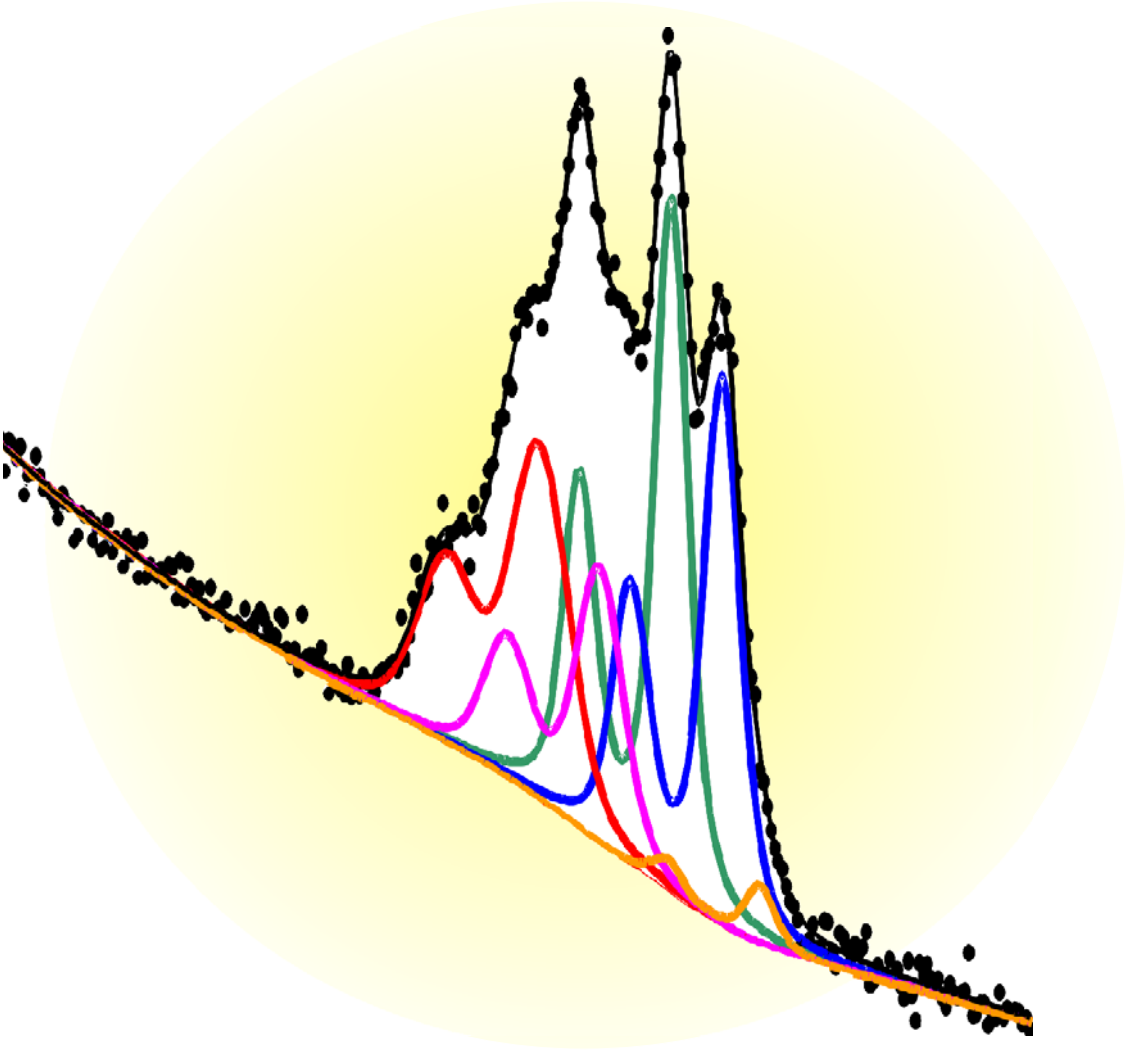
unifit FOR WINDOWS



Line Positions and Data Formats

Version 2018

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Unifit for Windows

Data Formats

Version 2018

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Content

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 directoies Unifit_2017_User_Files\lines. The second part gives the chemical shifts of some compounds.

line positions.pos

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Ag (M4N45N45).pos

357.8 Ag
356.7 Ag2O
356.6 AgO

354.2 Ag2SO4

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

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

Ag 3d5.pos

367.3 AgF2
367.4 AgO
367.5 Ag2CO3
367.7 AgF
367.8 Ag2O
367.8 CuAgSe
367.8 Ag2Se
367.8 Ag2SO4
368.0 AgI
368.1 Ag2S
368.2 Ag
368.4 Ag(OAc)
368.8 Ag2Yb
368.8 AgOOCCF3
368.8 Mg97Ag3

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

1393.1 Al
1391.2 AlAs
1389.4 Al2O3/Al
1389.0 AlN
1388.4 Al2O3
1388.2 Al2O3/alpha
1388.1 Al2FeO4
1387.9 Al2O3/sapphire
1387.8 Al2O3/gamma
1387.7 Al2O3/anhydride
1387.7 Al(OH)3/bayerite
1387.6 AlO(OH)/boehmite
1387.1 KAl2(AlSi3O10)2(OH)2/muscovite
1387.1 LiAlSi2O6/spodumene
1386.9 Mol Sieve A
1386.9 Al2SiO5/sillimannite
1386.9 Al6Si2O13/mullite
1386.8 Al2SiO5
1386.8 Al2Si4O10(OH)2/pyrophyllite
1386.7 Al4Si4O10(OH)8/kaolinite
1386.5 Na[AlSi3O8]/albite
1386.5 Na2Al2Si3O10.2H2O/natrolite
1386.3 Mol Sieve X
1385.9 Mol Sieve Y
1385.5 H Zeolon

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

67.2 Al
53.4 Al2O3/Al
66.4 Al2O3/Al

Al 2p.pos

71.0 AlB2
72.9 Al
73.4 Fe3Al
73.6 AlAs
73.6 AlGaAs
73.6 CoAl2O4
73.7 Mol Sieve A
73.7 Al2O3/gamma
73.9 Al2O3/alpha
74.0 AlN
74.1 Al2O3/sapphire
74.2 AlO2H/boehmite
74.2 Al2(MoO4)3
74.2 NiAl2O4
74.2 AlO2H
74.2 Al(OH)3/bayerite
74.3 Al2(WO4)3
74.3 Mica/muskovite
74.6 Al2S3
74.6 AlI3
74.6 Al2SiO5/sillimanite
74.7 AlCl3
74.7 MgAl2O4
74.8 Al2SiO5/mullite
74.8 H Zeolon
75.2 AlBr3
75.6 LiAlH4
76.3 AlF

Ar (L3M23M23).pos

211.0 Ar

Ar (L3M23M23;3P).pos

212.8 Ar

Ar 2p.pos

241.5 Ar in graphite

As (L2M45M45).pos

1254.9 As2O3
1254.6 NaAsO2
1252.9 Na2HAsO4

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

1225.1 GaAs
1224.8 As
1222.1 As2S3
1221.1 Ph3As
1219.5 Ph3AsO
1218.8 As2O3
1217.5 As2O5
1213.8 KAsF6
1218.1 AsBr3
1222.9 AsI3

As 3d.pos

40.6 InAs
41.0 AlGaAs
41.0 AlAs
41.2 GaAs
41.5 As
42.8 Ph3As
43.4 As2S3
43.4 AsI3
44.3 Ph3AsO
44.9 As2O3
45.3 AsBr3
46.2As2O5
47.8 KAsF6

As 2p3.pos

1323.1 GaAs
1324.3 As
1325.7 AsO
1326.4 As2O3
1327.4 As2O5

Au (M4N67N67).pos

2101.5 Au

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

2015.7 Au

Au (N7VV).pos

69.8 Au

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

71.2 Au

Au 4f7.pos

84.0 Au
84.5 AuSn
85.1 AuSn4
85.3 ClAuPh3P

B 1s.pos

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

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

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

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

59.5 BaF2/Au

56.0 BaCl2
57.8 BaBr2
55.4 BaBr2
55.3 BaTiO3

Ba (N45O23V).pos

71.4 BaBr2
71.2 BaCl2
68.6 BaTiO3

Ba 3d5.pos

778.9 BaCrO4
779.1 BaMoO4
779.8 BaS
779.9 BaO
779.9 BaCO3
780.6 Ba
780.7 Ba(NO3)2
780.8 BaSO4
781.7 BaF2

Be 1s.pos

111.8 Be
113.7 BeO
115.3 BeF2
115.3 NaBeF3

Bi (N6O45O45).pos, Bi (NOO)

103.7 Bi

Bi (N7O45O45).pos

100.1 Bi

Bi 4f7.pos

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

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

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

Br 3d.pos

66.7 Ph4AsBr
68.3 CsBr
68.4 RbBr
68.7 KBr
68.8 NaBr
68.9 LiBr
68.9 CuBr2
69.2 K2PtBr6
69.3 K2PtBr4
70.1 Bromanil
74.8 KBrO3

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

262.0 Graphite

C 1s.pos

281.6 TiC
282.8 WC
283.9 Fe3C
283.9 K3Fe(CN)6
284.5 Graphite
284.6 PhNH2
284.7 Benzene
285.0 -CH2-
285.5 C5H5N
285.6 C6H5F(C*H)
285.6 EtNH2
285.7 C6H5Cl(C*H)
285.7 (-C*H2CFH-)n
285.9 PVC(-C*H2CHCl-)
286.1 KCN
286.3 CH3C*H2OH
286.3 C*H3CN
286.4 (-C*H2CF2-)
286.5 (CH3C*H2)2O
286.5 PVA(-CH2C*HOH-)n
286.9 CH3COOC*H2CH3
287.0 CS2
287.0 PVC(-CH2C*HCl-)
287.1 C6H5Cl(C*Cl)
287.2 CH3C*N

287.8 C6H5F(C*F)
287.9 (-CH2C*FH-)n
287.9 CH3C*OCH3
288.0 Fe(CO)5
288.0 H2NCSNH2
288.2 CH3C*OONa
288.4 CH3C*ONH2
288.7 H2NCONH2
289.3 CH3C*OOH
289.4 Na2CO3
289.5 Cl3C*COONa
289.6 CaCO3
289.6 HCCl3
290.0 NaHCO3
290.9 (-CH2C*F2-)n
291.9 CO2
292.2 Teflon(-CF2CF2-)n
292.4 CCl4
292.9 C*F3COOEt
294.7 HCF3
296.7 CF4

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

298.2 Ca
292.5 CaO
291.9 CaCO3
291.9 CaCl2
288.9 CaF2

Ca 2p3.pos

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

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

383.6 Cd
382.5 CdO
382.4 CdTe
382.2 CdSe0.65Te0.35
381.4 Zn0.30Cd0.70Se
381.5 Zn0.50Cd0.50Se
381.2 Zn0.70Cd0.30Se
381.0 Zn0.90Cd0.10Se
381.3 CdS
381.0 CdSe
380.5 CdI2
380.0 Cd(OH)2
380.0 CdBr2.4H2O
379.8 (CdCl2)2.5H2O
378.5 CdF2
378.3 Ba/Ca/Cd/Sr/in_montmorillonite

Cd (M5N45N45).pos

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

Cd 3d5.pos

404.2 CdO
404.6 Hg0.8Cd0.2Te
405.0 CdSe
405.1 Cd
405.1 Cd(OH)2
405.1 CdCO3
405.2 CdTe
405.3 CdS
405.4 CdI2
405.9 CdF2
406.0 CdBr2
406.1 CdCl2

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

771.0 CeO2

Ce (M5N45N67).pos

755.0 CeO2

Ce 3d5.pos

881.9 CeO2
883.5 CeAl2
883.6 CeCu2Si2

883.9 Ce
884.3 CePd3
884.3 CeSe
886.0 CeH3

Cl (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.H20
181.0 KCl
181.0 KClO3
180.7 KClO4

Cl 2p3.pos

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

Co (L3M45M45).pos

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

Co (LMM).pos

770.7 Co((C6H5)3PO)2(NO3)2

Co (M23VV).pos

53.6 Co

Co 2p3.pos

778.1 CoS2
778.3 Co
779.9 Co3O4
780.3 CoOOH
780.4 CoO
781.3 Co(OH)2
781.3 CoAl2O4
781.7 Co(NH3)6Cl3
781.9 K3Co(CN)6
782.4 CoF3
783.0 CoF2
783.6 CoSiF6
784.0 CoSO4

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

528.8 Cr2O3
527.2 Cr
525.5 CrF3

Cr 2p3.pos

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

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

568.7 CsOH
568.4 Cs2SO4

Cs (N5O23O23).pos

46.3 Cs

Cs (N45O23O23).pos

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

Cs (N45O23V).pos

61.6 CsBr
61.4 CsCl

Cs 3d5.pos

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

Cu (L2M45M45).pos

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

Cu (L2VV).pos

938.3 Cu
934.7 Cu

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

918.6 Cu
918.6 Cu64Zn36
918.5 Ag28.6Au17.1Cu54.3
918.4 CuSe
918.1 CuS
918.0 CuCr2O4
917.9 CuO
917.8 CuFeS2
917.7 Cu2Se
917.7 AgCuSe
917.6 CuInSe2
917.1 Cu2S
917.0 Cu2CO3(OH)2
917.0 CuIn3Se5
917.0 CuGa5Se8
916.8 Cu(OH)2
916.8 Al2CuO4
916.7 Cu2O
916.7 CuInS2
916.6 CuMoO4
916.6 Cu3Mo2O9
916.3 CuCO3
916.3 CuBr2
916.1 CuI
916.1 CuSO4
915.3 CuCl
915.5 CuCl2
915.3 Cu(NO3)2
915.2 CuSiO3
915.1 CuF2
914.6 CuCN
914.5 [CuC(CN)3]
914.4 Cu2S

Cu (L3VV).pos

921.2 Cu
918.4 Cu
916.0 Cu
914.1 Cu
911.0 Cu

Cu (M23VV).pos, Cu (MVV).pos

62.4 Cu
63.7 6-8A Fe/Cu
60.8 6-8A Fe/Cu

Cu 2p3.pos

931.9 CuInSe2
932.3 CuS
932.5 Cu2O
932.5 Cu2S
932.5 CuCl
932.6 Cu64Zn36
932.7 Cu
933.1 CuCN
933.8 CuO
935.2 CuCl2
934.5 Cu(acac)2

934.9 CuSO4
935.1 Cu(OH)2
936.1 CuF2

Dy (M4N67N67).pos

1318.0 Dy

Dy (M5N45N45).pos

960.0 Dy

Dy (M5N67N67).pos

1280.0 Dy

Dy (M45N45N67).pos, Dy (MNN).pos

1115.0 Dy

Dy 3d5.pos

1295.5 Dy
1298.9 Dy2O3

Dy 4d.pos

152.4 Dy
167.7 Dy2O3

Er (M4N67N67).pos

1428.0 Er
1429.0 Er2O3

Er (M5N45N45).pos

1035.0 Er
1037.0 Er2O3

Er (M5N67N67).pos

1387.0 Er
1386.0 Er2O3

Er (M45N45N67).pos, Er (MNN).pos

1218.0 Er
1221.0 Er2O3

Er 4d.pos

167.3 Er
168.7 Er2O3

Eu (M4N67N67).pos

1150.0 Eu

Eu (M5N45N45.pos

846.0 Eu

Eu (M5N67N67).pos

1120.0 Eu

Eu (M45N45N67).pos, Eu (MNN).pos

980.0 Eu

Eu 3d5.pos

1125.6 Eu

Eu 4d.pos

128.2 Eu
135.9 Eu2O3

F (KL1L1).pos

608.0 LiF

F (KL1L23).pos

627.4 LiF

F (KL23L23).pos, F (KLL).pos

659.3 AgF
658.5 PbF2
658.0 LaF3
657.2 PrF3
657.0 SmF3
657.0 NdF3
657.0 ThF4
656.6 CuF2
656.4 InF3
656.3 SrF2
656.2 BaF2
656.1 GdF3

656.0 CdF2
656.0 K3FeF6
655.8 YF3
655.7 K2TiF6
655.6 ZnF2
655.6 CrF3
655.5 MnF2
655.5 NiF2
655.4 CaF2
655.3 HfF4
655.2 K2NbF7
655.1 Na2TiF6
655.1 Na2ZrF6
655.0 NaF
655.0 K2TaF7
654.7 LiF
654.4 MgF2
654.4 NaSnF3
654.1 Na3AlF6
654.0 Na2GeF6
653.9 KSbF6
653.8 CsF
653.5 SiF6 monolayer/Ni
653.0 Na2SiF6
653.0 SiF6 monolayer/O2/Ni
652.9 [Ni(CF3COO)2]
652.8 NaBF4
652.6 Al2.3(OH)0.3.H2O
652.4 (-CF2-CF2-)n
651.7 AlF3

F 1s.pos

683.9 KF
684.5 CuF2
684.5 NaF
684.6 CdF2
684.8 CaF2
684.8 UF2
685.0 LiF
685.5 MgF2
685.5 Na3AlF6
685.9 CsF
686.2 Na2SiF6
686.9 (-CHF-CH2-)n
687.0 NaBF4
688.2 (-CF2-CH2-)n
689.7 (-CF2-CF2)n
694.2 NF4BF4

Fe (L3M45M45).pos, Fe (LMM).pos

703.0 FeS2
702.9 FeB
702.9 Fe2B
702.7 Fe
702.6 CuFeS2

Fe (M23VV).pos, Fe (MVV).pos

48.6 8-9A Fe/Cu

Fe 2p3.pos

706.7 Fe
707.1 K4Fe(CN)6
707.2 FeS2
707.4 FeB
708.1 Fe3C
709.6 FeO
709.6 K3Fe(CN)6
710.6 Fe3O4
710.9 Fe2O3
712.1 FeSO4

Ga (L2M4M4).pos

1091.5 GaN

Ga (L3M45M45).pos, Ga (LMM).pos

1068.0 Ga
1066.3 GaAs
1065.6 GaP
1065.3 Ga2Se3
1065.3 CuGa5Se8
1064.3 GaN
1062.3 Ga2O3

Ga (M23VV).pos, Ga (MVV).pos

56.1 Ga

Ga 2p3.pos

1116.7 Ga
1116.8 GaP
1116.9 Ga2O3

Ga 3d.pos

18.7 Ga

19.0 AlGaAs
19.3 GaAs
19.3 GaP
19.5 GaN
20.5 Ga2O3

Gd (M4N67N67).pos

1202.0 Gd

Gd (M5N45N45).pos

884.0 Gd

Gd (M5N6N67).pos

1170.0 Gd

Gd (M45N45N67).pos, Gc (MNN).pos

1020.0 Gd

Gd 3d5.pos

1187.0 Gd
1189.0 Gd2O3
1190.0 Gd2(SO4)3

Gd 4d.pso

140.4 Gd
143.8 Gd2O3
143.8 Gd2(SO4)3

Ge (L3M45M45).pos, Ge (LMM).pos

1145.2 Ge
1144.8 GeTe
1143.7 GeS
1143.5 GeSe
1142.8 Ge2Se3
1141.8 GeSe2
1141.7 GeSe3
1137.8 GeO2
1136.6 Si0.4Ge0.9O0.6
1135.7 Na2GeF6 1135.7 Na2GeF6

Ge 2p3.pos

1217.2 Ge
1219.8 GeS2
1220.4 GeO2
1221.3 Na2GeF6

Ge 3d.pos

29.3 Ge
30.5 GeS
30.7 GeSe
32.7 GeO2
33.3 Na2GeF6

Hf (M4N67N67).pos

1669.0 Hf

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

1615.0 Hf

Hf (M45N45N67).pos

1420.0 Hf

Hf 4f7.pos

14.2 Hf
16.7 HfO2

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

2159.8 Hg

Hg 4f7.pos

99.9 Hg
100.2 Hg0.8Cd0.2Te
100.8 Hg2Cl2
100.8 HgO
101.0 HgS/cinnabar
101.4 HgCl2

Ho (M4N67N67).pos

1372.0 Ho

Ho (M5N45N45).pos

998.0 Ho

Ho (M5N67N67).pos

1332.0 Ho

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

1165.0 Ho

Ho 4d.pos

159.6 Ho

I (M4N45N45).pos

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

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

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

I 3d5.pos

618.4 NaI
618.8 KI
619.2 CdI
619,4 AgI
619.7 LiI
619.9 I2
620.3 UI3
621.5 ICl
622.5 ICl3
623.3 I2O5
623.5 NaIO3
624.0 NaIO3

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

410.2 In
409.3 InP
408.9 In2Te3
408.5 CuInSe2
408.0 InP
408.1 In2Se3
407.4 CuIn3Se5
407.3 In2S3
407.3 CuInS2
406.5 In2O3
405.8 InI3
405.7 In(OH)3.nH20
405.3 In(OH)3
404.8 InBr3
404.7 InPO4
404.6 InCl3
404.6 In(PO3)3
404.4 In(PO3)4
404.1 (NH4)3[InF6]
403.7 InF3
401.6 InSb

In (M5N45N45).pos

397.5 In
393.0 In
397.5 InP
396.0 InP

In (M5N45N45;1G).pos

402.6 In

In 3d5.pos

443.8 In
444.1 CuInSe2
444.3 InSb
444.5 InP
444.5 In2Te3
444.8 In2Se3
444.8 In2O3
444.9 In2S3
444.9 InCl
445.0 In(OH)3
445.4 In(acac)3
445.8 InI3
446.0 InBr3
446.0 InCl3
446.2 InF3

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).pos

728.0 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 Lu2O3
196.6 Lu
198.5 Lu2(SO4)3

Lu 4f7.pos

6.3 Lu

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

1185.6 Mg
1180.7 MgBr2.6H2O
1180.6 (Mg/Fe)2SiO4
1180.5 KMg3Si3AlO10(OH/F)2
1180.5 Mg3H2(SiO3)4
1180.5 (Mg/Fe)SiO3
1180.4 MgO
1179.0 (Na/Al/Mg)Si4O10(OH)2.nH2O
1178.8 MgSO4.7H2O
1178.5 MgCl2/Au
1178.2 MgF2

Mg (L23VV).pos

43.0 Mg/Ru
31.0 O2/Mg/Ru

Mg 1s.pos

1302.7 Mg(OH)2
1303.2 Mg
1304.0 MgAl2O3
1305.0 MgF2

Mg 2p.pos

49.5 Mg(OH)2
49.6 Mg
50.4 MgAl2O4
50.4 MgO
51.0 MgF2
51.6 MgSO4.7H2O

Mn (L3M23M45).pos, Mn (LMM).pos

586.4 Mn
585.7 MnO2
585.0 Mn2O3
584.8 MnS
583.7 Mn3O4
581.0 MnSO4

Mn 2p3.pos

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

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

2137.4 MoOx
2143.6 Mo

Mo (L3M45M45).pos

2039.0 MoSi2
2038.8 Mo
2032.2 MoOx

Mo 3d5.pos

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

N (KVV).pos

396.6 Gd(NO3)3.5H2O
385.0 GaN
383.0 Fe2N
379.2 BN
376.6 NH3

N 1s.pos

397.0 GaN
397.7 Si3N4
398.0 K4Fe(CN)6
398.1 BN
398.5 Na(N*NN*)
398.7 NH3
398.8 C5H5N/Pyridine
398.9 EtNH2
399.2 PhCN
399.5 H2NCONH2
399.4 C6H12N4/Urotropin
399.8 KCN
400.2 C4H5N/Pyrrole
401.3 (NH4)2SO4
401.4 Et4NCl
401.7 NH4Cl
402.2 Bu4NHSO4
402.9 Na(NN*N)
403.1 Pyridine N-oxide
403.8 NaNO2
404.7 K2Pt(NO2)6
405.5 R-NO2
407.3 NaNO3
408.2 R-ONO2

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

994.3 Na
991.2 NaI
990.6 NaBr
990.5 Na2C2O4
990.3 NaCl
990.1 Na3PO4
989.9 NaOAc
989.8 Na2CO3
989.8 Na2SO4
989.8 Na2O
989.7 Na2HPO4
989.4 NaNO3
989.4 NaPO3
989.1 NaH2PO4
988.6 NaF
987.7 Na2SiF6
987.1 NaBF4

Na (L23VV).pos

23.8 NaI
23.1 NaBr
21.6 NaCl
20.2 NaF

Na 1s.pos

1070.8 NaN3
1070.8 Na2C2O4
1071.1 Na3PO4
1071.1 NaOAc
1071.2 NaF
1071.2 Na2SO4
1071.4 NaNO3
1071.5 Na2CO3
1071.5 Na2HPO4
1071.6 NaI
1071.6 NaPO3
1071.6 NaCl
1071.7 Na2SiF6
1071.7 NaBr
1071.8 Na
1072.0 NaH2PO4
1072.5 Na2O
1072.7 NaBF4

Nb (M45N23V).pos, Nb (MNV).pos

167.8 Nb
165.6 NbHx
161.6 Nb2O5

Nb 3d5.pos

202.4 Nb
203.2 NbHx
203.7 NbO
203.8 NbN
206.5 KNbO3
207.1 NbBr5
207.6 Nb2O5
207.7 NbS2
208.0 NbCl5

Nd (M5N45N45).pos, Nd (MNN).pos

733.0 Nd

Nd (M45N45N67).pos

840.0 Nd

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)3.2H2O
862.9 NiOOH
862.7 KNiIO6

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/Ca0.166Ni0.833
845.2 Al70Co15Ni15
844.9 AlNi
843.2 ((P2O5)0.40(V2O5)0.60)0.90(NiO)0.10
842.9 NiO/Ca0.166Ni0.833
842.9 NiO
842.9 (Ni(OH)2)3.2H2O
842.4 NiF2
842.4 Ni(acac)2
841.7 Ni(OH)2/Ca0.166Ni0.833

Ni 2p3.pos

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

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

515.1 PbO2
513.1 PbO
513.2 Ag2O
511.8 H2MoO4
511.6 H2WO4
511.3 PbCO3
510.8 ZrO2
510.6 (CH3)2CH(CH2)CH(NH2)COOH
510.2 C6H5C(O)C(O)C6H5
510.0 NaC2H3O2
510.0 ZnO
509.9 CuCo3
509.7 CaCO3
509.5 COOH(CH2)4COOH
509.3 CaO
509.3 Mg(OH)2
509.3 [Mg(CH3C(O)CHC(O)CH3)2]
509.7 Na2Co3
509.4 HOCH2(CH2)8CH2OH
509.1 Na8(AlSiO4)6Cl2(OH)n
509.0 [Mg(C6H10OC(O)C3H7)]
508.8 CaSiO3
508.7 CaSO4
508.6 Al(OH)3
508.6 LiOH
508.5 Al2O3
508.5 Mol-Sieve-A
508.3 NaOh
508.1 KAl2(AlSi3O10)2(OH)2
507.9 NaPO3
507.7 H2O
507.7 NaAlSi3O8
507.6 -C6H5Si2O3C6H5-
507.4 Al2Si4O10(OH)2

507.0 H zeolon
506.8 SiO2

O 1s.pos

529.3 CrO2
529.5 NiO
529.6 Fe2O3
529.8 FeO
529.9 Co2O3
530.0 Fe3O4
530.1 K4P2O7
530.2 Co3O4
530.2 CrO3
530.2 CoO
530.4 K3PO4
530.6 Na2SiO*3.H2O
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.pos

1033..5 PmCl3

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

695.0 Pr

Pr (M45N45N67).pos

795.0 Pr

Pr 3d5.pos

931.8 Pr
933.6 Pr2O3
935.3 PrO2

Pr 4d.pos

116.1 Pr2O3
116.2 PrO2

Pt (M4N67N67).pos

2040.5 Pt
2035.2 K2PtCl4

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

1960.7 Pt

Pt 4f7.pos

71.2 Pt
71.4 Pt(Ph3P)3
71.4 Pt(Ph3P)4
72.5 Pt2Si
72.6 I2Pt(Me3P)2/cis
72.6 K2PtBr4
72.6 Pt(OH)2
72.7 I2Pt(Me3P)2/trans
73.0 PtSi
73.0 Cl2Pt(Ph3P)2/cis
73.4 K2PtCl4
73.4 K2PtI6
73.4 Pt(NH3)4Cl2
73.6 PtCl2
74.2 PtO
74.6 K2PtBr6
75.0 PtO2
75.4 K2PtCl6
75.5 PtCl4
75.9 Cl4Pt(Et3P)2
76.3 Pt(NH3)6Cl4
77.6 K2PtF6

Rb 3d5.pos

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

Re 4f7.pos

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

Rh 3d5.pos

307.2 Rh
307.4 ClRh(Ph3P)3
308.5 KRhO2
308.6 RhI3
308.7 Rh2O3
308.8 CaRh2O4
309.4 Rh2WO6
309.8 K3RhCl6
310.0 RhCl3.3H2O
310.1 RhCl3
310.5 K3Rh(NO2)6
312.2 K3RhF6

Ru 3d5.pos

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

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

2119.9 FeS

2119.9 NiS
2119.9 PbS
2119.1 Ag2S
2119.1 FeAsS
2118.9 Sb2S3
2118.4 MoS2
2118.2 HgS
2118.1 Cu2S
2117.6 CdS
2117.1 ZnS
2116.7 K2S
2116.1 S
2116.1 S8
2116.1 Na2S.9H2O
2116.0 FeS2
2115.9 Na((C2H5)2NCS2).3H2O
2115.9 NiWS2
2115.2 Na2S2O3.5H2O
2115.1 H2CH2CH(NH2)C(O)OH
2114.8 (CH3)S
2114.8 WS2
2114.6 NH4SCN
2114.3 (C10H12AuClN2S)n
2114.0 ZnSO4
2114.0 K(CH(CH3)2OCS2)
2113.9 C4H3S(CH)5C(CN)2
2113.9 CH3SCH2CH2CH(NH2)C(O)OH
2111.6 CS2
2111.2 NaSCN
2110.7 (C10H12AuClN2S)n
2110.6 Na2S2O3.5H2O
2110.5 CoSO4
2110.5 Na2SO3
2110.4 CuSO4
2110.4 NaHSO3
2110.3 FeSO4.7H2O
2110.3 NiSO4
2110.2 Fe2(SO4)3.nH2O
2110.2 MnSO4
2109.9 BaSO4
2109.7 (NH4)2SO4.FeSO4.6H2O
2109.7 CaSO4.2H2O
2109.6 HgSO4
2109.5 (NH4)2SO4
2109.3 (NH4)2(SO4)2
2109.3 SrSO4
2109.3 Al(NH4)(SO4)2.12H2O
2109.2 KAl(SO4)2.12H2O
2109.2 MgSO4.7H2O
2109.1 K2S2O7
2109.1 BeSO4
2109.1 Al2(SO4)3.18H2O
2109.0 SnSO4
2108.9 K2(SO4)2
2108.8 Li2SO4
2108.5 Na2SO4
2108.2 K2SO4
2107.8 Na2S2O3
2105.9 CaSO4
2103.9 (CH3)2S
2103.7 [PS(CH3O)3]
2103.3 [PSCl2(CH3O)]
2103.2 [PSCl2(CH3)]
2102.9 [PSCl3]
2102.5 (CH3S)2
2102.5 (CH3S)2
2100.9 (CF3S)2
2100.7 [PSF3]
2100.5 CH3SH
2100.4 SF6
2099.9 (CH3)2SO
2098.7 SO(CH3O)2
2098.6 H2S
2098.1 SOCl2
2097.6 (CH3O)2SO2
2097.0 SO2Cl2
2095.5 SO2ClF
2095.5 SO2
2094.5 SOF2
2094.3 SClF5
2093.9 SF4
2093.8 SO2F2
2092.6 SF6

S 2p.pos

160.8 PbS
161.6 FeS
161.7 CdS
162.1 NH2CSNH2
162.3 ZnS
162.8 NiS
162.8 Na2S*SO3
162.8 WS2
163.0 FeS2/Pyrite
163.2 Ph2S
163.2 Cysteine
163.7 CS2
163.8 S
164.3 Thiophene
164.4 PhSSPh
166.3 PhSO2Na

166.5 Me2SO
167.4 SO2
167.6 Na2SO3
168.1 p-NH2C6H4SO3Na
168.6 Na2SS*O3
169.0 Me2SO2
169.1 CuSO4
169.4 Na2SO4
169.7 CaSO4
174.4 SF6

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

464.5 Sb
462.2 Sb2S5
462.1 Sb2S3
459.7 Sb2O3
454.4 KSbF6

Sb 3d5.pos

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

Sc 2p3.pos

398.6 Sc
400.7 ScN
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 Zn0.30Cd0.70Se
1307.2 Zn0.42Cd0.58Se
1307.0 Se
1306.8 CdSe
1306.7 Zn0.50Cd0.50Se
1306.5 Zn0.70Cd0.30Se
1305.9 Zn0.90Cd0.10Se
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.pos

1241.4 TbO2
1241.5 Tb2O3
1242.0 Tb

Tb 4d.pos

146.0 Tb
148.7 Tb2O3
149.2 TbO2

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

492.1 Te
491.1 CdSe0.65Te0.35
490.8 CdTe
488.5 Ph2Te2
487.6 TeI2(C2H5)2]
487.3 TeBr4
487.1 TeO2
486.7 [TeBr2(C6H5)2]
486.6 [TeI2(CH3)2]
486.6 [TeBr2(C6H5CH3)]
486.4 (NH4)2TeCl6
486.3 Cl2TePh2
486.3 TeCl2(C6H5)2]
486.1 TeCl4
485.5 Na2TeO4
485.5 TeO3
485.1 Te(OH)6

Te 3d5.pos

572.3 Hg0.8Cd0.2Te
572.7 CdTe
572.7 GeTe
572.9 Te
573.9 Ph2Te2
575.5 K2TeO3
575.8 TeI4
576.1 TeO2
576.2 Cl2TePh2
576.7 TeBr4
576.8 Na2TeO4
576.9 TeCl4
576.9 (NH4)2TeCl6
577.1 Te(OH)6
577.3 TeO3

Th (N67O45O45).pos

154.0 Th

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

249.0 Th

Th 4d5.pos

675.2 Th
675.5 ThO2

Th 4f7.pos

333.1 Th
334.4 ThO2
336.5 ThF4

Ti (KL23L23).pos

4002.0 TiO2

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

419.0 Ti
418.2 TiC
409.8 Na2TiF6

Ti 2p3.pos

454.0 Ti
454.4 TiB2

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

Tl 4f7.pos

117.5 Tl2O3
117.7 Tl
118.5 TlI
118.7 Tl2S
118.7 Tl4S3
119.0 TlCl
119.2 TlBr
119.2 TlF

Tm (M4N67N67).pos

1487.0 Tm

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

85.1 Tl

Tm (M5N45N45).pos

1080.0 Tm

Tm (M5N67N67).pos

1440.0 Tm

Tm (M45N45N67).pos, Tm (MNN).pos

1270.0 Tm

Tm 4d.pos

175.4 Tm
176.6 Tm2O3
178.3 Tm2(SO4)3

U (N67O45N45).pos

190.0 U

U (N67O45V).pos

284.0 U

U 4f7.pos

377.4 U
378.3 UCl3
378.4 UBr3
379.1 USe3
379.4 US3
379.9 UBr4
380.0 UOCl
380.1 US
380.1 UF3
380.1 UOBr
380.2 UCl4
380.2 UO2
380.3 UOCl2
380.3 USe
380.4 UOBr2
380.5 UO2Br
380.5 U2Te3
380.7 U3O8
380.7 CaUO4
381.1 UO2Br2
381.3 UTe3
381.3 UO3
381.6 UO2Cl2
381.6 U(SO4)2
381.9 UCl5
382.2 UF4
382.4 K2UF6
383.0 UO2F2
384.9 UF6

V (L3M23M45).pos, V (LMM).pos

472.0 V
468.0 V2O5
468.6 VO2

V 2p3.pos

512.2 V
512.9 V(C5H5)2
513.3 K4V(CN)6
514.2 V(acac)3
514.4 VN

515.1 VO(acac)2
516.3 VO2
516.4 VOCl2
517.3 Na3VO4
517.6 V2O5

W (M5N67N67).pos, W (MNN).pos

1727.8 WS2
1723.9 H2WO4
1723.8 WO3
1722.0 Na2WO4

W 4f7.pos

31.3 W
31.5 WC
32.7 WO2
33.2 WS2
35.1 CaWO4
35.7 WO3
35.9 WBr6
36.2 H2WO4
36.3 Na2WO4
36.3 WBr5
36.3 Al2(WO4)3
36.9 WCl6
37.2 WOCl4

Xe (M4N45N45).pos

545.2 Xe in graphite
544.8 Xe in Fe
545.2 Xe in graphite
545.2 Xe
544.8 Xe in Fe
543.7 Xe/Ni
541.4 Na4XeO6

Xe 3d5.pos

668.9 Xe in Au
669.6 Xe in Cu
669.7 Xe in graphite
670.2 Xe in Fe
674.1 Na4XeO6

Y (M45N23V).pos, Y (MNV).pos

124.3 Y
123.3 YHx
117.8 Y2O3

Y 3d5.pos

155.8 Y
156.2 YHx
157.0 Y2O3
160.0 Y2(SO4)3

Yb (M4N67N67).pos

1549.0 Yb

Yb (M5N67N67).pos

1500.0 Yb

Yb (M45N45N67).pos

1320.0 Yb

Yb 4d5.pos

182.4 Yb
185.4 Yb2O3
187.3 Yb2(SO4)3

Zn (L3M45M45).pos, Zn (LMM).pos

992.7 Cu64Zn36
992.2 Zn
991.3 ZnTe
989.7 ZnS
989.5 ZnSe
989.4 ZnCl2
989.3 ZnFe2O4
988.7 ZnI2
988.6 ZnO/SiO2
988.2 ZnO/Si
988.0 Zn5(CO3)2(OH)6
987.8 Al2ZnO4
987.7 [Zn(CH3C(O)CHC(O)CH3)2]
987.7 Zn(acac)2
987.7 ZnAl2O4
987.7 ZnO
987.4 ZnCO3
987.3 Zn4Si2O7(OH)2.2H2O
987.3 ZnBr2
987.0 Zn2SiO4
986.5 Zn(OH)2
986.2 ZnF2

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 ZrHx
141.9 ZrO2

Zr 3d5.pos

179.0 Zr
179.6 ZrHx
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 directoriy Unifit_2017_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 Eclipes(.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_DATASTORAGEID_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 devided 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 Al12/20
date      :
time      :
source    :
MessMode  : EDC
max_energy  :  561.62557
min_energy  :  511.60555
pass_energy :    20
step_w      :    0.06100
anz_scans   :     3
count_time  :   100
num_of_data :   821
E_kin;resCh;secCh
511.60555;8202;1.0000
511.66655;9032;1.0000
511.72755;9055;1.0000
511.78855;8922;1.0000
511.84955;9028;1.0000
...
561.50355;5248;1.0000
561.56455;5183;1.0000
561.62555;5123;1.00001
```

3.1.5 VSI (*.GPH)

Comment:

- Excitation energy not available
- Example: single region, survey, excitation energy: 1253.6 eV
- Folder: Install-CD:\XPS_Measurement_Reference_Data\ 04-VSI(.GPH)\ VSI-SingleReg-survey-EP=1253.6.GPH

```
%%%%% 001   #     General data
 2.10  0.40 HSA FFFFFE1F      #     P-Version, C-Version, Type
05.12.1997 11:00  #     Date, Time
14    #     Unit TYPE
%%%%% 010   #     Comment
```

```
%%%%% 002   #     Modul data
KINETIC       1000.0000000000   1   1     1.0000000000     0.0000000000 FFFFF529
CHANNELT      2000.0000000000   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 forUNIFIT!)
11. row to 20. row no relevance for UNIFIT!

21. row: lowest binding energy in eV, highest bindig 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 imput of all aqcusition 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 measuement 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,Al
SourceEnergy(eV),1486.6
Power(W),400
[ION GUN INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
SputterRate(nm/min),1.00
BeamVoltage(kV),3.0
GridSupply(V),200
Emission(mA),25.00
Float(V),0
Condenser(%),80.0
Objective(%),65.0
Bend(%),0.0
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
SputterTime(sec),30
[ION GUN NEUTRALIZE INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
BeamVoltage(kV),0.5
GridSupply(V),120
Emission(mA),25.00
Float(V),450
Condenser(%),80.0
Objective(%),65.0
Bend(%),5.0
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
FilamentStatus,OFF
[NEUTRALIZER INFO]
EmissionCurrent(mA),0.000
BiasVoltage(V),0.0
Extractor(V),0.0
XSteering(%),0.0
YSteering(%),0.0
FilamentStatus,OFF
[STAGE INFO]
X(mm),0
Y(mm),0
Z(mm),0
Rotate(deg),0
Tilt(deg),45
DirectionOfRotation,CCW
[DETECTOR INFO]
```

```
MultiplierOffset(V),80
MultiplierVoltage(V),1830
[ENERGY SCAN INFO]
EnergyScanMode,Scanned
[IMAGE INFO]
ImageSize(mm),2.000
FileName,
[REGION INFO]
RegionNumber,RegionName,Lower(eV),Range(eV),PassEnergy(eV),EnergyStep(eV),Time/S
tep(ms),Repeats
1,SUR,0.000,1400.000,187.850,1.000,20,1
2,Ag3d,362.000,20.000,11.750,0.100,20,8
3,Au4f,79.000,20.000,11.750,0.100,20,8
[POINT INFO]
PointNumber,Xposition,Yposition
1,1024,1024
[SPECTRA DATA]
PointNumber,1
RegionName,SUR
Cycle,16
Data(Counts)
1400.000,47766
1399.000,47046
1398.000,46461
1397.000,45741
1396.000,44900
...
4.000,7848
3.000,6246
2.000,4812
1.000,3701
0.000,2933
RegionName,Ag3d
Cycle,16
Data(Counts)
382.000,9121
381.900,9355
381.800,9547
381.700,9231
...
362.300,7560
362.200,7536
362.100,7557
362.000,7506
RegionName,Au4f
Cycle,16
Data(Counts)
99.000,4387
98.900,4193
98.800,4221
...
79.200,2247
79.100,2278
79.000,2251
ddd
```

3.1.11.2 Standard Format, Version 2 (*.csv)

Comment:

- All acquisition parameters (dwell time, number of scans, pass energy, excitation energy, analyser mode) are not saved and has to be defined manually
- First column: binding energies, second column: intensities
- Example: measurement of 2 regions (Ag 3d, Au 4d3)

- Folder: Install-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,DEPTHPLOFILE
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,Omni3
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,C1s,278.000,20.000,11.750,0.100,20,2
2,O1s,523.000,20.000,11.750,0.100,20,5
3,Pt4f,66.000,20.000,11.750,0.100,20,2
4,Cu2p3,927.000,30.000,11.750,0.050,20,15
5,Si2p,94.000,20.000,11.750,0.100,20,2
[POINT INFO]
PointNumber,Xposition,Yposition
1,1024,1024
[PEAK DATA]
PointNumber,1
RegionName,C1s,,O1s,,Pt4f,,Cu2p3,,Si2p,
,Time(min),Data(CPS),Time(min),Data(CPS), … ,Time(min),Data(CPS),
,0.000,46142,0.000,57711,0.000,207322,0.000,54401,0.000,12444,
,0.000,39895,0.000,55214,0.000,238795,0.000,71552,0.000,12498,
...
,32.000,1531,32.000,240005,32.000,1938,32.000,6482,32.000,48073,
,33.000,1582,33.000,242800,33.000,1089,33.000,4961,33.000,49444,
[SPECTRA DATA]
PointNumber,1
RegionName,C1s
Cycle,1,2,3,4,5,6,7,8,9,10,11, ... ,34,35,
Energy(eV),Data(Counts),Data(Counts) ...
,Data(Counts),Data(Counts),Data(Counts),Data(Counts),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
8
Region 1
sample id
2007
7
11
12
15
0
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
```

```
0
As2p3

-1
kinetic energy
eV
151.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
401
0
10000
16389.1800000041
16569.0600000015
16452.1600000039
16071.5800000038
15940.9000000052
...
12967.2800000033
12998.0600000011
12904.8600000032
Region 2
sample id
2007
7
11
11
45
43
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
As3d

-1
kinetic energy
eV
1436.6
0.05
1
```

```
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
281
0
10000
238.659999999962
239.639999999449
233.739999999547
245.179999999964
...
193.099999999989
200.540000000061
Region 3
sample id
2007
7
11
11
37
34
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
C1s

-1
kinetic energy
eV
1191.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
401
```

```
0
10000
2948.54000000032
2975.69999999348
3025.5599999944
3080.79999999792
...
3039.59999999812
3074.74000000033
3136.04000000021
Region 4
sample id
2007
7
11
12
26
15
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
Ga2p3

-1
kinetic energy
eV
356.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
401
0
10000
8753.79999999996
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
O1s

-1
kinetic energy
eV
946.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
301
0
10000
6797.37999999294
6775.21999999325
6831.79999999088
...
6678.09999999377
6699.85999999812
6626.33999999272
Region 7
sample id
2007
7
11
11
26
13
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
50
1
4.444
```

```
0
0
0
0
0
Survey

-1
kinetic energy
eV
86.5999999999999
0.5
1
counts per channel
d
pulse counting
0.3
2
0
0
0
0
0
2801
0
10000
113668.31
113261.39
111981.53
111248.01
...
444.849999999974
197.139999999988
68.0399999999922
Region 8
sample id
2007
7
11
12
33
29
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
VB

-1
kinetic energy
eV
```

```
1476.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
241
0
10000
37.259999999985
30.539999999924
35.5399999999286
...
4.14000000000136
2.25999999999409
2.180000000005
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
FAT
20
1E+37
4.61
0
0
0
0
0
C1s
C1s
-1
Kinetic Energy
eV
1196.6
0.1
1

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

1998
12
21
10
33
19
255
0
XPS
```

```
360
Al K-alpha
18
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
C1s
C1s
-1
Kinetic Energy
eV
1196.6
0.1
1

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

1998
12
21
9
47
3
255
0
XPS
0
Al K-alpha
```

```
18
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
O1s
O1s
-1
Kinetic Energy
eV
947.6
0.1
1

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

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

```
1
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
O1s
O1s
-1
Kinetic Energy
eV
947.6
0.1
1

Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
111
7187.1
8566.98
7359.68
...
7362.26
7240
7220.72
7265.28
Region 2

1998
12
21
9
47
1
255
0
XPS
0
Al K-alpha
18
1
```

```
1
1486.6
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
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
Si2p
Si2p
-1
Kinetic Energy
eV
1378.6
0.1
1

Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
131
1976.72
25878.7
3811.28
3780.16
...
1976.72
1980.54
Region 2

1998
12
21
10
33
19
255
0
XPS
360
Al K-alpha
18
1
1
1486.6
0
0
0
```

```
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
Si2p
Si2p
-1
Kinetic Energy
eV
1378.6
0.1
1

Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
131
1940.86
25983.9
3690
...
1969.58
1991.7
2053.38
end of experiment
```

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

Comment:

- Multipoint measurement (area scan), MAP in the 6. row means: Mapping
- Example consists of 211 spectra, i.e. 3 regions (O 1s, Ag 3d, Bi 4f) at 70 recording points (210 single spectra with x and y position) and one survey
- sequence of spectrea: 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
O 1s/2
Not Specified
2013
9
23
11
28
51
0
3
   XPS   Spectrum
  Acqn. Time(s): 65   Sweeps: 2   Anode:Mono(Al (Mono))(150 W)
Step(meV): 100.0
   Dwell Time(ms): 180   Charge Neutraliser :On   Acquired On :13/09/23
11:28:51
XPS
51.31
1.241
0
Mono(Al (Mono))
1486.69
150
1E+37
1E+37
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
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
1127
2334
0.709544
0.712206
1127
0.709544
1140
0.709558
1163
0.709573
1141
0.709588
1156
0.709603
...
1281
0.712162
1316
0.712177
1330
0.712192
1333
0.712206
Ag 3d/3
Not Specified
2013
9
23
11
28
51
0
3
   XPS     Spectrum
   Acqn. Time(s): 65         Sweeps: 2        Anode:Mono(Al (Mono))(150 W)
Step(meV): 100.0
   Dwell Time(ms): 180        Charge Neutraliser :On   Acquired On :13/09/23
11:28:51
XPS
51.31
1.241
0
Mono(Al (Mono))
1486.69
150
1E+37
1E+37
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
```

```
1E+37
Ag
3d
-1
Kinetic Energy
eV
1109.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
2
0
1E+37
1E+37
1E+37
0
362
359
6763
0.741829
0.746462
844
0.741829
845
0.741855
817
0.741881
840
0.741907
842
0.741932
...
398
0.74641
395
0.746436
383
0.746462
Bi 4f/4
Not Specified
2013
9
23
11
28
51
0
3
   XPS     Spectrum
   Acqn. Time(s): 98         Sweeps: 3        Anode:Mono(Al (Mono))(150 W)
Step(meV): 100.0
   Dwell Time(ms): 180        Charge Neutraliser :On   Acquired On :13/09/23
11:28:51
XPS
51.31
1.241
0
Mono(Al (Mono))
1486.69
150
1E+37
```

```
1E+37
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
Bi
4f
-1
Kinetic Energy
eV
1317.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
3
0
1E+37
1E+37
1E+37
0
362
427
912
0.783451
0.786926
517
0.783451
574
0.783462
516
0.783473
...
603
0.786891
592
0.786926
O 1s/7
Not Specified
2013
9
23
11
35
24
0
3
   XPS     Spectrum
   Acqn. Time(s): 65         Sweeps: 2        Anode:Mono(Al (Mono))(150 W)
Step(meV): 100.0
   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
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
```

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

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

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

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

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

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

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

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

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

```
    xrs_voltage =  0;
    xrs_emission_current =  0.02;
}
EnergyAnalyser: ea200
{
    ea_mode =  esca_c_ep;
    ea_serial =  0;
    ea_vers =  0;
    ea_const =  48;
    ea_ampl_fact =  0;
    ea_particle_polarity =  -1;
    ea_detector_U =  2249.9;
    ea_conversion_U =  0;
    ea_aperture =  13;
    ea_is_small_spot =  0;
}
Manipulator: Max
{
    ma_type =  Max;
    ma_x =  0;
    ma_y =  0;
    ma_sample =  6;
    ma_z =  0;
    ma_tilt =  0;
    ma_rot =  0;
}
MiscAcqInfo:
{
    mi_sample_ampere =  0;
    mi_sample_kelvin =  283;
    mi_acp_pascal =  1.7e-07;
    mi_tcp_pascal =  6.8e-06;
}
flood_gun_U: 0
tag: "O 1s_2"
ManipulationProtocol:
{
    mp_nstrings =  0;
    mp_strings =  {
    }
}
measure_date: 13 09 2005 11 14
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 351 long 2081
10501
10265
10450
...
9563
10156
9816
enddata
background: 351 double 3463
10413.160
10413.160
10413.121
...
9768.989
9806.995
9845.000
endbackground
original: 351 long 2081
10501
```

```
10265
10450
...
9563
10156
9816
endoriginal
endregion
region: 9
method: XPS
active: 1
range: 1160 1173 0.2
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode =  Mg;
    xrs_voltage =  0;
    xrs_emission_current =  0.02;
}
EnergyAnalyser: ea200
{
    ea_mode =  esca_c_ep;
    ea_serial =  0;
    ea_vers =  0;
    ea_const =  192;
    ea_ampl_fact =  0;
    ea_particle_polarity =  -1;
    ea_detector_U =  2249.9;
    ea_conversion_U =  0;
    ea_aperture =  13;
    ea_is_small_spot =  0;
}
Manipulator: Max
{
    ma_type =  Max;
    ma_x =  0;
    ma_y =  0;
    ma_sample =  6;
    ma_z =  0;
    ma_tilt =  0;
    ma_rot =  0;
}
MiscAcqInfo:
{
    mi_sample_ampere =  0;
    mi_sample_kelvin =  283;
    mi_acp_pascal =  1.7e-07;
    mi_tcp_pascal =  6.8e-06;
}
flood_gun_U: 0
tag: "Au 4f_3"
ManipulationProtocol:
{
    mp_nstrings =  5;
    mp_strings =  {
         "Default Background applied",
         "Default Background applied",
         "No Background [1191.6..1191.6]",
         "Tougaard Background  B/C 2866/1643 [1191.6..1191.6]",
         "Shirley Background [1191.6..1191.6]"
    }
}
```

```
measure_date: 13 09 2005 11 20
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 66 long 430
67216
67186
67441
...
48517
47882
47434
enddata
background: 66 double 660
67360.999
67360.999
67360.651
...
47944.353
47941.887
47942.145
47944.333
endbackground
original: 66 long 430
67216
67186
67441
...
48517
47882
47434
endoriginal
endregion
region: 10
method: XPS
active: 1
range: 880 935 0.2
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
Source: XRayGun
{
    xrs_anode =  Mg;
    xrs_voltage =  0;
    xrs_emission_current =  0.02;
}
EnergyAnalyser: ea200
{
    ea_mode =  esca_c_ep;
    ea_serial =  0;
    ea_vers =  0;
    ea_const =  192;
    ea_ampl_fact =  0;
    ea_particle_polarity =  -1;
    ea_detector_U =  2249.9;
    ea_conversion_U =  0;
    ea_aperture =  13;
    ea_is_small_spot =  0;
}
Manipulator: Max
{
    ma_type =  Max;
    ma_x =  0;
```

```
    ma_y =  0;
    ma_sample =  6;
    ma_z =  0;
    ma_tilt =  0;
    ma_rot =  0;
}
MiscAcqInfo:
{
    mi_sample_ampere =  0;
    mi_sample_kelvin =  283;
    mi_acp_pascal =  1.7e-07;
    mi_tcp_pascal =  6.8e-06;
}
flood_gun_U: 0
tag: "Au 3d_3"
ManipulationProtocol:
{
    mp_nstrings =  0;
    mp_strings =  {
    }
}
measure_date: 13 09 2005 11 20
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 276 long 1709
77278
77950
77600
...
52072
52506
52648
enddata
background: 276 double 2760
77610.974
77609.295
77609.341
77608.179
77606.895
77605.696
...
52131.467
52270.067
52408.667
endbackground
original: 276 long 1709
77278
77950
77600
...
52072
52506
52648
endoriginal
endregion
region: 11
method: XPS
active: 1
range: 695 720 0.2
scans: 2
dwell: 0.3
x_shift: 0
x_gain: 1
work_function: 4
```

```
Source: XRayGun
{
    xrs_anode =  Mg;
    xrs_voltage =  0;
    xrs_emission_current =  0.02;
}
EnergyAnalyser: ea200
{
    ea_mode =  esca_c_ep;
    ea_serial =  0;
    ea_vers =  0;
    ea_const =  192;
    ea_ampl_fact =  0;
    ea_particle_polarity =  -1;
    ea_detector_U =  2249.9;
    ea_conversion_U =  0;
    ea_aperture =  13;
    ea_is_small_spot =  0;
}
Manipulator: Max
{
    ma_type =  Max;
    ma_x =  0;
    ma_y =  0;
    ma_sample =  6;
    ma_z =  0;
    ma_tilt =  0;
    ma_rot =  0;
}
MiscAcqInfo:
{
    mi_sample_ampere =  0;
    mi_sample_kelvin =  283;
    mi_acp_pascal =  1.7e-07;
    mi_tcp_pascal =  6.8e-06;
}
flood_gun_U: 0
tag: "O 1s_3"
ManipulationProtocol:
{
    mp_nstrings =  0;
    mp_strings =  {
    }
}
measure_date: 13 09 2005 11 22
filename: "050913_Au_Mg_13"
visible: 1
depth: 1
sputter_def: 0
data: 126 long 768
82388
82946
82067
...
78573
78518
78679
enddata
background: 126 double 1260
82467.000
82412.977
82358.954
...
78852.292
78721.146
78590.000
```

```
endbackground
original: 126 long 768
82388
82946
82067
...
78573
78518
78679
endoriginal
endregion
```

3.1.16 VSW-Tübingen (*.dat)

Comment:

- Regions separeted 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
```

```
74455.000000
75405.000000
...
62980.000000
62970.000000
65290.000000
*
*
```

3.1.17 VGS2000 (*.xps)

Comment::

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

```
30308IA       1 Bereich
tv30308 interkaliert ungesputtert
24 19,35 158 33,5 Mg
-
1. Bereich: SURV1   BE
10 Scans     100 ms Dwell-Time    50 eV Pass-Energie   4000 Kanäle
Start  1000.00 eV       Step  0.25 eV
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
-
 1000.00   58228
  999.75   58404
  999.50   58170
     ...
    1.00    1210
    0.75    1214
    0.50    1078
```

```
    0.25    1208
```

3.1.18 ScientaSES-Signals (*.txt)

Comment::

- Excitation energy was transferred from the synchrotron in case ‚Monochromator Energy' is zero
- Excitation energy in Line: 'Ph. energy=1099.995'
- Example: 2 regions, VB and Ce, La,_Co
- Versions 1.2.2 and 1.3.1 are loadable
- Folder: Install-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 C1s 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 0.00
NoSpatialArea: 1
SpatialAreaDef: 1 1 1 (-279.7 -8247.6 18557.9 45.0 -90.1)
SpatialAreaDesc: 1 Bi2Te3
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 0
XrayPower: 25.61 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 15000.0 V
XRayCondenserLensVoltage: 8230.0 V
XRayObjectiveCoilCurrent: 0.748 A
XRayBlankingVoltage: 325.0 V
XRayFilamentCurrent: 1.576 A
XRayStigmator: 0.0 0.0
XRayHighPower: no
EgunNeutMode: Off
NeutralizerCurrent: 0.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 30.0 V
EgunNeutXSteering: 0.0
EgunNeutYSteering: 0.0
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 1458.6 eV
SxiPassEnergy: 376 eV
SxiLens2: 476 V
SxiLens3: 406 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 350.0 V
SxiDisplayMode: 2
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.698
Channel Info: 2 1 1.467
Channel Info: 3 1 1.392
Channel Info: 4 1 1.320
Channel Info: 5 1 1.251
Channel Info: 6 1 1.103
Channel Info: 7 1 1.074
Channel Info: 8 1 1.026
Channel Info: 9 1 1.001
Channel Info: 10 1 0.941
Channel Info: 11 1 0.824
Channel Info: 12 1 0.819
Channel Info: 13 1 0.750
Channel Info: 14 1 0.650
Channel Info: 15 1 0.674
Channel Info: 16 1 1.266
StagePosition: 8.0986 0.7914 18.5579 45.0062 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 1
DefectPosComment: Bi2Te3
DefectPosU: -0.2797
DefectPosV: 8.2476
DefectPosX: 8.0986
```

```
DefectPosY: 0.7914
DefectPosZ: 18.5579
DefectPosTilt: 45.0063
DefectPosRotation: -90.0500
DefectPosAligment: None
DefectPosReferenceImage: 120685.7.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
    ┐   À   ┼                        -           pnt     sar      + ’+┬ä@c/s àø'⌅
f4  ´┘  Ð               ┐           ┐       É           pnt     sar
+□’+┬ä@c/s àø'⌅        f4  $└  „│              Uå—D«:“D«J˜D € D«*”DUu“D Ð–D Ð˜D
p”DU┴”D«°•DUe“D«→•D«j‘DUÅŽD«:’DUu’DU5“DUµ DU┴“DU…•D p‘DUõ‘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
    └       ┼                       y│          chn     sar             c/s
f8  È+  0               ┐           ┐       É          chn     sar
c/s             f8  H¯  ø,                └           └       É           chn
sar             c/s             f8  H¯  @3               ¿hR'¢8┐A¯
4±Mò AØÅ »0¹ A»hèƒàr AM┤G┘¾  AŽ.²‰│Þ A┐ %ÚPÌ AÂèR└fY A┐ púÿM AØEÎ¨O? Aí¢nÞü└
...
```

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
        `└  ┼                          _           chn     sar             c/s
f8  ø
  p└              ┐            ┐        ¡           chn     sar             c/s
¹@Ÿø†µ/┘¹@ ó" /k¹@DUtÑ…8¹@ÒJž↨´f°@ç(Až↨¹¸@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   ┼                        «           chn     sar             c/s
f8  X|  ð               ┐           ┐       ©┐           chn     sar
c/s             f8  H└  H•               └           └       é└           chn
sar             c/s             f8  H                   ┘           ┘       ì
    chn     sar             c/s             f8  H
  Ø;              |           |       —           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 ﾌﾌﾌﾌsar ﾌﾌﾌﾌ ﾌﾌﾌﾌﾌﾌﾌﾌc/s ﾌﾌﾌﾌﾌﾌﾌﾌ
ﾌﾌﾌﾌﾌf8 ﾌ8*  p            ｨ*        ﾑ>ﾘ@      ﾞ ﾘ@    ・・ﾘ@
ｽeﾘ@      ﾑﾚﾗ@    瑾ﾘ@     phﾘ@    ・{｀ﾘ@    ﾀ8ｱﾘ@    ﾀh湍@    ・←華@      1Hﾘ@      ~瞹@    @7
↕ﾘ@    ﾀﾈｮﾗ@    @j､ﾗ@    `DZﾗ@      >ﾗ@      !@ﾗ@
・ﾛｴ@      Nｴｴ@    @:葷@     瑜ｴ@    ・鰒@     ｀・@    ｀¶袒@    @z ﾗ@      ｮ・@      聡ｴ@
・ﾚｴ@    療ﾓｴ@    ・+ﾕｴ@     ・ｴ
...
```

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
        `   ┼                        '            chn e~1\sar ni~2
2005\06c/s05\XPS2.PCS f8 €^  p                      °³@     à³@     ¶´@     `³@
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
    ┘   €   ┼                       Ý|          pts     sar             c/s
f8  è.  ▪               ┐           ┐       -          pts     sar
c/s             f8  h     x0                └           └        -           pts
sar             c/s             f8  h       à9                ┘           ┘        -
          pts     sar             c/s              f8  h     HC
À‰Ú@      Ú@    À¬Ú@    €_Û@     ◘Û@     ŸÚ@    @ Ú@    À‰Ú@    ÀÛ@    €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 Vl1s 112 401 -0.1250 30.0 -20.0 30.0 -20.0    1.200000
69.00 AREA
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (21339.2 37232.7 24019.0 45.0 0.0)
SpatialAreaDesc: 1 sample-A
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH
    −   @┐  ┼                        ‘           pnt ª~o¤sar ┘      k¤h
Ï c/s Té↨ ┘   Ä¢r¤f8  ˆ
...  P┐          Ø
...
```

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⌘sar ┘     *k⌘h
È c/s Té↨ ┘    ìÂr⌘f8  h"  p           Ø"      € å@     ↑å@     ¯ä@    @ûä@
  €└å@    @çä@    àûä@    @⌘å@    ÀRå
...
```

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
    ┘    €   ┼                        È           pnt ┘    sar ´þ↑     ┐   c/s  ┼
 ┘   f4    └  ▪                ┐            ┐       È           pnt ┘    sar ´þ↑
...
```

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@    €┴Éf8  (└  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 O1s 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000
0.600000 23.50 HEIGHT
SpectralRegDef2: 2 20.0 1 0 6 500
SpectralRegBackground: 2 0.0 533.0 0.0
SpectralRegHero: 2 533.0 0.0 0.0 0.00
SpectralRegIR: 2 0 0.000 0.000 0.0
SpectralRegDef: 3 1 Si2s 14 101 -0.2000 163.0000 143.0000 162.0000 144.0000
10.500000 23.50 HEIGHT
SpectralRegDef2: 3 20.0 3 0 6 500
SpectralRegBackground: 3 0.0 153.0 0.0
SpectralRegHero: 3 153.0 0.0 0.0 0.00
SpectralRegIR: 3 0 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 1 4 (-4373.3 -5907.8 16187.4 45.0 -0.1) (-3073.3 -5907.8
16187.4 45.0 -0.1) (-3073.3 -5507.8 16187.4 45.0 -0.1) (-4373.3 -5507.8
16187.4 45.0 -0.1)
SpatialAreaDesc: 1 Tool matching VP II
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 6
XrayPower: 90.80 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 20000.0 V
XRayCondenserLensVoltage: 9550.0 V
XRayObjectiveCoilCurrent: 0.938 A
XRayBlankingVoltage: 430.0 V
XRayFilamentCurrent: 1.645 A
XRayStigmator: 0.0 0.0
XRayHighPower: yes
EgunNeutMode: Neutralize
NeutralizerCurrent: 20.0 uA
NeutralizerEnergy: 3.00 V
EgunNeutExtractor: 40.0 V
EgunNeutXSteering: 0.0
EgunNeutYSteering: -3.0
EgunNeutFilament: 0.90 A
EgunNeutPulseLength: 50.0 msec
SxiPersistence: 4 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 534.0 eV
SxiPassEnergy: 376 eV
SxiLens2: -711 V
SxiLens3: -673 V
SxiLensBias: 200 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 439.8 V
SxiDisplayMode: 0
Detector Acq Time: 100.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.600
Channel Info: 2 1 1.237
Channel Info: 3 1 1.144
Channel Info: 4 1 1.112
Channel Info: 5 1 1.029
Channel Info: 6 1 0.973
Channel Info: 7 1 0.953
Channel Info: 8 1 0.959
Channel Info: 9 1 1.096
Channel Info: 10 1 1.081
Channel Info: 11 1 0.916
```

```
Channel Info: 12 1 0.804
Channel Info: 13 1 0.770
Channel Info: 14 1 0.722
Channel Info: 15 1 0.750
Channel Info: 16 1 0.820
StagePosition: -4.2486 6.0367 16.1874 45.0031 -0.0500
StageCurrentRotationSpeed: 1.0000
DefectPosID: 1
DefectPosComment: Tool matching VP II
DefectPosU: -3.7246
DefectPosV: 5.7082
DefectPosX: -4.2486
DefectPosY: 6.0367
DefectPosZ: 16.1874
DefectPosTilt: 45.0031
DefectPosRotation: -0.0500
DefectPosAligment: None
DefectPosReferenceImage: SiO2_25nm_01.101.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 23.50 eV
XRaySetting: 100u100W_HP
EOFH
    └       ┼
...
```

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 O1s 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000
0.000000 46.95 AREA
SpectralRegDef2Full: 2 20.0 1 0 4 1
SpectralRegBackgroundFull: 2 0.0 533.0 0.0
SpectralRegHeroFull: 2 533.0 0.0 0.0 0.00
SpectralRegDefFull: 3 1 La3d5 57 126 -0.2000 850.0000 825.0000 849.0000 826.0000
0.000000 46.95 AREA
SpectralRegDef2Full: 3 25.0 1 0 4 1
SpectralRegBackgroundFull: 3 0.0 837.5 0.0
SpectralRegHeroFull: 3 837.5 0.0 0.0 0.00
NoSpectralReg: 3
SpectralRegDef: 1 1 F1s 9 101 -0.2000 699.0000 679.0000 698.0000 680.0000
0.200000 46.95 AREA
SpectralRegDef2: 1 20.0 1 0 4 1 0.00
SpectralRegBackground: 1 0.0 689.0 0.0
SpectralRegHero: 1 689.0 0.0 0.0 0.00
```

```
SpectralRegDef: 2 1 O1s 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000
0.200000 46.95 AREA
SpectralRegDef2: 2 20.0 1 0 4 1 0.00
SpectralRegBackground: 2 0.0 533.0 0.0
SpectralRegHero: 2 533.0 0.0 0.0 0.00
SpectralRegDef: 3 1 La3d5 57 126 -0.2000 850.0000 825.0000 849.0000 826.0000
0.200000 46.95 AREA
SpectralRegDef2: 3 25.0 1 0 4 1 0.00
SpectralRegBackground: 3 0.0 837.5 0.0
SpectralRegHero: 3 837.5 0.0 0.0 0.00
NoSpatialArea: 1
SpatialAreaDef: 1 1 1 (10354.5 2256.9 18760.0 45.0 -90.0)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 0
XrayPower: 25.61 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 15000.0 V
XRayCondenserLensVoltage: 8230.0 V
XRayObjectiveCoilCurrent: 0.748 A
XRayBlankingVoltage: 325.0 V
XRayFilamentCurrent: 1.577 A
XRayStigmator: 0.0 0.0
XRayHighPower: no
EgunNeutMode: Neutralize
NeutralizerCurrent: 0.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 40.0 V
EgunNeutXSteering: 1.0
EgunNeutYSteering: 4.0
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 694.0 eV
SxiPassEnergy: 188 eV
SxiLens2: -591 V
SxiLens3: -560 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 349.9 V
SxiDisplayMode: 1
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.698
Channel Info: 2 1 1.467
Channel Info: 3 1 1.392
Channel Info: 4 1 1.320
Channel Info: 5 1 1.251
Channel Info: 6 1 1.103
Channel Info: 7 1 1.074
Channel Info: 8 1 1.026
Channel Info: 9 1 1.001
Channel Info: 10 1 0.941
Channel Info: 11 1 0.824
Channel Info: 12 1 0.819
Channel Info: 13 1 0.750
Channel Info: 14 1 0.650
Channel Info: 15 1 0.674
Channel Info: 16 1 1.266
StagePosition: -2.6672 -9.4501 18.7598 45.0094 -90.0500
StageCurrentRotationSpeed: 0.6700
```

```
DefectPosID: 1
DefectPosComment:
DefectPosU: 10.3546
DefectPosV: -2.2577
DefectPosX: -2.6672
DefectPosY: -9.4501
DefectPosZ: 18.7598
DefectPosTilt: 45.0094
DefectPosRotation: -90.0500
DefectPosAligment: None
DefectPosReferenceImage: 120530.20.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
    |   à   ┼                       e   ┴       pnt     cyc             c/s
ñDnw|   ◘   f4 5$!  ð               ┐           ┐       e   ┴       pnt     cyc
...
```

Software Version 4: XPS V1.30

- Example. sputter depth profile with 41 sputter steps (sputter time: 30 s, -30 ... 1170) and 6 regions: C 1s, O 1s, Ni $2p_{3/2}$, Fe $2p_{3/2}$, Cr $2p_{3/2}$, Mo 3d,
- Folder: Install-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
    ◘    └  ┼                  ◘   )   ¯       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
    ◘    └  ┼                    ◘
   ¯       cyc ┐┐┐┐reg ┐┐┐┐ ┐┐┐┐┐┐┐s ┐┐┐┐┐┐┐┐┐┐┐┐┐┐┐f8 ┐┼┐  ┼└  ┐            ┐
      ┐
...
```

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
c/s * eV        f8  ↑   È└               └                     ‡   •       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
DefectPosAligment: None
DefectPosReferenceImage: 20kV.1.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 200u50W15KV
EOFH
    |   à   ┼                          ¡   H        pnt      cyc              c/s
ñDNv|   ◘   f4 1 µ  ð               ┐           ┐        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: 1400.0000000
EBeamCurrent: -2.2 nA
ImageSizeXY: 1400.0000 200.0000
IonGunMode: Neutralize
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 0.110 kV
FloatVolt: -100.0 V
FloatEnable: yes
GridVolt: 120.0
CondensorVolt: 69.30
ObjectiveVolt: 101.20
BendVolt: 1.43
SputterRaster: 0.00 0.00 mm
SputterRasterOffset: 1.950 -0.200 mm
TargetSputterTime: 10.0 min
SputterEmission: 7.00 mA
DeflectionBias: 71.0 V
XpsScanMode: scanned
AnalyserMode: FAT
SurvNumCycles: 15
SurvTimePerStep: 50.000000
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2197 3136
PhotoOffsetInPixel: 1519 200
PhotoSizeInMm: 35.000 50.000
PhotoOffsetInMm: -38.354 -50.000
NoSpectralRegFull: 1
SpectralRegDefFull: 1 1 survey 111 938 -0.8000 745.0000 -5.0000 744.0000 -4.0000
0.000000 187.85 AREA
SpectralRegDef2Full: 1 750.0 1 0 1 1
SpectralRegBackgroundFull: 1 0.0 370.0 0.0
SpectralRegHeroFull: 1 370.0 0.0 0.0 0.00
SpectralRegIRFull: 1 0 0.000 0.000 0.0
NoSpectralReg: 1
```

```
SpectralRegDef: 1 1 survey 111 938 -0.8000 745.0000 -5.0000 744.0000 -4.0000
0.750000 187.85 AREA
SpectralRegDef2: 1 750.0 1 0 1 1
SpectralRegBackground: 1 0.0 370.0 0.0
SpectralRegHero: 1 370.0 0.0 0.0 0.00
SpectralRegIR: 1 0 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 13 4 (8215.5 5905.4 19312.7 46.0 -90.1) (9615.5 5905.4 19312.7
46.0 -90.1) (9615.5 6105.4 19312.7 46.0 -90.1) (8215.5 6105.4 19312.7 46.0 -
90.1)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 1
XrayPower: 92.65 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 20000.0 V
XRayCondenserLensVoltage: 9250.0 V
XRayObjectiveCoilCurrent: 0.929 A
XRayBlankingVoltage: 400.0 V
XRayFilamentCurrent: 1.621 A
XRayStigmator: 0.0 0.0
XRayHighPower: yes
EgunNeutMode: Neutralize
NeutralizerCurrent: 20.0 uA
NeutralizerEnergy: 1.01 V
EgunNeutExtractor: 50.0 V
EgunNeutXSteering: 2.0
EgunNeutYSteering: 4.1
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 534.0 eV
SxiPassEnergy: 188 eV
SxiLens2: -711 V
SxiLens3: -673 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 342.0 V
SxiDisplayMode: 1
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.661
Channel Info: 2 1 1.490
Channel Info: 3 1 1.499
Channel Info: 4 1 1.268
Channel Info: 5 1 1.149
Channel Info: 6 1 1.100
Channel Info: 7 1 1.148
Channel Info: 8 1 1.079
Channel Info: 9 1 1.118
Channel Info: 10 1 1.021
Channel Info: 11 1 0.942
Channel Info: 12 1 0.803
Channel Info: 13 1 0.730
Channel Info: 14 1 0.627
Channel Info: 15 1 0.634
Channel Info: 16 1 1.028
StagePosition: -5.8668 -8.6215 19.3127 46.0031 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 13
DefectPosComment:
```

```
DefectPosU: 8.9165
DefectPosV: -6.0062
DefectPosX: -5.8668
DefectPosY: -8.6215
DefectPosZ: 19.3127
DefectPosTilt: 46.0031
DefectPosRotation: -90.0500
DefectPosAligment: None
DefectPosReferenceImage: 140420.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 100u100W20kV_HP
EOFH
        `   ┼                        ªL          pnt     sar     äéè¯_ä@c/s  □¸¤
...
```

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
DefectPosAligment: None
DefectPosReferenceImage: 120749.17.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
    ◘     └  ┼                        L   ¤       pnt     ang             c/s ñD—
w│   ◘    f4 ;Ð◄  ┼└
...
```

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

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f8  À   Ð└ ┐           ┐               ┐   └   ◘       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 Area1 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
    ◘    └  ┼                   ◘   |   –       ang ÌÌÌÌreg ÌÌÌÌ ÌÌÌÌÌÌÌÌdeg ÌÌÌÌ
ÌÌÌÌÌÌÌÌf8 Ìğ   ┼└  ┐           ┐               ┐   |   –       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
    •    ┐  ┼                        ¡   │        pnt ↑ ↑ ang      A→     c/s Ð
Ìú↑ f4  ”
...
```

3.1.20.4 PHI Spectrometer/Mapping (*.map)

Comment:

- With respect to the multi region files (*.spe) the header contains additional profile and mapping information (e.g. angle values, number and position of mappimg 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
DefectPosAligment: None
DefectPosReferenceImage: ASKim150122-1.13.sxi
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 10u1.25W15KV
EOFH
    ┐   À   ┼                    ┘   ö
...
```

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: 1000.0000000
EBeamCurrent: -2.2 nA
ImageSizeXY: 1000.0000 1000.0000
IonGunMode: Off
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 0.100 kV
FloatVolt: 0.0 V
FloatEnable: no
GridVolt: 150.0
CondensorVolt: 71.00
ObjectiveVolt: 68.50
BendVolt: 1.50
SputterRaster: 3.00 3.00 mm
SputterRasterOffset: 0.000 0.000 mm
TargetSputterTime: 10.0 min
```

```
SputterEmission: 0.00 mA
DeflectionBias: 0.0 V
XpsScanMode: unscanned
AnalyserMode: FAT
SurvNumCycles: 1
SurvTimePerStep: 1000.000000
NoMapPixelsXY: 256 256
MapFramesPerFCC: 1
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2197 3136
PhotoOffsetInPixel: 1519 200
PhotoSizeInMm: 35.000 50.000
PhotoOffsetInMm: -38.354 -50.000
NoSpectralRegFull: 2
SpectralRegDefFull: 1 1 Al2p 13 16 -1.0000 81.5000 66.5000 80.0000 68.0000
0.000000 117.40 AREA
SpectralRegDef2Full: 1 15.0 5 0 1 1
SpectralRegBackgroundFull: 1 0.0 74.0 0.0
SpectralRegHeroFull: 1 74.0 0.0 0.0 0.00
SpectralRegIRFull: 1 0 0.000 0.000 0.0
SpectralRegDefFull: 2 0 Mn2p3 25 16 -1.0000 648.5000 633.5000 647.0000 635.0000
0.000000 117.40 AREA
SpectralRegDef2Full: 2 15.0 10 0 1 1
SpectralRegBackgroundFull: 2 0.0 641.0 0.0
SpectralRegHeroFull: 2 641.0 0.0 0.0 0.00
SpectralRegIRFull: 2 0 0.000 0.000 0.0
NoSpectralReg: 1
SpectralRegDef: 1 1 Al2p 13 16 -1.0000 81.5000 66.5000 80.0000 68.0000 0.200000
117.40 AREA
SpectralRegDef2: 1 15.0 5 0 1 1
SpectralRegBackground: 1 0.0 74.0 0.0
SpectralRegHero: 1 74.0 0.0 0.0 0.00
SpectralRegIR: 1 0 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 10 4 (9787.3 7171.0 11701.4 46.0 -90.1) (10787.3 7171.0
11701.4 46.0 -90.1) (10787.3 8171.0 11701.4 46.0 -90.1) (9787.3 8171.0 11701.4
46.0 -90.1)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 3
XrayPower: 0.98 W
XrayBeamDiameter: 5.0 um
XRayBeamVoltage: 15000.0 V
XRayCondenserLensVoltage: 11850.0 V
XRayObjectiveCoilCurrent: 0.723 A
XRayBlankingVoltage: 325.0 V
XRayFilamentCurrent: 1.577 A
XRayStigmator: 0.0 0.0
XRayHighPower: no
XrayScanIncXY: 3.906250 3.906250 um
EgunNeutMode: Off
NeutralizerCurrent: 1.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 30.0 V
EgunNeutXSteering: 0.0
EgunNeutYSteering: 0.0
EgunNeutFilament: 1.11 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 1458.6 eV
SxiPassEnergy: 376 eV
```

```
SxiLens2: 476 V
SxiLens3: 406 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 342.0 V
SxiDisplayMode: 2
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.661
Channel Info: 2 1 1.490
Channel Info: 3 1 1.499
Channel Info: 4 1 1.268
Channel Info: 5 1 1.149
Channel Info: 6 1 1.100
Channel Info: 7 1 1.148
Channel Info: 8 1 1.079
Channel Info: 9 1 1.118
Channel Info: 10 1 1.021
Channel Info: 11 1 0.942
Channel Info: 12 1 0.803
Channel Info: 13 1 0.730
Channel Info: 14 1 0.627
Channel Info: 15 1 0.634
Channel Info: 16 1 1.028
StagePosition: -7.5750 -9.9215 11.7014 46.0000 -90.1000
StageCurrentRotationSpeed: 0.6700
DefectPosID: 10
DefectPosComment:
DefectPosU: 10.2873
DefectPosV: -7.6710
DefectPosX: -7.5750
DefectPosY: -9.9215
DefectPosZ: 11.7014
DefectPosTilt: 46.0000
DefectPosRotation: -90.1000
DefectPosAligment: None
DefectPosReferenceImage: 140438.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 9u1.0W15KV
EOFH
    ┐   À   ┼                    ┘                pnt     pnt      ‹Ù¼ `ä@    c/s
    f4     ┘ Ð               ┐                    ┼           chn     pnt
...
```

3.1.21 Focus CSA (*.dat)

Comment:

- the header includes the acquisition parameters
- data: 1. column: energy, 2. column: intensities, 3.-5. column: data for normalization
- after [DATA] intensities of the sum spectrum
- from [DATA 1] to [DATA 20] intensities of the single scans
- Example. valence band, 20 scans
- Folder: Install-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 (*.pesp)

Comment:

- Measurement data format of the Universiy 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[HWType 31:60, 32:63, 33:64,
                     542:511] DLD
# Analyzer Lens:     SmallArea:3.5kV
# Analyzer Slit:     4:3x20\2:open
# Scan Mode:         FixedAnalyzerTransmission
# Number of Scans:   1
# Curves/Scan:       1
# Values/Curve:      2008
# Dwell Time:        0.3
# Excitation Energy: 5900
# Kinetic Energy:    4900
# Pass Energy:       40
# Bias Voltage:      50
# Detector Voltage:  2650
# Eff. Workfunction: 4.658
# Source:            UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
4900  1090
4900.5  1063.3333
...
5903  0
5903.5  0

# values in kinetic energy
# Region:            VB
# Analysis Method:   UPS
# Analyzer:          PHOIBOS HSA15000 DLD 225 R6-HV[HWType 31:60, 32:63, 33:64,
                     542:511] DLD
```

```
# Analyzer Lens:     SmallArea:1.5kV
# Analyzer Slit:     4:3x20\2:open
# Scan Mode:         FixedAnalyzerTransmission
# Number of Scans:   5
# Curves/Scan:       1
# Values/Curve:      281
# Dwell Time:        2
# Excitation Energy: 5900
# Kinetic Energy:    5890
# Pass Energy:       20
# Bias Voltage:      50
# Detector Voltage:  2650
# Eff. Workfunction: 4.658
# Source:            UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
5890  17.5
5890.05  25.5
...
5903.95  1.5
5904  0

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

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

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

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

```
5904  2.5

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

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

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

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

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

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

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

```
5903.95  1
5904  2

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

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

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

3.1.25 Energy-Intensity (*.dat)

Comment:

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

- Only one region seved 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 manuelly

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 enenry, pass energy, dwell time, comment, step width
- Deciaml delimiter: comma
- Columns: 1. kinetic energies, 2. binding energies, 3.sum of scans, 4. - n. intensities of the scans
- Scan direction: increasing kinetic energies
- Only one region seved in the data file
- Peak name, number of scans, analyser mode, x position, y position has to be defined manuelly

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

Kommentar:
Probe auf altem Halter

Messwerte:
kin. Energie      Bindungsenergie   Scan Summe  Scans    (Counts    pro    Sekunde)
      Scan 1      Scan 2      Scan 1 (Counts pro Sekunde)   Scan  2  (Counts  pro
Sekunde)
[eV]  [eV]  [1/eV]      [1/(s*eV)]  [1/eV]      [1/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
      Cold Cathode Gauge      SR Energy
19:44:21    4.61600000  334.98152024      246.03768190      1.00000000
      0.32811574  0.00000000  217188.00000000   286835.00000000   0.00000000
      0.00000000  0.00000000  0.00000000  0.00000000  0.00000000  0.00000000
      0.00000000  0.00000000  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  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  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  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
```

```
6
1st block id
1st sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
C

-1
kinetic energy
eV
245.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.0
1110704128.0
270
0.0
0
48
88991
92272
89655
89357
...
91940
92057
92272
2nd block id
2nd sample id
2011
8
15
12
0
45
9
0
```

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

-1
kinetic energy
eV
454.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.000000
1.10625e+009
270
0
0
86
110295
123403
110295
110499
...
114918
114537
3rd block id
3rd sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
```

```
0.0
0.0
0.000000
0.000000
55.0
270.0
Mg

-1
kinetic energy
eV
1139.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
5
0.000000
1.10625e+009
270
0
0
64
154883
160094
154958
...
157743
157784
4th block id
4th sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
Al

-1
kinetic energy
eV
1347.000000
1.000000
```

```
1
Intensity
c/s
pulse counting
0.100000
5
0.000000
1.10625e+009
270
0
0
61
169114
172551
169114
...
171943
172261
5th block id
5th sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
Si

-1
kinetic energy
eV
1570.000000
1.000000
1
Intensity
c/s
pulse counting
0.100000
6
0.000000
1.10625e+009
270
0
0
75
185302
```

```
190447
185302
185576
...
189879
189924
6th block id
6th sample id
2011
8
15
12
0
45
9
0
AES dir
0
electron gun
10000
10.349999
0.000000
0.000000
0.0
0.0
FRR
1.700000
3.0
0.0
0.0
0.000000
0.000000
55.0
270.0
Pb

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

3.3.2 PHI Spectrometer

Comment:

- Header in ASCII from SOFH to EOFH

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

3.3.2.1 Multiregion Measurements (*.spe)

Software Version 1: Without software specification

- Example PHI 700. multiregion measurement, 4 regions (C, O, Fe, Ni)
- Folder: Install-USB-Memory-Card:\AES_Measurement_Reference_Data\ 03-PHI-NORM(.SPE)\PHI-MultiReg-V1-without_software_specification-PHI-700-C-O-Fe-Ni.SPE

```
SOFH
Platform: PC
Technique: AES
FileType:  SPECTRUM
FileDesc: Stainless Steel
AcqFilename: C:\Datafiles\StainlessSteel\Stahl.101.spe
FileDate: 2011 5 2
AcqFileDate: 2011 5 2
Institution: PHI
Operator: phiuser
ExperimentID: IntroPhoto
EnergyReference: none 0.0
RegisterImage: no
RegImageInterval: 1
RegImageMode: 1
NegativeData: yes
PlatenID: apr26a
PhotoFilename:
SXIFilename:
HERO Mode: no
EBeamScanIncXY: 1.73007813 1.29755860 um
SemFieldOfView: 885.8000040
ImageShift: 0.000 0.000
Focus: 50.000 V
Stigmation: -0.3 -6.9
Rotation: 0.0
Tilt: 0.0
Detector: 1
BseEnergy: 0.0
AesMultiplier: 2150.0 V
Contrast: 15.0
Brightness: 50.0
Gamma: 0.0
DcOffset: 50.0
InverseVideo: no
HoldImage: no
VideoCalibrate: no
PseudoColor: no
EBeamEnergy: 10.0 kV
EBeamCurrent: (null)
ExtractorSteering: -1.2 2.9
FocusSteering: -4.4 -16.7
GunLensVoltage: 0.510
ImageSizeXY: 100.0000 75.0000
IonGunMode: Blank
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 150.000 A/min
SputterEnergy: 2.000 kV
```

```
FloatVolt: 0.0 V
FloatEnable: no
GridVolt: 150.0
CondensorVolt: 1518.00
ObjectiveVolt: 1475.00
BendVolt: 75.00
SputterRaster: 1.00 1.00 mm
SputterRasterOffset: 0.050 -0.510 mm
TargetSputterTime: 0.5 min
SputterEmission: 15.00 mA
DeflectionBias: 0.0 V
ScanMode: scan
AnalyserMode: FRR
MultNumCycles: 30
MultTimePerStep: 20.000000
NumSpatialLines: 3
SpatialLine: 1 1 1 251.0 251.0
SpatialLine: 2 1 1 68.0 68.0
SpatialLine: 3 1 1 318.0 318.0
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2570 2660
PhotoOffsetInPixel: 778 56
PhotoSizeInMm: 57.702 59.690
PhotoOffsetInMm: -50.000 -50.000
NoSpectralRegFull: 4
SpectralRegDefFull: 1 1 C1 6 0 1.0000 231.0 311.0 249.0 283.0 0.000000 0.00 none
SpectralRegDef2Full: 1 80.0 5 8 1 1
SpectralRegBackgroundFull: 1 243.0 266.0 287.0
SpectralRegHeroFull: 1 266.0 266.0 0.0 0.50
SpectralRegDefFull: 2 1 O1 8 0 1.0000 472.0 552.0 490.0 524.0 0.000000 0.00 none
SpectralRegDef2Full: 2 80.0 5 8 1 1
SpectralRegBackgroundFull: 2 496.0 507.0 525.0
SpectralRegHeroFull: 2 507.0 507.0 0.0 0.50
SpectralRegDefFull: 3 1 Fe2 26 0 1.0000 612.5 672.5 630.5 664.5 0.000000 0.00
none
SpectralRegDef2Full: 3 60.0 10 8 1 1
SpectralRegBackgroundFull: 3 616.0 647.0 669.0
SpectralRegHeroFull: 3 647.0 266.0 0.0 0.50
SpectralRegDefFull: 4 1 Ni1 28 0 1.0000 811.0 871.0 829.0 863.0 0.000000 0.00
none
SpectralRegDef2Full: 4 60.0 20 8 1 1
SpectralRegBackgroundFull: 4 827.0 846.0 873.0
SpectralRegHeroFull: 4 846.0 266.0 0.0 0.50
NoSpectralReg: 4
SpectralRegDef: 1 1 C1 6 81 1.0000 231.0 311.0 249.0 283.0 0.300000 0.00 none
SpectralRegDef2: 1 80.0 5 8 0 0 0.00
SpectralRegBackground: 1 243.0 266.0 287.0
SpectralRegHero: 1 266.0 266.0 0.0 0.50
SpectralRegDef: 2 2 O1 8 81 1.0000 472.0 552.0 490.0 524.0 0.300000 0.00 none
SpectralRegDef2: 2 80.0 5 8 0 0 0.00
SpectralRegBackground: 2 496.0 507.0 525.0
SpectralRegHero: 2 507.0 507.0 0.0 0.50
SpectralRegDef: 3 3 Fe2 26 61 1.0000 612.5 672.5 630.5 664.5 0.600000 0.00 none
SpectralRegDef2: 3 60.0 10 8 0 0 0.00
SpectralRegBackground: 3 616.0 647.0 669.0
SpectralRegHero: 3 647.0 266.0 0.0 0.50
SpectralRegDef: 4 4 Ni1 28 61 1.0000 811.0 871.0 829.0 863.0 1.200000 0.00 none
SpectralRegDef2: 4 60.0 20 8 0 0 0.00
SpectralRegBackground: 4 827.0 846.0 873.0
SpectralRegHero: 4 846.0 266.0 0.0 0.50
NumRefImages: 2
ImageReference: 1 1 1.0 0.0 0.0 0.0 0.0 0.0
ImageReference: 2 0 1.0 0.0 0.0 0.0 0.0 0.0
NumSpatialAreas: 1
SpatialArea: 1 1 1 257.9 261.6 467.9 444.6
DefectPosID: 0
```

```
DefectPosComment:
DefectPosU: -11.9814
DefectPosV: -0.2549
DefectPosX: -10.7949
DefectPosY: 0.2203
DefectPosZ: 15.0001
DefectPosTilt: 14.9875
DefectPosRotation: 1.0000
DefectPosRotationSpeed: 1.0000
DefectPosAligment:
DefectPosReferenceImage:
EOFH
    ┘   €   ┼                       Q           pnt     sar      O^f.Ûã@c/s àñ;
f4  D
...
```

3.3.2.2 PHI Spectrometer/Profile (*.pro)

Comment:

- With respect to the multiregion files (*.spe) the header contains additional profile information (e.g. number of parameter steps, sputter time)
- Example PHI 680. multiregion measurement, 4 regions (C, O, Fe, Ni)
- Folder: Install-USB-Memory-Card:\AES_Measurement_Reference_Data\05-PHI-Profile(.PRO)\ PHI-Profile-V1-without_software_specification-PHI680-SiO2

```
SOFH
Platform: PC
Technique: AES
FileType:  DEPTHPRO
FileDesc: 55 nm SiO2 0.5kV 0,5 uA 1x1
FileDate: 113 11 22
AcqFileDate: 113 11 22
AcqFilename: SiO2104.pro
ScanMode: scan
EBeamEnergy: 10.0 keV
EBeamCurrent: 0.000000e+00 A
EBeamDiameter: 0.00 nm
SourceAnalyserAngle: 0.0 d
AnalyserMode: FRR
AnalyserWorkFcn: 4.5 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon:
SputterEnergy: 2.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 1 s
PreAcqSputterRate: 1.0 A/s
NoSpectralReg: 4
SpectralRegDef: 1 1 Si4 14 41 1.0000 1590.0 1630.0 1590.0 1620.0 0.100000 0.00
none
SpectralRegDef: 2 2 O1 8 41 1.0000 487.0 527.0 490.0 524.0 0.100000 0.00 none
SpectralRegDef: 3 3 Si1 14 41 1.0000 73.0 113.0 76.0 110.0 0.100000 0.00 none
SpectralRegDef: 4 4 C1 6 41 1.0000 246.0 286.0 249.0 283.0 0.100000 0.00 none
NoDPDataCyc: 60
NoPreSputterCyc: 2
SputterInterval: 0.500 s
SputterMode: alt
SampleRotation: off
DepthRecal: no
EBeamScanIncXY: 6.3826 4.8189 um
```

```
Magnification: 122.4
NoSpatialArea: 1
SpatialAreaDef: 1 Full 1 (0.0 0.0 0.0 0.0 0.0)
EOFH
    −   @┐  ┼                        )   <       pnt øëý cyc @    úî l
ñwc/s @   Äúî Ôúî f4  p&  P┐
...
```

3.3.2.3 PHI Spectrometer/Mapping (*.map)

Comment:

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

Software Version 1: Without software specification

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

```
SOFH
Platform: PC
Technique: AES
FileType:  MAP
FileDesc: Pad 41
SoftwareVersion:
Institution: PHI
FileDate: 112 9 22
AcqFileDate: 2012 9 22
ScanMode: scan
AcqFilename: C:\Datafiles\IC.412~2_1.map
Operator:
ExperimentID: Pad_41
StagePosition: 0.0000 0.0000 0.0000 0.0000 0.0000
PhotoFilename:
SXIFilename:
EBeamEnergy: 10.0 kV
EBeamCurrent: 10.00 nA
EBeamDiameter: 0.0
NeutralizerEnergy: 0.0
NeutralizerCurrent: 0.0
SourceAnalyserAngle: 0.0 d
AnalyserSolidAngle: 0.0 sr
AnalyserMode: FRR
AnalyserWorkFcn: 3.8 eV
IntensityCalCoeff: 0.000 0.000
SputterIon: Ar+
SputterEnergy: 2.000 kV
SputterCurrent: 0.0 uA
SputterRaster: 2.0 2.0 mm
PreAcqSputterTime: 0
PreAcqSputterRate: 0.0
NoSpectralReg: 1
SpectralRegDef: 1 1 Si4 14 51 0.5000 1628.00000 1603.00000 1627.00000 1604.00000
0.000000 0.00 PEAK_TO_PEAK
ImageParam: 1 1.0000 7465.28 32297.05 7465.28 32297.05
NoMapPixelsXY: 256 256
EBeamScanIncXY: 0.7813 0.7813 um
Magnification: 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 -1 1 (-495.6 -15.3 16854.5 0.0 315.1)
SpatialAreaDesc: 1
NoHistory: 1
History: 1 SPEC 1 -1 ""
EOFH
```

```
    ┘    €    ┼                    ┘                pnt     pnt             c/s
f4
```

3.4 RAMAN Data

3.4.1 S_I VistaComtrol (*.tvf)

Comment:

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

3.4.2 S_I VistaComtrol XY Multipoint/Batch Parameter Measurement (*.csv)

Comment:

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

1. Batch-Parameter measrement

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

```
Frame 1
44.475;605.000
46.007;616.000
47.540;606.000
49.072;609.000

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

Frame 2
44.475;599.000
46.007;616.000
47.540;622.000
49.072;595.000
50.603;596.000
52.136;615.000
53.667;614.000
55.199;617.000
...
2221.600;5628.000
```

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

Frame 3
44.475;614.000
46.007;615.000
47.540;611.000
49.072;613.000
50.603;611.000
52.136;602.000
53.667;612.000
55.199;624.000
...
2228.932;3034.000
2230.154;3133.000
2231.374;2935.000
2232.597;2943.000

Frame 300
44.475;594.000
46.007;590.000
47.540;607.000
49.072;580.000
50.603;574.000
52.136;587.000

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

2. XY multipoint measurement

- Examples includes 10201 spectra (101x101 frames)
- Batch parameter: Frame number or x|y values generated from the frame number
- Following acqisition 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 aqcusition parameters are available: Name of the reference sample, chemical informations
- Examples saved on the USB memory installation card: RAMAN_Measurement_Referecnce_Data\ 04-RRUFF(.TXT)\ Magnetite__R060191-3__Raman__514__0__ccw__Raman_Data_RAW__29858.txt

```
##NAMES=Magnetite
##RRUFFID=R060191
##IDEAL CHEMISTRY=Fe^2+^Fe^3+^_2_O_4_
```

```
##LOCALITY=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 formatl: 1. column: wavelength (increasing or decreasing), 2. column: intensities
- No aqcusition 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 specta 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 availble 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 wisth of exported data: 0.01 eV,
- Not available intensities are interpolated,
- 1. row: energy, series name of spectrum 1, series name spectrum 2, …,
- 1. column: energy, 2-13 columns: intensities

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

4.1.1.5 Parameter Plot

Comment:

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

```
Energy      0     1     2     3     ...   9     10

Parameter C1s Peak1  O1s Peak1  O1s Peak2  Si2p Peak1  Si2p Peak2  Si2p Peak3
0     199.999999999994  1.00000000000031  999.99999999999   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  999.99999999999   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 ratiol 1. peak 1. doublet,
5. column: Lorentzian mixing ratio 2. peak 1. doublet
...
12. column: intensity 1. peak 2. douublet
…
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_2017_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_2017_User_Files\examples\Calibration_Intensity_Cu.ufp
- Example of 3 lines (Cu 2p, Cu 3p and survey), Cu 2p3 and Cu 3p fitteted, project comment, quantification
- Data structure: ,space’+,Auger parameter’+,=’+,position photoelectron peaks as BE’+,+’+,position Auger peak as KE’+,space’+,space’+,name of Auger parameter’

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frei
Calibration of intensity scale
```

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Acquisition conditions:
Twin, LAX, 50eV pass
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FAT

3-5-2004

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Kurve 1
Kurve 2
Kurve 3
Kurve 4
Kurve 5
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frei
frei
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 suctracted, 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_2017_User_Files\design\GaAs-survey.dsg

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Ga (L3M45M45)
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Ga 2p1
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As 2p3
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As 2p1
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Curve 285
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Curve 289
Curve 290
Curve 291
Curve 292
Curve 293
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_2017_User_Files\cross section*.cro
- example: estimated inelastic electron scattering cross section of SiO_2

```
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_2017_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-Intensitiy-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
```

5 Data Banks Integrated in UNIFIT

5.1 Auger Parameter (*.AUP)

Comment:
- Saved in Unifit_2017_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 Unidt_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  AgOOCCF3
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\sensifivity factors
- Example: Wagner factors
- If the file name starts with WAG, than the values are empirical data and the mean free path and transmission function in the quantification are setteled to one.

```
Sensitivity Factors
Ag3p3,1.52,Ag3d3,2.10,Ag3d5,3.10,Ag3d,5.20,Al2s,0.23,Al2p,0.185,Ar2s,0.4,Ar2p,0.
96,As3p1,0.97,As3d,0.53,As2p3,6.8
Au4d5,2.05,Au4f5,2.15,Au4f7,2.8,Au4f,4.95,B1s,0.13,Ba3d5,7.9,Ba4d,2.35,Be1s,0.05
9,Bi4d5,2.5,Bi4f5,3.15,Bi4f7,4.25
Bi4f,7.4,Bi5d,1.1,Br3p,0.14,Br3d,0.83,C1s,0.25,Ca2s,0.47,Ca2p1,0.53,Ca2p3,1.05,C
a2p,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,Cr
2p3,1.5,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,Er4
d,2.0,Eu3d,5.0,Eu4d,2.0,F1s,1.0,F2s,0.04
Fe2p1,1.0,Fe2p3,2.0,Fe2p,3.0,Fe3p,0.26,Ga2p3,5.4,Ga3p,0.84,Ga3d,0.31,Gd3d5,3.0,G
d4d,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,K2p1,0.4
1,K2p3,0.83,K2p,1.24,Kr3p1,0.39,Kr3p3,0.82
Kr3p,1.23,La3d,10.0,La4d,2.0,Li1s,0.02,Lu4p3,0.6,Lu4d,2.0,Mg1s,3.5,Mg2s,0.2,Mg2p
,0.12,Mn2p1,0.9,Mn2p3,1.7,Mn2p,2.6,Mn3p,0.22
Mo3p3,1.17,Mo3d3,1.09,Mo3d5,1.66,Mo3d,2.75,N1s,0.42,Na1s,2.3,Na2s,0.13,Nb3p3,1.1
,Nb3d3,0.96,Nb3d5,1.44,Nb3d,2.4
Nd3d,7.0,Nd4d,2.0,Ne1s,1.5,Ne2s,0.07,Ni2p1,1.5,Ni2p3,3.0,Ni2p,4.5,Ni3p,0.5,O1s,0
.66,O2s,0.25,Os4d3,0.85,Os4d5,1.75,Os4d,2.9
Os4f,3.5,P2s,0.29,P2p,0.39,Pb4d5,2.35,Pb4f5,2.95,Pb4f7,3.85,Pb4f,6.7,Pb5d,1.0,Pd
3p3,1.43,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,Rb
3p1,0.43,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,1.2
3,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,T
l4f,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,W4d3,1.0
3,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,Zn3
p,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. hights and energy-positions of the exitation satellites.
Comment:

- 1st row: name of satellite linie (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. hight of the satellite 1. set
- 4th row: energy position of the satellite 2. set
- 5th row: rel. hight 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
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 dounlet peaks.
Comment:

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

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

```
Mn2p,0.5,11.25,Mn3p,0.5,1.0,Mo3p,0.5,16.6,Mo3d,0.666,3.15,Nb3p,0.5,15.5,Nb3d,0.6
66,2.8,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,Pr4
d,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,Ti2
p,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 (AES-LinePositionsTargetIonisationSubshell.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 Coversion 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,Be1s
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)
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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
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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,Mb3d5
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
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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
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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
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```
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)
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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)
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```
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)
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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)
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Tl1,Tl(N6O45O45)
Tl2,Tl(N5N7O5)
Tl6,Tl(M5N5N5)
Tl5,Tl(M5N5N67)
Tl3,Tl(M5N67N67)
Tl4,Tl(M4N67N67)
Th1,Th(N6O3O5)
Th2,Th(N67O45V)
Th5,Th(M5N5N7)
Th3,Th(M5N7N7)
Th4,Th(M4N7N7)
Tm1,Tm(N45N67N67)
Tm4,Tm(M5N45N45)
Tm3,Tm(M45N45N67)
Tm2,Tm(M5N67N67)
Sn1,Sn(M5N45N45)
Sn2,Sn(L3M5M5)
Ti1,Ti(L3M23M23)
Ti2,Ti(L3M23M45)
W1,W(N4N7N7)
W5,W(N45O23O45)
W4,W(M5N5N5)
W3,W(M5N5N7)
W2,W(M5N67N67)
U1,U(OPV)
U2,U(N67O45V)
U5,U(M5N5N7)
U3,U(M5N7N7)
U4,U(M4N6N7)
V1,V(L3M23M23)
V2,V(L3M23M45)
Yb1,Yb(N5N67N67)
Yb4,Yb(M5N5N5)
Yb3,Yb(M45N45N67)
Yb2,Yb(M5N67N67)
Y1,Y(M45N23V)
Y4,Y(L3M23M45)
Y2,Y(L3M45M45)
Y3,Y(L2M45M45)
Zn4,Zn(LVV)
Zn3,Zn(L3M23M23)
Zn2,Zn(L3M23M45)
Zn1,Zn(L3M45M45)
Zr1,Zr(M45N23V)
Zr4,Zr(L3M3M45)
Zr2,Zr(L3M45M45)
Zr3,Zr(L2M45M5)
frei,frei
frei,frei
frei,frei
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