 KBr
 250.1 KF
 249.3 KSbF₆

K (L3M23M23).pos, K (LMM).pos

250.1 KF
 249.3 KSbF₆
 248.3 KBr

K 2p3.pos

292.2 K₄P₂O₇
 292.8 KCl
 292.8 KI
 292.5 KF
 293.1 KBr
 293.5 K₃PO₄
 293.7 KSbF₆
 294.6 K
 294.7 KCN

Kr (L3M45M45).pos

1460.4 Kr(gas)(vac)

Kr 3d.pos

87.0 Kr in graphite

La (M4N45N67).pos728.0 La₂O₃**La (M5N45N67).pos**711.0 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 O₂
 43.6 Li-O/1L O₂
 37.6 Li-O/1L O₂
 42.3 Li-O/5L O₂
 36.0 Li-O/5L O₂

Li 1s.pos

54.8 Li
 54.9 LiOH
 55.2 Li₂CO₃
 55.6 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.pos

196.5 Lu ₂ O ₃	581.0 MnSO ₄
196.6 Lu	Mn 2p3.pos
198.5 Lu ₂ (SO ₄) ₃	638.3 Na ₄ Mn(CN) ₆
Lu 4f7.pos	638.5 Mn(C ₅ H ₅) ₂
6.3 Lu	638.8 Mn
Mg (KL23L23).pos, Mg (KLL).pos	640.9 MnO
1185.6 Mg	640.9 MnS
1180.7 MgBr ₂ ·6H ₂ O	641.4 Mn ₃ O ₄
1180.6 (Mg/Fe) ₂ SiO ₄	641.6 Mn ₂ O ₃
1180.5 KMg ₃ Si ₃ AlO ₁₀ (OH/F) ₂	641.7 MnOOH
1180.5 Mg ₃ H ₂ (SiO ₃) ₄	642.0 MnCl ₂
1180.5 (Mg/Fe)SiO ₃	642.1 MnBr ₂
1180.4 MgO	642.6 MnO ₂
1179.0 (Na/Al/Mg)Si ₄ O ₁₀ (OH) ₂ ·nH ₂ O	642.6 MnF ₂
1178.8 MgSO ₄ ·7H ₂ O	644.9 MnSO ₄
1178.5 MgCl ₂ /Au	647.0 KMnO ₄
1178.2 MgF ₂	Mo (L2M45M45).pos, Mo (LMM).pos
Mg (L23VV).pos	2137.4 MoO _x
43.0 Mg/Ru	2143.6 Mo
31.0 O ₂ /Mg/Ru	Mo (L3M45M45).pos
Mg 1s.pos	2039.0 MoSi ₂
1302.7 Mg(OH) ₂	2038.8 Mo
1303.2 Mg	2032.2 MoO _x
1304.0 MgAl ₂ O ₃	Mo 3d5.pos
1305.0 MgF ₂	227.7 MoSi ₂
Mg 2p.pos	227.9 Mo
49.5 Mg(OH) ₂	227.9 MoB ₂
49.6 Mg	229.0 MoS ₂
50.4 MgAl ₂ O ₄	229.6 MoO ₂
50.4 MgO	230.0 MoCl ₃
51.0 MgF ₂	230.6 MoCl ₄
51.6 MgSO ₄ ·7H ₂ O	231.0 MoCl ₅
Mn (L3M23M45).pos, Mn (LMM).pos	232.1 (NH ₄) ₂ MoO ₄
586.4 Mn	232.7 MoO _x
585.7 MnO ₂	232.8 MoO ₃
585.0 Mn ₂ O ₃	N (KVV).pos
584.8 MnS	396.6 Gd(NO ₃) ₃ ·5H ₂ O
583.7 Mn ₃ O ₄	385.0 GaN
	383.0 Fe ₂ N
	379.2 BN
	376.6 NH ₃

N 1s.pos	23.1 NaBr
397.0 GaN	21.6 NaCl
397.7 Si ₃ N ₄	20.2 NaF
398.0 K ₄ Fe(CN) ₆	Na 1s.pos
398.1 BN	1070.8 NaN ₃
398.5 Na(N*NN*)	1070.8 Na ₂ C ₂ O ₄
398.7 NH ₃	1071.1 Na ₃ PO ₄
398.8 C ₅ H ₅ N/Pyridine	1071.1 NaOAc
398.9 EtNH ₂	1071.2 NaF
399.2 PhCN	1071.2 Na ₂ SO ₄
399.5 H ₂ NCONH ₂	1071.4 NaNO ₃
399.4 C ₆ H ₁₂ N ₄ /Urotropin	1071.5 Na ₂ CO ₃
399.8 KCN	1071.5 Na ₂ HPO ₄
400.2 C ₄ H ₅ N/Pyrrole	1071.6 NaI
401.3 (NH ₄) ₂ SO ₄	1071.6 NaPO ₃
401.4 Et ₄ NCl	1071.6 NaCl
401.7 NH ₄ Cl	1071.7 Na ₂ SiF ₆
402.2 Bu ₄ NHSO ₄	1071.7 NaBr
402.9 Na(NN*N)	1071.8 Na
403.1 Pyridine N-oxide	1072.0 NaH ₂ PO ₄
403.8 NaNO ₂	1072.5 Na ₂ O
404.7 K ₂ Pt(NO ₂) ₆	1072.7 NaBF ₄
405.5 R-NO ₂	Nb (M45N23V).pos, Nb (MNV).pos
407.3 NaNO ₃	167.8 Nb
408.2 R-ONO ₂	165.6 NbH _x
Na (KL23L23).pos, Na (KLL).pos	161.6 Nb ₂ O ₅
994.3 Na	Nb 3d5.pos
991.2 NaI	202.4 Nb
990.6 NaBr	203.2 NbH _x
990.5 Na ₂ C ₂ O ₄	203.7 NbO
990.3 NaCl	203.8 NbN
990.1 Na ₃ PO ₄	206.5 KNbO ₃
989.9 NaOAc	207.1 NbBr ₅
989.8 Na ₂ CO ₃	207.6 Nb ₂ O ₅
989.8 Na ₂ SO ₄	207.7 NbS ₂
989.8 Na ₂ O	208.0 NbCl ₅
989.7 Na ₂ HPO ₄	Nd (M5N45N45).pos, Nd (MNN).pos
989.4 NaNO ₃	733.0 Nd
989.4 NaPO ₃	Nd (M45N45N67).pos
989.1 NaH ₂ PO ₄	840.0 Nd
988.6 NaF	
987.7 Na ₂ SiF ₆	
987.1 NaBF ₄	
Na (L23VV).pos	
23.8 NaI	

Nd 3d5.pos

980.8 Nd
982.0 Nd₂O₃
984.9 Nd₂(SO₄)₃

Nd 4d.pos

120.8 Nd₂O₃
122.5 Nd₂(SO₄)₃

Ne (KL23L23).pos

818.0 Ne in Fe

Ne 1s.pos

861.6 Ne in Au
863.1 Ne in graphite
863.4 Ne in Fe

Ni (L2VV).pos

866.6 NiO
863.7 Ni(OH)₂
863.3 (Ni(OH)₂)_{0.75}(H₂O)_{0.16}(NiCO₃)_{0.09}
863.3 (Ni(OH)₂)_{3.2}H₂O
862.9 NiOOH
862.7 KNiO₆

Ni (L3M45M45).pos, Ni (LMM).pos

856.0 ((P₂O₅)_{0.40}(V₂O₅)_{0.60})_{0.95}(NiO)_{0.05}
855.7 ((P₂O₅)_{0.40}(V₂O₅)_{0.60})_{0.98}(NiO)_{0.02}
855.7 ((P₂O₅)_{0.40}(V₂O₅)_{0.60})_{0.90}(NiO)_{0.10}
855.3 ((P₂O₅)_{0.40}(V₂O₅)_{0.60})_{0.85}(NiO)_{0.15}
849.8 NiO
848.1 Ni(OH)₂
848.1 NiOOH
847.3 (Ni(OH)₂)_{0.75}(H₂O)_{0.16}(NiCO₃)_{0.09}
846.2 Ni
846.0 Ni/Ca_{0.166}Ni_{0.833}
845.2 Al₇₀Co₁₅Ni₁₅
844.9 AlNi
843.2 ((P₂O₅)_{0.40}(V₂O₅)_{0.60})_{0.90}(NiO)_{0.10}
842.9 NiO/Ca_{0.166}Ni_{0.833}
842.9 NiO
842.9 (Ni(OH)₂)_{3.2}H₂O
842.4 NiF₂
842.4 Ni(acac)₂
841.7 Ni(OH)₂/Ca_{0.166}Ni_{0.833}

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)]
1843.4 [PCl₂(N(CH₃)₂)]
1842.8 [PCl(CH₃)₂]
1842.1 [PCl₂(CH₃O)]
1842.1 [P(O)(CH₃O)(CH₃)]
1841.3 [PSF₂(N(CH₃)₂)]
1841.2 [PF(N(CH₃)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.pos1033..5 PmCl₃**Pr (M5N45N45).pos, Pr (MNN).pos**

695.0 Pr

Pr (M45N45N67).pos

795.0 Pr

Pr 3d5.pos931.8 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.pos71.2 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 PtO₂75.4 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	2109.1 Al ₂ (SO ₄) ₃ ·18H ₂ O
2119.9 PbS	2109.0 SnSO ₄
2119.1 Ag ₂ S	2108.9 K ₂ (SO ₄) ₂
2119.1 FeAsS	2108.8 Li ₂ SO ₄
2118.9 Sb ₂ S ₃	2108.5 Na ₂ SO ₄
2118.4 MoS ₂	2108.2 K ₂ SO ₄
2118.2 HgS	2107.8 Na ₂ S ₂ O ₃
2118.1 Cu ₂ S	2105.9 CaSO ₄
2117.6 CdS	2103.9 (CH ₃) ₂ S
2117.1 ZnS	2103.7 [PS(CH ₃ O) ₃]
2116.7 K ₂ S	2103.3 [PSCI ₂ (CH ₃ O)]
2116.1 S	2103.2 [PSCI ₂ (CH ₃)]
2116.1 S ₈	2102.9 [PSCI ₃]
2116.1 Na ₂ S·9H ₂ O	2102.5 (CH ₃ S) ₂
2116.0 FeS ₂	2102.5 (CH ₃ S) ₂
2115.9 Na((C ₂ H ₅) ₂ NCS ₂) ₃ ·3H ₂ O	2100.9 (CF ₃ S) ₂
2115.9 NiWS ₂	2100.7 [PSF ₃]
2115.2 Na ₂ S ₂ O ₃ ·5H ₂ O	2100.5 CH ₃ SH
2115.1 H ₂ CH ₂ CH(NH ₂)C(O)OH	2100.4 SF ₆
2114.8 (CH ₃) ₂ S	2099.9 (CH ₃) ₂ SO
2114.8 WS ₂	2098.7 SO(CH ₃ O) ₂
2114.6 NH ₄ SCN	2098.6 H ₂ S
2114.3 (C ₁₀ H ₁₂ AuClN ₂ S) _n	2098.1 SOCl ₂
2114.0 ZnSO ₄	2097.6 (CH ₃ O) ₂ SO ₂
2114.0 K(CH(CH ₃) ₂ OCS ₂)	2097.0 SO ₂ Cl ₂
2113.9 C ₄ H ₃ S(CH) ₅ C(CN) ₂	2095.5 SO ₂ ClF
2113.9 CH ₃ SCH ₂ CH ₂ CH(NH ₂)C(O)OH	2095.5 SO ₂
2111.6 CS ₂	2094.5 SOF ₂
2111.2 NaSCN	2094.3 SCIF ₅
2110.7 (C ₁₀ H ₁₂ AuClN ₂ S) _n	2093.9 SF ₄
2110.6 Na ₂ S ₂ O ₃ ·5H ₂ O	2093.8 SO ₂ F ₂
2110.5 CoSO ₄	2092.6 SF ₆
2110.5 Na ₂ SO ₃	
2110.4 CuSO ₄	S 2p.pos
2110.4 NaHSO ₃	
2110.3 FeSO ₄ ·7H ₂ O	160.8 PbS
2110.3 NiSO ₄	161.6 FeS
2110.2 Fe ₂ (SO ₄) ₃ ·nH ₂ O	161.7 CdS
2110.2 MnSO ₄	162.1 NH ₂ CSNH ₂
2109.9 BaSO ₄	162.3 ZnS
2109.7 (NH ₄) ₂ SO ₄ ·FeSO ₄ ·6H ₂ O	162.8 NiS
2109.7 CaSO ₄ ·2H ₂ O	162.8 Na ₂ S*SO ₃
2109.6 HgSO ₄	162.8 WS ₂
2109.5 (NH ₄) ₂ SO ₄	163.0 FeS ₂ /Pyrite
2109.3 (NH ₄) ₂ (SO ₄) ₂	163.2 Ph ₂ S
2109.3 SrSO ₄	163.2 Cysteine
2109.3 Al(NH ₄)(SO ₄) ₂ ·12H ₂ O	163.7 CS ₂
2109.2 KAl(SO ₄) ₂ ·12H ₂ O	163.8 S
2109.2 MgSO ₄ ·7H ₂ O	164.3 Thiophene
2109.1 K ₂ S ₂ O ₇	164.4 PhSSPh
2109.1 BeSO ₄	166.3 PhSO ₂ Na

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
 401.4 ClSc(C₅H₅)₂
 401.8 Sc₂O₃
 401.9 Sc₂O₃

Sc (L3M23M23).pos, Sc (LMM).pos

334.9 Sc₂O₃
 333.5 Sc oxalate
 333.4 Sc acetylacetonate
 329.8 ScF₃

Se (L3M45M45).pos

1307.3 Zn_{0.30}Cd_{0.70}Se
 1307.2 Zn_{0.42}Cd_{0.58}Se
 1307.0 Se

1306.8 CdSe
 1306.7 Zn_{0.50}Cd_{0.50}Se
 1306.5 Zn_{0.70}Cd_{0.30}Se
 1305.9 Zn_{0.90}Cd_{0.10}Se
 1305.8 ZnSe
 1304.3 Ph₂Se₂
 1304.0 Ph₂Se
 1302.9 Cl₂SePh₂
 1302.1 I₂SePh₂
 1301.9 Ph₂SeO
 1301.6 SeO₂
 1301.0 H₂SeO₃
 1298.1 H₂SeO₄

Se 3d5.pos

53.4 PbSe
 53.8 CuInSe₂
 54.5 GeSe₂
 54.6 Ga₂Se₃
 54.8 In₂Se₃
 54.9 As₂Se₃
 55.1 Se
 55.8 Ph₂Se
 55.8 Ph₂Se₂
 57.6 Ph₂SeO
 57.7 Cl₂SePh₂
 58.1 I₂SePh₂
 58.8 SeO₂
 58.8 PhSeO(OH)
 59.0 H₂SeO₃
 61.0 H₂SeO₄

Si (KL23L23).pos, Si (KLL).pos

1617.2 MoSi₂
 1616.6 Si
 1613.8 SiC
 1611.5 Si₃N₄
 1610.1 Mol Sieve A
 1610.0 Penthylsilicone
 1609.6 Mica/Muscovite
 1609.5 AlSiO₅/Sillimanite
 1609.4 Mol Sieve X
 1609.0 Kaolinite
 1608.8 SiO₂
 1608.8 Methylsilicone
 1608.6 Mol Sieve Y
 1608.6 SiO₂/Quartz
 1606.4 Na₂SiF₆

Si 2p.pos

98.8 NiSi
 99.5 Si
 99.5 Fe₃Si
 99.6 MoSi₂
 99.8 PdSi
 100.5 PtSi
 100.6 SiC
 100.9 Me₃SiOSiMe₃
 101.0 Ph₄Si
 101.1 Et₃SiOH
 101.3 Ph₃SiOSiPh₃
 101.4 Mol Sieve A
 102.0 Si₃N₄
 102.2 Mol Sieve X
 102.4 Mica/Muscovite
 102.6 Al₂SiO₅/Sillimanite
 102.7 Phenylsilicone
 102.8 Mol Sieve Y
 102.9 EtSiCl₃
 102.9 Methylsilicone
 103.0 Al₂SiO₅/Mullite
 103.0 Kaolinite
 103.3 SiO₂
 103.7 SiO₂/Quartz
 104.3 Na₂SiF₆

Sm (M4N67N67).pos

1094.0 Sm₂O₃

Sm (M5N45N45).pos

808.0 Sm₂O₃

Sm (M5N67N67).pos

1068.0 Sm₂O₃

Sm (M45N45N67).pos

950.0 Sm₂O₃

Sm 3d5.pos

1081.1 Sm
 1083.2 Sm₂O₃
 1083.4 Sm₂(SO₄)₃

Sn (M4N45N45).pos, Sn (MNN).pos

437.3 Sn
 435.7 SnS
 434.1 SnO
 432.6 SnO₂
 431.7 Na₂SnO₃
 430.8 NaSnF

Sn 3d5.pos

484.9 Sn
 485.6 SnS
 485.6 Ph₃SnOH
 485.7 SnSe
 486.6 Ph₄Sn
 486.6 SnO₂
 486.7 SmCl₂
 486.7 (NH₄)₂SnCl₆
 486.7 KSnF₃
 486.7 Na₂SnO₃
 486.9 SnBr₂
 486.9 SnO
 487.0 Ph₃SnCl
 487.4 SnF₂
 487.4 NaSnF₃
 487.6 K₂SnF₆
 488.2 SnF₄

Sr 3d5.pos

133.2 SrCO₃
 133.8 SrF₂
 134.3 SrSO₄
 134.4 Sr
 134.7 Sr(NO₃)₂
 135.3 SrO

Ta (M5N67N67).pos, Ta (MNN).pos

1674.7 Ta

Ta 4f7.pos

21.9 Ta
 25.9 KTaO₄
 26.5 Ta₂O₅
 26.6 TaS
 26.7 TaS₂
 26.9 TaBr₅
 27.3 TaCl₅
 27.8 TaF₅

29.4 K₂TaF₇**Tb (M4N67N67).pos**

1256.0 Tb

Tb (M5N45N45).pos

920.0 Tb

Tb (M5N67N67).pos

1223.0 Tb

Tb (M45N45N67).pos, Tb (MNN).pos

1068.0 Tb

Tb 3d5.pos1241.4 TbO₂1241.5 Tb₂O₃

1242.0 Tb

Tb 4d.pos

146.0 Tb

148.7 Tb₂O₃149.2 TbO₂**Te (M4N45N45).pos, Te (MNN).pos**

492.1 Te

491.1 CdSe_{0.65}Te_{0.35}

490.8 CdTe

488.5 Ph₂Te₂487.6 TeI₂(C₂H₅)₂]487.3 TeBr₄487.1 TeO₂486.7 [TeBr₂(C₆H₅)₂]486.6 [TeI₂(CH₃)₂]486.6 [TeBr₂(C₆H₅CH₃)]486.4 (NH₄)₂TeCl₆486.3 Cl₂TePh₂486.3 TeCl₂(C₆H₅)₂]486.1 TeCl₄485.5 Na₂TeO₄485.5 TeO₃485.1 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 Ph₂Te₂575.5 K₂TeO₃575.8 TeI₄576.1 TeO₂576.2 Cl₂TePh₂576.7 TeBr₄576.8 Na₂TeO₄576.9 TeCl₄576.9 (NH₄)₂TeCl₆577.1 Te(OH)₆577.3 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 ThO₂336.5 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	190.0 U
455.1 TiO	
455.8 TiN	U (N67O45V).pos
457.1 Cl ₂ Ti(C ₅ H ₅) ₂	
458.5 TiCl ₄	284.0 U
458.5 BaTiO ₃ (cubic/tetra)	
458.7 TiO ₂	U 4f7.pos
459.2 TiO ₂ (anatase/rutile)	
462.6 Na ₂ TiF ₆	377.4 U
Tl 4f7.pos	378.3 UCl ₃
	378.4 UBr ₃
	379.1 USe ₃
117.5 Tl ₂ O ₃	379.4 US ₃
117.7 Tl	379.9 UBr ₄
118.5 TlI	380.0 UOCl
118.7 Tl ₂ S	380.1 US
118.7 Tl ₄ S ₃	380.1 UF ₃
119.0 TlCl	380.1 UOBr
119.2 TlBr	380.2 UCl ₄
119.2 TlF	380.2 UO ₂
	380.3 UOCl ₂
Tm (M4N67N67).pos	380.3 USe
	380.4 UOBr ₂
1487.0 Tm	380.5 UO ₂ Br
	380.5 U ₂ Te ₃
Tl (N6O45O45).pos, Tl (NOO).pos	380.7 U ₃ O ₈
	380.7 CaUO ₄
85.1 Tl	381.1 UO ₂ Br ₂
	381.3 UTe ₃
	381.3 UO ₃
Tm (M5N45N45).pos	381.6 UO ₂ Cl ₂
	381.6 U(SO ₄) ₂
1080.0 Tm	381.9 UCl ₅
	382.2 UF ₄
Tm (M5N67N67).pos	382.4 K ₂ UF ₆
	383.0 UO ₂ F ₂
1440.0 Tm	384.9 UF ₆
Tm (M45N45N67).pos, Tm (MNN).pos	V (L3M23M45).pos, V (LMM).pos
1270.0 Tm	472.0 V
	468.0 V ₂ O ₅
Tm 4d.pos	468.6 VO ₂
175.4 Tm	V 2p3.pos
176.6 Tm ₂ O ₃	
178.3 Tm ₂ (SO ₄) ₃	512.2 V
	512.9 V(C ₅ H ₅) ₂
U (N67O45N45).pos	513.3 K ₄ V(CN) ₆
	514.2 V(acac) ₃
	514.4 VN

515.1 VO(acac) ₂	117.8 Y ₂ O ₃
516.3 VO ₂	
516.4 VOCl ₂	Y 3d5.pos
517.3 Na ₃ VO ₄	
517.6 V ₂ O ₅	155.8 Y
	156.2 YH _x
W (M5N67N67).pos, W (MNN).pos	157.0 Y ₂ O ₃
	160.0 Y ₂ (SO ₄) ₃
1727.8 WS ₂	
1723.9 H ₂ WO ₄	Yb (M4N67N67).pos
1723.8 WO ₃	
1722.0 Na ₂ WO ₄	1549.0 Yb
W 4f7.pos	Yb (M5N67N67).pos
31.3 W	1500.0 Yb
31.5 WC	
32.7 WO ₂	Yb (M45N45N67).pos
33.2 WS ₂	
35.1 CaWO ₄	1320.0 Yb
35.7 WO ₃	
35.9 WBr ₆	Yb 4d5.pos
36.2 H ₂ WO ₄	
36.3 Na ₂ WO ₄	182.4 Yb
36.3 WBr ₅	185.4 Yb ₂ O ₃
36.3 Al ₂ (WO ₄) ₃	187.3 Yb ₂ (SO ₄) ₃
36.9 WCl ₆	
37.2 WOCl ₄	Zn (L3M45M45).pos, Zn (LMM).pos
Xe (M4N45N45).pos	992.7 Cu ₆₄ Zn ₃₆
	992.2 Zn
545.2 Xe in graphite	991.3 ZnTe
544.8 Xe in Fe	989.7 ZnS
545.2 Xe in graphite	989.5 ZnSe
545.2 Xe	989.4 ZnCl ₂
544.8 Xe in Fe	989.3 ZnFe ₂ O ₄
543.7 Xe/Ni	988.7 ZnI ₂
541.4 Na ₄ XeO ₆	988.6 ZnO/SiO ₂
	988.2 ZnO/Si
Xe 3d5.pos	988.0 Zn ₅ (CO ₃) ₂ (OH) ₆
	987.8 Al ₂ ZnO ₄
668.9 Xe in Au	987.7 [Zn(CH ₃ C(O)CHC(O)CH ₃) ₂]
669.6 Xe in Cu	987.7 Zn(acac) ₂
669.7 Xe in graphite	987.7 ZnAl ₂ O ₄
670.2 Xe in Fe	987.7 ZnO
674.1 Na ₄ XeO ₆	987.4 ZnCO ₃
	987.3 Zn ₄ Si ₂ O ₇ (OH) ₂ ·2H ₂ O
Y (M45N23V).pos, Y (MNV).pos	987.3 ZnBr ₂
	987.0 Zn ₂ SiO ₄
124.3 Y	986.5 Zn(OH) ₂
123.3 YH _x	986.2 ZnF ₂

986.2 ZnSO₄

Zn 2p3.pos

1020.9 ZnP₂

1021.4 Zn(acac)₂

1021.6 ZnS

1021.7 Zn

1021.8 ZnF₂

1021.9 ZnCl₂

1022.1 ZnO

1022.5 ZnI₂

1023.1 ZnSO₄

1023.4 ZnBr₂

Zr (M45N23V).pos, Zr (MNV).pos

148.6 Zr

145.3 ZrH_x

141.9 ZrO₂

Zr 3d5.pos

179.0 Zr

179.6 ZrH_x

183.3 ZrO₂

184.2 K₂ZrF₆

185.3 ZrF₄

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_2019_User_Files\auger parameters*.aup.

Ag 3d5 + Ag (M4N45N45).aup

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

2099.7=84.0+2015.7 Au

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 NbHx

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 YHx
 276.4=158.6+117.8 Y₂O₃

Zn 2p₃ + Zn (L3M45M45).aup

2013.8=1021.7+992.1 Zn
 2012.9=1021.6+991.3 ZnTe
 2011.5=1022.0+989.5 ZnSe
 2011.3=1021.6+989.7 ZnS
 2011.3=1021.9+989.4 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 VG ESCALAB 220i-XL (*.TAP;*.TXT)

Comment:

- All necessary acquisition parameters are available
- Example: multiregion measurement with 8 spectra
- Folder: Install-CD:\XPS_Measurement_Reference_Data\01-ESCALAB Eclipses(.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 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 are saved
- Example: profile measurement with 5 Zn2p_{3/2} spectra
- Folder: Install-CD:\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 VG 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-CD:\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-CD:\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 A112/20
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-CD:\XPS_Measurement_Reference_Data\ 04-VSI(.GPH)\ VSI-SingleReg-survey-EP=1253.6.GPH

```

%%%%% 001 # General data
 2.10 0.40 HSA FFFFFFFF # 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 FFFFF529
CHANNELT 2000.000000000 6 1 1.0000000000 0.0000000000 FFFFF651
%%%%% 003 # Segment
0 # Flag für Segmentauswahl
865.0000000000 890.0000000000 0.0500000007 # min max inc
2 # Segmentanzahl
0.0099999998 860.0000000000 885.0000000000 0.2999999821
0.2000000030 # wait start stop inc
0.0099999998 1100.0000000000 1130.0000000000 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 865.0000000000 890.0000000000 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-CD:\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-CD:\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-CD:\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-CD:\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
O1           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-CD:\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-CD:\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-CD:\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-CD:\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,Omni2
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,A1
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-CD:\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-CD:\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/S
tep (ms) , Repeats
1, Cls, 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, Cls, , 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, Cls
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) , 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-CD:\XPS_Measurement_Reference_Data\09-VGX-900 (.1)\ Install-CD:\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-CD:\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
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
0
281
0
10000
238.6599999999962
239.6399999999449
233.7399999999547
245.1799999999964
...
193.0999999999989
200.5400000000061
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
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
1.0E37
FAT
10
1
4.444
0
0
0
0
0
Ga2p3

-1
kinetic energy
eV
356.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
401
0
10000
8753.79999999996
8611.96000000445
8614.64000000418
8670.04000000134
...
7040.82000000105
7134.21999999996
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
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
01s

-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
Survey
-1
kinetic energy
eV
86.59999999999999
0.5
1
counts per channel
d
pulse counting
0.3
2
0
0
0
0
0
0
2801
0
10000
113668.31
113261.39
111981.53
111248.01
...
444.8499999999974
197.1399999999988
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
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
37.2599999999985
30.5399999999924
35.53999999999286
...
4.14000000000136
2.25999999999409
2.1800000000005
end of experiment

```

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

Comment:

- SDP' 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-CD:\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
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
0
FAT
20
1E+37
4.61
0
0
0
0
0
01s
01s
-1
Kinetic Energy
eV
947.6
0.1
1

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

1998
12
21
10
33
19
255
0
XPS
360
Al K-alpha
18
```

```
1
1
1486.6
0
0
0
0
0
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
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
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
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
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-CD:\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
0 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
0 1s/7
Not Specified
2013
9
23
11
35
24
0
3
XPS Spectrum
Acqn. Time(s): 65
Step(meV) : 100.0
Dwell Time(ms) : 180
11:35:24
XPS

Sweeps: 2 Anode:Mono (Al (Mono)) (150 W)
Charge Neutraliser :On Acquired On :13/09/23

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-CD:\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 b4f_3, Au 3d_3, O 1s_3
- Folder: Install-CD:\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
```

```
dwll: 0.1
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 192;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Survey1"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 10 22
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 2201 long 12558
46488
46693
45865
...
2176
2127
enddata
background: 2201 double 21247
46348.667
46211.736
46074.805
...
```

```
2157.193
2158.667
endbackground
original: 2201 long 12558
46488
46693
45865
...
2176
2127
endoriginal
endregion
region: 2
method: XPS
active: 0
range: 200 1560 0.5
scans: 1
dwell: 0.1
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode = Al;
    xrs_voltage = 0;
    xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
    ea_mode = esca_c_ep;
    ea_serial = 0;
    ea_vers = 0;
    ea_const = 192;
    ea_ampl_fact = 0;
    ea_particle_polarity = -1;
    ea_detector_U = 2249.9;
    ea_conversion_U = 0;
    ea_aperture = 13;
    ea_is_small_spot = 0;
}
Manipulator: Max
{
    ma_type = Max;
    ma_x = 0;
    ma_y = 0;
    ma_sample = 6;
    ma_z = 0;
    ma_tilt = 0;
    ma_rot = 0;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = 283;
    mi_acp_pascal = 1.7e-07;
    mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Survey2"
ManipulationProtocol:
{
    mp_nstrings = 3;
    mp_strings = {
        "Smooth Golay",
        "Smooth Golay",
        "Smooth Golay"
    }
}
```

```
    }
}
measure_date: 13 09 2005 10 15
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 2721 long 13508
15347
15255
15413
...
265
252
enddata
background: 2721 double 24363
15425.250
15425.250
15375.775
...
257.420
256.000
endbackground
original: 2721 long 13508
15347
15255
15413
...
265
252
endoriginal
endregion
region: 3
method: XPS
active: 0
range: 1160 1173 0.1
scans: 3
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 24;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
```

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

```
    ma_y = 0;
    ma_sample = 6;
    ma_z = 0;
    ma_tilt = 0;
    ma_rot = 0;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = 283;
    mi_acp_pascal = 1.7e-07;
    mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 3d_1"
ManipulationProtocol:
{
    mp_nstrings = 5;
    mp_strings = {
        "Default Background applied",
        "Default Background applied",
        "No Background [1191.6..1191.6]",
        "Tougaard Background B/C 2866/1643 [1191.6..1191.6]",
        "Shirley Background [1191.6..1191.6]"
    }
}
measure_date: 13 09 2005 10 53
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 551 long 2755
3842
4039
3827
...
2509
2518
2565
enddata
background: 551 double 4959
3902.809
3902.490
3902.667
...
2534.058
2532.362
2530.667
endbackground
original: 551 long 2755
3842
4039
3827
...
2509
2518
2565
endoriginal
endregion
region: 5
method: XPS
active: 0
range: 690 725 0.1
scans: 3
dwell: 0.3
x_shift: 0
```



```
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 24;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "0 1s_1"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 10 56
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 351 long 1755
5390
5231
5249
...
4642
4894
4759
enddata
background: 351 double 3159
5290.000
5264.830
5239.660
...
4760.143
```

```
4762.571
4765.000
endbackground
original: 351 long 1755
5390
5231
5249
...
4642
4894
4759
endoriginal
endregion
region: 6
method: XPS
active: 1
range: 1160 1173 0.1
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 48;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 4f_2"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
}
```

```
measure_date: 13 09 2005 11 10
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 131 long 720
6816
7071
6798
...
4423
4275
4408
enddata
background: 131 double 1179
6895.175
6894.786
6895.000
...
4368.547
4368.753
4368.667
endbackground
original: 131 long 720
6816
7071
6798
...
4248
4423
4275
4408
endoriginal
endregion
region: 7
method: XPS
active: 1
range: 880 935 0.1
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
  xrs_anode = Mg;
  xrs_voltage = 0;
  xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 48;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
```

```
    ma_y = 0;
    ma_sample = 6;
    ma_z = 0;
    ma_tilt = 0;
    ma_rot = 0;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = 283;
    mi_acp_pascal = 1.7e-07;
    mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "Au 3d_2"
ManipulationProtocol:
{
    mp_nstrings = 0;
    mp_strings = {
    }
}
measure_date: 13 09 2005 11 11
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter def: 0
data: 551 long 3022
9426
9444
9495
...
6275
6399
6238
enddata
background: 551 double 4959
9455.037
9455.052
9455.000
...
6177.532
6240.766
6304.000
endbackground
original: 551 long 3022
9426
9444
9495
...
6275
6399
6238
endoriginal
endregion
region: 8
method: XPS
active: 1
range: 690 725 0.1
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode = Mg;
```

```
xrs_voltage = 0;
xrs_emission_current = 0.02;
}
EnergyAnalyser: ea200
{
  ea_mode = esca_c_ep;
  ea_serial = 0;
  ea_vers = 0;
  ea_const = 48;
  ea_ampl_fact = 0;
  ea_particle_polarity = -1;
  ea_detector_U = 2249.9;
  ea_conversion_U = 0;
  ea_aperture = 13;
  ea_is_small_spot = 0;
}
Manipulator: Max
{
  ma_type = Max;
  ma_x = 0;
  ma_y = 0;
  ma_sample = 6;
  ma_z = 0;
  ma_tilt = 0;
  ma_rot = 0;
}
MiscAcqInfo:
{
  mi_sample_ampere = 0;
  mi_sample_kelvin = 283;
  mi_acp_pascal = 1.7e-07;
  mi_tcp_pascal = 6.8e-06;
}
flood_gun_U: 0
tag: "0 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-CD:\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

```


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-CD:\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-CD:\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-CD:\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 0.00
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 0.00
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 0.00
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 0.00
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 0.00
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 0.0
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
f4  7  À  †  -  pnt  sar  +  '+Tä@c/s àø'ÿ
f4  7  È  7  É  pnt  sar
+[]'+Tä@c/s àø'ÿ  f4  $L  „|  Uâ-D«: "D«J~D € D«*"DUu"D È-D È~D
p"DUL"D«°•DUe"D«↔•D«j 'DUÅŽD«: 'DUu' DU5"DUµ DUL"DU...•D p 'DUö'D 0"D ð D
...

```

Software Version 2: XPS V1.00

- Example of 3 regions: survey, Ag 3d, Au 4f
- Folder: Install-CD:\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
L + y| chn sar c/s
f8 È+ 0 1 É chn sar c/s
c/s f8 H- ø, L É chn
sar c/s f8 H- @3 ;hR`ç81A-
4±Mò AØÅ »0¹ A»hèfàr AM|G³¼ AŽ.²%|Ð A1 %ÚPÌ AÂèR¹fY A1 púÿM AØEÍ`O? AíçnÈù¹
...

```

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-CD:\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
      \L +
      -          chn      sar          c/s
f8  ø
  pL
  1@ÿø†µ/11@ ó" /k1@DUtÑ...81@ÒJž1' f°@ç (Až11, @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-CD:\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  †
f8 x|  ð
c/s
sar
  chn  sar
  c/s
    f8  H⊥  H•
    f8  H
      f8  H
        f8  H
          chn  sar
            c/s
              f8  ,  G
              ñ↑d  ~|°@-dÃöît_@ÀE@o
...

```

Software Version 5: XPS V2.0

- Example of 1 regions: survey
- Folder: Install-CD:\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 1* M>77e * 77e . . 77e
λe77e M77e 瑾77e ph77e . {`77e 7877e 7h端77e . ←華77e 1H77e ~曖77e @7
↓77e 7777e @j.77e `DZ77e >77e !@77e
. 077e N377e @:葦77e 瑜77e . 鯨77e ` . @ `77祖77e @z 77e 3 . @ 聡77e
. 77e 潦77e . +177e . 3
...

```

Software Version 6: XPS V3.5s

- Example of 1 region: survey
- Folder: Install-CD:\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@   ¨³@   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-CD:\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 è.   |   Ý|   pts   sar   c/s
c/s   |   f8 h   |   |   |   |   |   |   |   |   |
sar   |   c/s   |   f8 h   |   |   |   |   |   |   |   |
À%Ú@   |   Ú@   |   À-Ú@   |   €_Ú@   |   □Ú@   |   ÝÚ@   |   @ Ú@   |   À%Ú@   |   ÀÚ@   |   €îÚ@
...

```

Software Version 8: Compass V7.2.2

- Example of 6 regions: Ni 2p, Al 2p, Al 2s, O 1s, C 1s, VB
- Folder: Install-CD:\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

```

Software Version 9: Compass V7.3

- Example of 1 region: survey
- Folder: Install-CD:\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
      +
      M
      pnt ° · o s ar
      *k h
È c/s Té
      iAr f8 h" p
      e
      çä
      àüä
      @
      ÀRå
      Ø"
      e ä
      ä
      -ä
      @üä
      ...

```

Software Version 10: Without software specification

- Example. multiregion measurement, 4 Ad 3d regions with different pass energies
- Folder: Install-CD:\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
  f4      e  +
          È      pnt  sar  'p↑
          È      pnt  sar  'p↑
          c/s  +
          sar  'p↑
...

```

Software Version 11: XPS 3.3

- Example of 5 region: C 1s, O 1s, Au 4f, N 1s, Si 2p
- Folder: Install-CD:\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@      e¹Éf8      (¹      ð
...

```

Software Version 12: SS 2.6.1.2

- Example of 3 region: O 1s, Si 2p, Si 2s
- Folder: Install-CD:\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: 1300.0000000
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 01s 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
DefectPosAlignment: None
DefectPosReferenceImage: SiO2_25nm_01.101.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 23.50 eV
XRaySetting: 100u100W_HP
EOFH
  L      +
...

```

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-CD:\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 F1s 9 101 -0.2000 699.0000 679.0000 698.0000 680.0000
0.200000 46.95 AREA
SpectralRegDef2: 1 20.0 1 0 4 1 0.00
SpectralRegBackground: 1 0.0 689.0 0.0
SpectralRegHero: 1 689.0 0.0 0.0 0.00
```

SpectralRegDef: 2 1 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 0.0
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 0.0
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$!  δ      1      1      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-CD:\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
  ▣      L  +                ▣  )  -          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-CD:\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
  ▣      L  +      ▣
  -      cyc 7777reg 7777 7777777s 77777777777777f8 7+1  +L  1
  ...

```

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-CD:\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
  @| +                È ¶                pnt øëý cy
  ...

```

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-CD:\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 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDesc: 1
EOFH
  •   °   †   □   •   |   •   cyc   reg   s
f8 ↑   °   †   □   •   |   •   cyc   reg   s
c/s * eV   f8 ↑   EL   |   •   cyc   reg   chn
  ...

```

Software Version 12: SS 2.6.1.2

- Example of 1 regions: survey

- Folder: Install-CD:\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
ñDNv|  à  +          i  H          pnt      cyc      c/s
      |  □  f4 1 µ ð          1          1          y  H          p
...

```

Software Version 13: SS 2.5.0.9

- Example of 1 regions: survey
- Folder: Install-CD:\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: 1400.000000
EBeamCurrent: -2.2 nA
ImageSizeXY: 1400.0000 200.0000
IonGunMode: Neutralize
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 0.110 kV
FloatVolt: -100.0 V
FloatEnable: yes
GridVolt: 120.0
CondensorVolt: 69.30
ObjectiveVolt: 101.20
BendVolt: 1.43
SputterRaster: 0.00 0.00 mm
SputterRasterOffset: 1.950 -0.200 mm
TargetSputterTime: 10.0 min
SputterEmission: 7.00 mA
DeflectionBias: 71.0 V
XpsScanMode: scanned
AnalyserMode: FAT
SurvNumCycles: 15
SurvTimePerStep: 50.000000
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2197 3136
PhotoOffsetInPixel: 1519 200
PhotoSizeInMm: 35.000 50.000
PhotoOffsetInMm: -38.354 -50.000
NoSpectralRegFull: 1
SpectralRegDefFull: 1 1 survey 111 938 -0.8000 745.0000 -5.0000 744.0000 -4.0000
0.000000 187.85 AREA
SpectralRegDef2Full: 1 750.0 1 0 1 1
SpectralRegBackgroundFull: 1 0.0 370.0 0.0
SpectralRegHeroFull: 1 370.0 0.0 0.0 0.00
SpectralRegIRFull: 1 0 0.000 0.000 0.0
NoSpectralReg: 1

SpectralRegDef: 1 1 survey 111 938 -0.8000 745.0000 -5.0000 744.0000 -4.0000
0.750000 187.85 AREA
SpectralRegDef2: 1 750.0 1 0 1 1
SpectralRegBackground: 1 0.0 370.0 0.0
SpectralRegHero: 1 370.0 0.0 0.0 0.00
SpectralRegIR: 1 0 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 13 4 (8215.5 5905.4 19312.7 46.0 -90.1) (9615.5 5905.4 19312.7
46.0 -90.1) (9615.5 6105.4 19312.7 46.0 -90.1) (8215.5 6105.4 19312.7 46.0 -
90.1)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 1
XrayPower: 92.65 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 20000.0 V
XRayCondenserLensVoltage: 9250.0 V
XRayObjectiveCoilCurrent: 0.929 A
XRayBlankingVoltage: 400.0 V
XRayFilamentCurrent: 1.621 A
XRayStigmator: 0.0 0.0
XRayHighPower: yes
EgunNeutMode: Neutralize
NeutralizerCurrent: 20.0 uA
NeutralizerEnergy: 1.01 V
EgunNeutExtractor: 50.0 V
EgunNeutXSteering: 2.0
EgunNeutYSteering: 4.1
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 534.0 eV
SxiPassEnergy: 188 eV
SxiLens2: -711 V
SxiLens3: -673 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 342.0 V
SxiDisplayMode: 1
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.661
Channel Info: 2 1 1.490
Channel Info: 3 1 1.499
Channel Info: 4 1 1.268
Channel Info: 5 1 1.149
Channel Info: 6 1 1.100
Channel Info: 7 1 1.148
Channel Info: 8 1 1.079
Channel Info: 9 1 1.118
Channel Info: 10 1 1.021
Channel Info: 11 1 0.942
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-CD:\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
  ▣      L  +
w|  ▣  f4 ;D◀  +L      L  ✕      pnt      ang      c/s ñD-
...

```

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-CD:\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

```

```

  ÅL †      □      L      □      ang      reg      sin
f8 Å  ΔL  γ      γ      □      L      □      ang      reg
...

```

Software Version 4: XPS V1.30

- Example. angle resolved measurement with 4 angles and 3 regions: O 1s, C 1s, Si 2p
- Folder: Install-CD:\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
  |  à  †                □  †  †                ang  reg                sin
  ...

```

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-CD:\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
  ▣      L  +          ▣  |  -          ang  ììììreg  ìììì  ìììììììdeg  ìììì
ììììììììf8  ìg  +L  1          1  |  -          ang  ììììreg  ìììì
  ìììììììc/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-CD:\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
•   1   +
i   |   pnt ↑ ↑ ang   A→   c/s Ⓓ
ù↑ 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-CD:\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
DefectPosAlignment: None
DefectPosReferenceImage: ASKim150122-1.13.sxi
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 10u1.25W15KV
EOFH
...
...
...

Software Version 13: SS 2.5.0.9

- Example. snap shot mapping of 256x256 points of one region
- Folder: Install-CD:\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
DefectPosAlignment: None
DefectPosReferenceImage: 140438.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 9u1.0W15KV
EOFH
      1      Å      †      †      pnt      pnt      <Û¼ `ä@      c/s
      f4      †      †      †      †      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-CD:\XPS_Measurement_Reference_Data\20-Focus CSA(.DAT)\FocusCSA-SingleReg-VB.DAT

```

[REGION_CONFIG]
TIMESTAMP="9/11/2009 / 10:17:40 AM"
USE=TRUE
E_START=10000.000000000000
E_STOP=10070.000000000000
E_STEP=0.318437500000

```

```

E_SCAN=1
EPASS=100.000000000000
N_SCAN=20
N_IMAGE=1000
PE=10050.000000
T_DWELL=5000.000000
SLIT=9
COMMENT=""
PATH_LENS_TAB=/C/Program Files/FOCUS ProCSA/lens tables/Mode2/M06_Mo2.lens
PATH_DATA_FILE=/C/Data/090910/STO10KeV/VBdef.dat
[DETECTOR]
CAMRES_X=1280
CAMRES_Y=1024
CAMRANGE_XMIN=100
CAMRANGE_XMAX=599
CAMRANGE_YMIN=115
CAMRANGE_YMAX=350
T_EXPOSURE=5.000000
K_DET=0.101900
WA=4.500000
NX0=337
BINNING=1
K_SPEC=0.859900
CHANNELS=25
U_MCP=2400.000000
U_SCR=4500.000000
IP=127.0.0.1
PORT=5555
[DATA_CONFIG]
TIMESTAMP="9/11/2009 / 3:20:44 AM"
T_EXPOSURE=5.000000
N_SCAN=20
N_Image=1000
PE=10050.000000
WA=4.500000
[DATA]
10000.00000 1537 41 0 0
10000.31844 1553 41 0 0
10000.63688 1538 41 0 0
...
10069.73781 702 43 0 0
10070.05625 688 42 0 0
[DATA_1]
10000.00000 77 2 0 0
10000.31844 96 2 0 0
...
10069.73781 26 3 0 0
10070.05625 45 2 0 0
[DATA_2]
10000.00000 90 2 0 0
10000.31844 85 2 0 0
...
10069.73781 46 2 0 0
10070.05625 31 2 0 0
[DATA_3]
10000.00000 79 2 0 0
10000.31844 65 2 0 0
...
10069.73781 33 2 0 0
10070.05625 38 2 0 0
[DATA_4]
10000.00000 81 2 0 0
10000.31844 84 2 0 0
...
10069.73781 38 2 0 0
10070.05625 39 2 0 0

```



```

[DATA_5]
10000.00000 78    2    0    0
10000.31844 83    2    0    0
...
10069.73781 39    2    0    0
10070.05625 26    2    0    0
...
[DATA_19]
10000.00000 63    2    0    0
10000.31844 78    2    0    0
...
10069.73781 31    2    0    0
10070.05625 28    2    0    0
[DATA_20]
10000.00000 81    2    0    0
10000.31844 60    2    0    0
...
10069.73781 20    2    0    0
10070.05625 33    2    0    0

```

3.1.22 Croissant (*.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-CD:\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-CD:\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 (*.xy)

Comment:

- Measurement data format generated via converter using the SPECSLab Software
- example has six regions:
 1. Survey, Scans 1, Pass 40 eV
 2. VB, Scans 5, Pass 20
 3. Sb2p3/2 Sb2p1/2, Scans 2, Pass 40
 4. Survey, Scans 1, Pass 40

5. VB, Scans 5, Pass 20

6. Sb3/2 Sb1/2, Scans 1, Pass 40

- the header of the region includes all important recording parameters
- Data: KE, two space characters, intensities (cps)
- the intensities are saved after the two lines: # ColumnLabels and #
- Example: multi region high energy measurement, excitation energy: 5900 eV, 6 regions: survey, VB, Sb 2p, survey 1, VB 1, Sb 2p
- Folder: Install-CD:\XPS_Measurement_Reference_Data\23-SPECS-Phoibos(.XY)\SPECS-Phoibos-MultiReg-HEXPS-Separatescans.XY

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

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

# Group: MS16
#
# values in kinetic energy
# Region: Survey
# Analysis Method: UPS
# Analyzer: PHOIBOS HSA15000 DLD 225 R6-HV[HWTtype 31:60, 32:63, 33:64,
542:511] DLD
# Analyzer Lens: SmallArea:3.5kV
# Analyzer Slit: 4:3x20\2:open
# Scan Mode: FixedAnalyzerTransmission
# Number of Scans: 1
# Curves/Scan: 1
# Values/Curve: 2008
# Dwell Time: 0.3
# Excitation Energy: 5900
# Kinetic Energy: 4900
# Pass Energy: 40
# Bias Voltage: 50
# Detector Voltage: 2650
# Eff. Workfunction: 4.658
```

```
# Source:          UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
4900 28060
4900.5 26963.333
...
5902.5 6.6666667
5903 3.3333333
5903.5 0

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

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

# Cycle: 0, Curve: 0, Scan: 2
#
# ColumnLabels: energy counts/s
#
5890 293
5890.05 304.5
...
```

```

5903.95  1
5904     2

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

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

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

```

3.1.25 Energy-Intensity (*.dat)

Comment:

- Simplest form of a measurement data format, 1. column: energies, 2. - n. column: intensities
- Scan direction: increasing or decreasing energies
- Energy form: binding or kinetic energies

- Only one region saved in the data file
- The reading of the spectrum starts from the first line with numbers
- Lines with characters are ignored
- Peak name, comment, excitation energy, dwell time, number of scans, analyser energy, analyser mode has to be defined manually

Version 1: BE decreasing

- Example: single region
- Folder: Install-CD:\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-CD:\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-CD:\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-CD:\XPS_Measurement_Reference_Data\24-EnergyIntensity(.DAT)\EnergyIntensity-SingleReg-KE-increasing.DAT

```
BE      Int
1458.61  583
1458.64  595
1458.67  598
...
1465.54  240
```

1465.57 252
1465.6 217

3.1.26 HTW-Berlin (*.dat)

Comment:

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

XPS

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

Kommentar:

Probe auf altem Halter

Messwerte:

kin. Energie	Bindungsenergie	Scan	Summe	Scans	(Counts	pro	Sekunde)
Scan 1	Scan 2	Scan 1	(Counts	Scan 2	(Counts	pro	Sekunde)
[eV]	[eV]	[1/eV]	[1/(s*eV)]	[1/eV]	[1/eV]	[1/(s*eV)]	[1/(s*eV)]
1,139099E+3	-1,100009E+2	9,510000E+2	1,585000E+2	4,750000E+2	4,760000E+2		
1,583333E+2	1,586667E+2						
1,139160E+3	-1,099398E+2	9,620000E+2	1,603333E+2	4,610000E+2	5,010000E+2		
1,536667E+2	1,670000E+2						
1,139191E+3	-1,099093E+2	9,540000E+2	1,590000E+2	4,990000E+2	4,550000E+2		
1,663333E+2	1,516667E+2						
1,139252E+3	-1,098483E+2	9,620000E+2	1,603333E+2	4,680000E+2	4,940000E+2		
1,560000E+2	1,646667E+2						
1,139313E+3	-1,097873E+2	9,040000E+2	1,506667E+2	4,530000E+2	4,510000E+2		
1,510000E+2	1,503333E+2						
1,139343E+3	-1,097567E+2	9,360000E+2	1,560000E+2	4,700000E+2	4,660000E+2		
1,566667E+2	1,553333E+2						
1,139404E+3	-1,096957E+2	9,380000E+2	1,563333E+2	4,600000E+2	4,780000E+2		
1,533333E+2	1,593333E+2						
1,139435E+3	-1,096652E+2	8,590000E+2	1,431667E+2	4,460000E+2	4,130000E+2		
1,486667E+2	1,376667E+2						
1,139496E+3	-1,096042E+2	8,770000E+2	1,461667E+2	4,540000E+2	4,230000E+2		
1,513333E+2	1,410000E+2						
1,139557E+3	-1,095431E+2	8,780000E+2	1,463333E+2	4,200000E+2	4,580000E+2		
1,400000E+2	1,526667E+2						

...

3.2 XAS Data

3.2.1 NEXAFS (*.dat)

Comment:

- Data format of a NEXAFS measurement with non-equidistant steps
- no header, only one region saved
- Data: 1. column: increasing Photon energy, 2. column: Intensity
- Example: single region, C K-edge
- Folder: Install-CD:\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-CD:\XAS_Measurement_Reference_Data\02-BESSY-EMP2\BESSY-EMP2-SingleReg-Ti L-edge.008

```
Comment      :
Probe        :
CfgTyp       : $627
Fileform     : $BF
Date         : 89.6545.14  22:11:26
Program      : EMP/2-M
Version      : 00.4A0
MeasTyp      : CFS
Analys.      : 1
Scans        : 1
Points       : 181
MonSta       : 4.540000000E+02
MonEnd       : 4.900000000E+02
AnaSta       : 2.000000000E+02
AnaEnd       : 6.000000000E+02
AnaRange     : 9.000000000E+03
AnaMin       : 0.000000000E+00
DacSta       : 0.000000000E+00
DacEnd       : 1.000000000E+01
DeltaE       : 0.000000000E+00
MonName      : UE56/2-PGM-1
```

```

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

```

3.2.3 MAXlab Scan Zeiss (*.sp7)

Comment:

- Data format of a MAXlab Scan Zeiss measurement with non-equidistant and non-monotone steps (Lund)
- Header includes number of start and end energy, number of scans, dwell time, number of points
- The intensities and reference data are saved in 12 columns with 11 characters after the line: start spectrum data, 1. columns: Photon energy, next columns intensities and reference data
- Example: 2 ML Co on BTO,
- Folder: Install-CD:\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-CD:\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
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 3000000000.00000000 1.89397613
19:44:45 29.03500000 336.00704614 245.81550468 1.00000000
0.32809361 0.00000000 218028.00000000 287125.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:44:49 33.17500000 336.20638998 245.77666413 1.00000000
0.32724433 0.00000000 216735.00000000 286256.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:44:55 39.18400000 336.38151877 245.72117112 1.00000000
0.32616590 0.00000000 216126.00000000 283649.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:44:59 42.89200000 336.60170582 245.67399892 1.00000000
0.32634440 0.00000000 215912.00000000 285105.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:04 48.39900000 336.78541472 245.62405239 1.00000000
0.32659269 0.00000000 216056.00000000 284616.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:11 54.60200000 336.98568085 245.56301724 1.00000000
0.32621503 0.00000000 215852.00000000 285602.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:15 58.73700000 337.20665757 245.53249966 1.00000000
0.32609984 0.00000000 215193.00000000 283313.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:18 62.43700000 337.40332407 245.49088478 1.00000000
0.32591437 0.00000000 215181.00000000 281131.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
19:45:22 66.38500000 337.60842840 245.46036720 1.00000000
0.32477547 0.00000000 214457.00000000 281865.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
...
20:05:45 1289.45100000 364.52621530 234.35718363 1.00000000
0.34323552 0.00000000 226474.00000000 289185.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:05:50 1293.59700000 364.65540722 234.29892280 1.00000000
0.34345527 0.00000000 225931.00000000 287053.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:05:53 1297.19900000 364.80385136 234.26008224 1.00000000
0.34483647 0.00000000 226430.00000000 290068.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:05:57 1301.47800000 364.95241610 234.22956467 1.00000000
0.34543259 0.00000000 227133.00000000 289884.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613
20:06:01 1305.26500000 365.10110157 234.19072411 1.00000000
0.34546582 0.00000000 227048.00000000 289365.00000000 0.00000000
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 0.00000000
0.00000000 0.00000000 3000000000.00000000 1.89397613

```

3.2.5 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-CD:\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-CD:\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
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
      J      €      +      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
- @1 + ) < pnt øëý cyc @ ú↑ 1
ñwc/s @ Äú↑ Ôú↑ f4 p& P1
...

```

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

```


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_O_4_
##PIN_ID=M01451
##ORIENTATION=Laser parallel to -a* (-1 0 0). Fiducial mark perpendicular to
laser is parallel to -c [0 0 -1]
126.5290, 41816.00
127.7630, 41778.00
128.9970, 41848.00
130.2300, 42065.00
131.4640, 41809.00
132.6970, 41542.00
133.9300, 41143.00
135.1630, 41653.00
136.3950, 41657.00
...
1539.354, 41909.00
1540.385, 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  199.9999999999994  1.000000000000031  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  99.9999999999967  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

C:\Users\rhesse\Documents\Unifit_2019_User_Files\My Unifit Projects\Test Project\example.tap

Window	Component	Peak name	Area/cps·eV	Sens. Fact.	Norm. Area	Quant./at. %
1	1	S2p -S- 9971.6329	33.07	301.53108	12.08	
1	2	S2p S6+	2070.0950	33.031	62.671279	2.51
2	1	C1s -CH2-	22369.343	18.991	1177.8917	47.19
2	2	C1s -C*-C-X	8839.5495	19.002	465.19048	18.64
2	3	C1s -CO-NH-/-CO-O-	708.40255	18.965	37.353153	1.5
3	1	N1s -N-CO-	2989.7457	32.894	90.890307	3.64
3	2	N1s -NH3+	1676.2427	32.859	51.013201	2.04
4	1	O1s >C=O	11035.866	50.925	216.70821	8.68
4	2	O1s -C-O-R	4728.4317	50.865	92.960419	3.72

4.1.5 Call: [Concentration - Concentration] and **Save 2** (*.DAT)

Comment:

- 1. column: series parameter, delimitation character
- next columns: intensities (number of columns corresponds to the number of components in peak fit))
- Example below: angle-dependent experiment (Si 2p) with 21 angle steps and peak fit with two components

```
-69.44;1502.07100;966.262289
-65.29;1706.82367;773.786431
-61.14;2038.14743;854.516160
...
-11.34;4104.58497;555.788140
-7.19;4298.24804;528.463500
-3.04;5067.81837;410.645179
1.11;5342.32652;383.560886
5.26;3764.66546;476.371478
9.41;4162.20312;90.0477212
```

4.2 Project File (*.UFP)

Comment:

- Saved in Unifit_2019_User_Files\examples\Calibration_Intensity_Cu.ufp
- Example of 3 lines (Cu 2p, Cu 3p and survey), Cu 2p3 and Cu 3p fitted, project comment, quantification
- Data structure: ,space'+,Auger parameter'+,='+,position photoelectron peaks as BE'+,+'+,position Auger peak as KE'+,space'+,space'+,name of Auger parameter'

```
3
0 2016
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-1
-1
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300
21
30
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0
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frei
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Calibration of intensity scale
```


FAT

3-5-2004

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23248.7
23117.2
23163.2
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23062.1
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23313.4
23224.6
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23299.8
23196.4
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23245.1
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23274.1
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23131.4
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24394.1
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24674.3
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25615.9
25914.5
25779.3
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26406.9
27010.9
27557.3
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43499.78
43151.8
42549.82
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21643.82
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4227200

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Kurve 3
Kurve 4
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Calibration of intensity scale
Acquisition conditions:
Twin, LAX, 50eV pass
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Doublet
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3-5-2004
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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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4.4 Annotation/Design File (*.DSG)

Remark:

- saved in Unifit_2019_User_Files\design\GaAs-survey.dsg

Annotation/Design 2014
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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
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0.794210195091252
0.757225433526012
1
GaAs_Ozone
0.262429200755192
0.0751445086705202
1
0
0
0
Messkurve
Untergrund
Komponenten
Summenkurve
Residuum
Curve 6
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Curve 294
Curve 295
Curve 296


```

Curve 297
Curve 298
Curve 299
Curve 300
  1
  1
  0
Binding Energy / eV
Intensity / kCounts
Batch parameter
  Intensity / kcps
  1936
  1031

```

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

Remark:

- saved in Unifit_2019_User_Files\cross section*.cro
- example: estimated inelastic electron scattering cross section of SiO₂

```

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_2019_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_2019_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 2019
 0
As2p3
 1
 1
-1
-1
-1
 0
 0
2866
1643
 1
 0
 0
0 0 0 0 0
0

```

```

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

```

0.05804748
0
0.000755178
0
0
0
0
0
0
0
0
0
0
0
2
1
1
Wahr
0
Peak
0
188357.2
30
370
1333.01
1316.01
NORM
Peak
405
GaAs
Dublett 1
1
0
5000000
36188.75
0
0
1
0
1
0.55
1
0.6423534
0
0
1
0
1
1322.9
1323.3
1322.907
0
0
1
1322.907
1
0.1
10
1.757303
0
0
1
0
1
0
1
0
1
0
1

0
1
0
1
As
Dublett 2
1
0
163743400000
4520.299
0
0
1
0
1
0.6002151
0.9177305
0.6423534
1
0
1
0
1
1323.707
1324.107
1324.107
0
0
1
1324.107
1
0.1676468
16.76661
1.757303
1
0
1
0
1
0
1
0
1
0
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0
1
1
AsO
Dublett 3
1
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163743400000
12283.88
0
0
1
0
1
0.6002151
0.9177305
0.6423534
1
0
1
0
1

1325.107
1325.507
1325.475
0
0
1
1325.475
1
0.1676468
16.76661
1.757303
1
0
1
0
1
0
1
0
1
0
1
0
1
0
1
As203
Dublett 4
1
0
163743400000
25805.46
0
0
1
0
1
0.6002151
0.9177305
0.6423534
1
0
1
0
1
1325.807
1326.207
1326.207
0
0
1
1326.207
1
0.1676468
16.76661
1.757303
1
0
1
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0

1
As205
Dublett 5
1
0
163743400000
2414.963
0
0
1
0
1
0.6002151
0.9177305
0.6423534
1
0
1
0
1
1326.807
1327.607
1327.323
0
0
1
1327.323
1
0.1676468
16.76661
1.757303
1
0
1
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1
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0
1
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1
0
1
93698.1733601024
Falsch
19.2268554676829
Falsch
0.0644971942770271
Falsch
0
Wahr
0.000755178
Falsch
0
Wahr
1643
1
0 0
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Wahr
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Wahr
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4227327
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2
32768
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2
255
0
2
8421504
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3
255
2
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16711935
1
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0
2
16711680
3
1
65280
0
1
64
0
2
255
0

2
8421504
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16711680
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Arial
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31
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8421440
Arial
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8421504
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Arial
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Arial
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Arial
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12632256

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8388863
7
16711680
8
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32896
10
8421440
11
12632256
12
16711935
13
12615680
14
16744448
15
8454016
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12615680
17
4259584
18
12615935
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12615808
20
4194432
21
10485760
22
8388736
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16711935
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8388863
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16711808
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16711680
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Summenkurve
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RegionEnd

5 Data Banks Integrated in UNIFIT

5.1 Auger Parameter (*.AUP)

Comment:

- Saved in Unifit_2019_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 Unifit2017_User_Files\sensitivity 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, Bls, 0.13, Ba3d5, 7.9, Ba4d, 2.35, Bel, 0.059, Bi4d5, 2.5, Bi4f5, 3.15, Bi4f7, 4.25
 Bi4f, 7.4, Bi5d, 1.1, Br3p, 0.14, Br3d, 0.83, Cls, 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, Fls, 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, Lils, 0.02, Lu4p3, 0.6, Lu4d, 2.0, Mgl, 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, Nls, 0.42, Nals, 2.3, Na2s, 0.13, Nb3p3, 1.1, Nb3d3, 0.96, Nb3d5, 1.44, Nb3d, 2.4
 Nd3d, 7.0, Nd4d, 2.0, Nel, 1.5, Ne2s, 0.07, Ni2p1, 1.5, Ni2p3, 3.0, Ni2p, 4.5, Ni3p, 0.5, Ols, 0.66, Os2s, 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:

- 1st row: name of satellite line (1 = α_3 , 2 = α_4 , 3 = α_5 , 4 = α_6 , 5 = β)
- 2nd row: energy position of satellite 1. set
- 3rd row: rel. height of the satellite 1. set
- 4th row: energy position of the satellite 2. set
- 5th row: rel. height of the satellite 2. set etc.

```
Aluminiumsatelliten 1
9.8
0.064
0
0
0
0
0
0
```



```

0
0
Magnesiumsatelliten 1
8.4
0.08
0
0
0
0
0
0
0
...
0
0
Aluminiumsatelliten 5
69.7
0.0055
0
0
0
0
0
0
0
0
0
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,0.666,1.0
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)\Unifit2017\phi-names\Phi_names.ele

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

As2, As3p
As3, As2p3
As4, AsLMM
As5, As2p1
As6, As (LMM)
Au1, Au4f
Au2, Au4d5
Au3, Au4f7
Au4, Au (MNN)
Au5, Au (NVV)
Au6, Au4p1
Au7, Au4p3
Au8, Au4d3
Au9, Au4f5
B1, B1s
B2, BKVV
Ba1, Ba3d5
Ba2, Ba4d
Ba3, Ba (MNN)
Ba4, Ba3d3
Ba5, Ba (MNN)
Ba6, Ba4p3
Be1, Bels
Bi1, Bi4f
Bi2, Bi4d5
Bi3, Bi5d
Bi4, Bi4f7
Bi5, Bi4p3
Bi6, Bi4d3
Bi7, Bi4f5
Br1, Br3d
Br2, Br3p
Br3, Br (LMM)
Br4, Br3s
Br5, Br3p1
Br6, Br3p3
C1, C1s
C2, C (KLL)
C3, C1s
Ca1, Ca2p
Ca2, Ca2s
Ca3, Ca (LMM)
Ca4, Ca2p3
Ca5, Ca2p1
Cd1, Cd3d5
Cd2, Cd3p3
Cd3, CdMNN
Cd4, Cd4d
Cd5, CdMNN
Cd6, Cd3p1
Cd7, Cd3d3
Ce1, Ce3d
Ce2, Ce4d
Ce3, Ce3d3
Ce4, Ce3d5
Ce5, Ce (MNN)
Cl1, Cl2p
Cl2, Cl2s
Cl3, Cl (LMM)
Co1, Co2p
Co2, Co2p3
Co3, Co3p
Co4, Co (LMM)
Co5, Co2p1
Co6, Co (LMM)
Co7, Co (LMM)

Co8, Co3s
Cr1, Cr2p
Cr2, Cr2p3
Cr3, Cr3p
Cr4, Cr (LMM)
Cr5, Cr (LMM)
Cr6, Cr (LMM)
Cr7, Cr2s
Cr8, Cr2p1
Cr9, Cr3s
Cs1, Cs3d5
Cs2, Cs4d
Cs3, Cs (MNN)
Cs4, Cs3p3
Cs5, Cs3d3
Cs6, Cs4p3
Cs7, Cs (MNN)
Cu1, Cu2p
Cu2, Cu2p3
Cu3, Cu3p
Cu4, Cu (LMM)
Cu5, Cu2p3
Cu6, Cu2p1
Cu7, Cu (LMM)
Cu8, Cu (LMM)
Cu9, Cu (LMM)
Dy1, Dy4d
Dy2, Dy4p3
Dy3, Dy3d5
Er1, Er4d
Er2, Er4p
Eu1, Eu3d
Eu2, Eu4d
F1, F1s
F2, F2s
F3, F (KLL)
F4, F (KLL)
F5, F (KLL)
F6, F (KLL)
Fe1, Fe2p
Fe2, Fe2p3
Fe3, Fe3p
Fe4, Fe (LMM)
Fe5, Fe2p1
Fe6, Fe (LMM)
Fe7, FeLMM
Ga1, Ga2p3
Ga2, Ga3p
Ga3, Ga (LMM)
Ga4, Ga3d
Ga5, Ga2p1
Ga6, Ga (LMM)
Ga7, Ga (LMM)
Ga8, Ga (LMM)
Ga9, Ga (LMM)
Gd1, Gd4d
Gd2, Gd3d
Ge1, Ge2p3
Ge2, Ge3p
Ge3, Ge3d
Ge4, Ge (LMM)
Ge5, Ge2p1
Ge6, Ge (LMM)
Ge7, Ge (LMM)
Ge8, Ge (LMM)
Ge9, Ge (LMM)

Hf1, Hf4f
Hf2, Hf4d
Hf3, Hf4d5
Hf4, Hf4p1
Hf5, Hf4p3
Hf6, Hf4d3
Hg1, Hg4f
Hg2, Hg4d5
Hg3, Hg4f7
Hg4, Hg4p3
Hg5, Hg4d3
H6, Hg4f5
Ho1, Ho4d
Ho2, Ho4p
I1, I3d5
I2, I4d
I3, I (MNN)
I4, I3p1
I5, I3p3
I6, I (MNN)
I7, I3d3
In1, In3d5
In2, In3p3
In3, In (MNN)
In4, In (MNN)
In5, In3p1
In6, In3d3
Ir1, Ir4f
Ir2, Ir4d5
Ir3, Ir4f7
Ir4, Ir4p1
Ir5, Ir4p3
Ir6, Ir4d3
Ir7, Ir4f5
K1, K2p
K2, K2s
K3, K (LMM)
K4, K2p3
K5, K2p1
Kr1, Kr3d
Kr2, Kr3p
Kr3, Kr3p3
La1, La3d
La2, La4d
La3, La (MNN)
La4, La3d3
La5, La3d5
La6, La4p3
Li1, Li1s
Lu1, Lu4d
Lu2, Lu4p
Mg1, Mg2s
Mg2, Mg2p
Mg3, Mg1s
Mg4, Mg (KLL)
Mn1, Mn2p
Mn2, Mn2p3
Mn3, Mn3p
Mn4, Mn (LMM)
Mn5, Mn2p1
Mn6, Mn (LMM)
Mn7, Mn (LMM)
Mo1, Mo3d
Mo2, Mo3p3
Mo3, Mo3d5
Mo4, Mo3s

Mo5, Mo3p1
Mo6, Mo3d3
N1, N1s
N2, N (KVV)
Na1, Na1s
Na2, Na2s
Na3, Na (KLL)
Na4, Na2p
Na5, Na (KLL)
Nb1, Nb3d
Nb2, Nb3p3
Nb3, Nb3d5
Nb4, Nb3s
Nb5, Nb3p1
Nb6, Nb3d3
Nd1, Nd3d
Nd2, Nd4d
Ne1, Ne1s
Ne2, Ne2s
Ne3, Ne (KLL)
Ni1, Ni2p
Ni2, Ni2p3
Ni3, Ni3p
Ni4, Ni (LMM)
Ni5, Ni2p1
Ni6, Ni3s
Ni7, Ni (LMM)
Ni8, Ni (LMM)
O1, O1s
O2, O2s
O3, O (KVV)
Os1, Os4f
Os2, Os4d
Os3, Os4d5
Os4, Os4d3
Os5, Os4p3
Os6, Os4p1
P1, P2p
P2, P2s
Pb1, Pb4f
Pb2, Pb4d5
Pb3, Pb5d
Pb4, Pb4f7
Pb5, Pb4p3
Pb6, Pb4d3
Pb7, Pb4f5
Pd1, Pd3d
Pd2, Pd3p3
Pd3, Pd (MNN)
Pd4, Pd3d5
Pd5, Pd3p1
Pd6, Pd3d3
Pm1, Pm3d
Pm2, Pm4d
Pr1, Pr3d
Pr2, Pr4d
Pt1, Pt4f
Pt2, Pt4d5
Pt3, Pt4f7
Pt4, Pt (MNN)
Pt5, Pt4p3
Pt6, Pt4d3
Pt7, Pt4f5
Rb1, Rb3d
Rb2, Rb3p
Rb3, Rb3p3

Rb4, Rb3p1
Rb5, Rb3s
Re1, Re4f
Re2, Re4d
Re3, Re4d5
Re4, Re4d3
Re5, Re4p3
Re6, Re4p1
Re7, Re4s
Rh1, Rh3d
Rh2, Rh3p3
Rh3, RhMNN
Rh4, Rh3d5
Rh5, Rh3p1
Rh6, Rh3d3
Ru1, Ru3d
Ru2, Ru3p3
Ru3, RuMNN
Ru4, Ru3d5
Ru5, Ru3p1
Ru6, Ru3d3
S1, S2p
S2, S2s
S3, S (LMM)
S4, S (KLL)
Sb1, Sb3d5
Sb2, Sb4d
Sb3, Sb (MNN)
Sb4, Sb3d3
Sb5, Sb (MNN)
Sb6, Sb3p1
Sb7, Sb3p3
Sc1, Sc2p
Sc2, Sc2s
Sc3, ScLMM
Sc4, Sc2p3
Sc5, Sc2p1
Sc6, Sc (LMM)
Se1, Se3d
Se2, Se (LMM)
Se3, Se (LMM)
Se4, Se3s
Se5, Se3p1
Se6, Se3p3
Se7, Se (LMM)
Se8, Se (LMM)
Se9, Se (LMM)
Si1, Si2p
Si2, Si2s
Si3, Si (KLL)
Sm1, Sm3d5
Sm2, Sm4d
Sn1, Sn3d5
Sn2, Sn3p3
Sn3, Sn (MNN)
Sn4, Sn4d
Sn5, Sn3d3
Sn6, Sn3p1
Sn7, Sn (MNN)
Sr1, Sr3d
Sr2, Sr3p
Sr3, Sr3p3
Sr4, Sr3p1
Sr5, Sr3s
Ta1, Ta4f
Ta2, Ta4d

Ta3, Ta4d5
Ta4, Ta (MNN)
Ta5, Ta (MNN)
Ta6, Ta4d3
Ta7, Ta4s
Ta8, Ta4p1
Ta9, Ta4p3
Tb1, Tb4d
Tb2, Tb3d
Tc1, Tc3d
Tc2, Tc3p3
Tc3, Tc3d5
Tc4, Tc (MNN)
Tc5, Tc3p1
Tc6, Tc3d3
Te1, Te3d5
Te2, Te4d
Te3, Te (MNN)
Te4, Te3p1
Te5, Te3p3
Te6, Te (MNN)
Te7, Te3d3
Th1, Th4f7
Th2, Th4d5
Th3, Th5d
Th4, Th5d5
Th5, Th4d3
Th6, Th4f5
Th7, Th5d3
Ti1, Ti2p
Ti2, Ti3p
Ti3, Ti (LMM)
Ti4, Ti2p3
Ti5, Ti2s
Ti6, Ti2p1
Ti7, Ti (LMM)
Tl1, Tl4f
Tl2, Tl4d5
Tl3, Tl5d
Tl4, Tl4f7
Tl5, Tl4p3
Tl6, Tl4d3
Tl7, Tl4f5
Tm1, Tm4d
Tm2, Tm4p
U1, U4f7
U2, U4d5
U3, U5d
U4, U5d5
U5, U4d3
U6, U4f5
U7, U5d3
V1, V2p
V2, V3p
V3, V (LMM)
V4, V2p3
V5, V (LMM)
V6, V (LMM)
V7, V2s
V8, V2p1
W1, W4f
W2, W4d
W3, W4d5
W4, W4s
W5, W4p1
W6, W4p3

W7, W4d3
 Xe1, Xe3d5
 Xe2, Xe4d
 Xe3, Xe (MNN)
 Xe4, Xe3d3
 Y1, Y3d
 Y2, Y3p
 Y3, Y3p3
 Y4, Y3s
 Y5, Y3p1
 Yb1, Yb4d
 Yb2, Yb4p
 Zn1, Zn2p3
 Zn2, Zn3p
 Zn3, ZnLMM
 Zn4, Zn2p1
 Zn5, Zn (LMM)
 Zn6, Zn (LMM)
 Zn7, Zn (LMM)
 Zr1, Zr3d
 Zr2, Zr3p
 Zr3, Zr3p3
 Zr4, Zr3p1
 Zr5, Zr3s

5.7.2 Data Set 2: AES

This file contains the peak name conversion of typical PHI-peak names to the correct scientific names. The data set 2 is for AES instruments (e.g. PHI700).

Comment:

- 1. column: PHI name of the line
- 2. column: correct scientific line name
- Folder: C:\Program Files (x86)\Unifit2017\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)

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