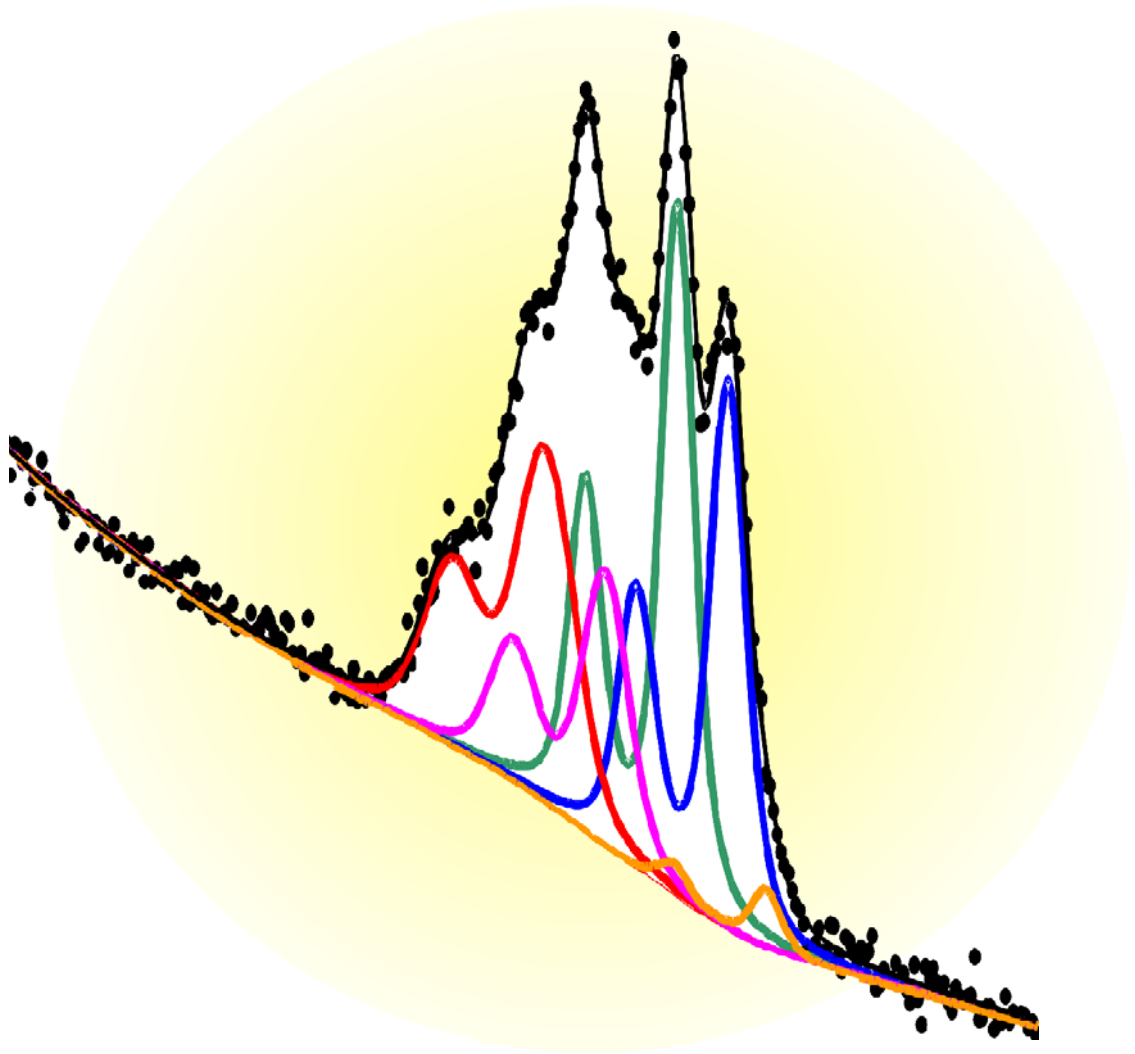


unifit FOR WINDOWS



Line Positions and Data Formats

Version 2016

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Unifit for Windows

Data Formats

Version 2016

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1 Line positions

All photoelectron lines are in BE, all Auger lines are in KE! [1, 2, 3] The main lines are marked by a star. The values are saved in the directories Unifit_2016_User_Files\lines. The second part gives the chemical shifts of some compounds.

line positions.pos

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

34 Eu 5s	56 Ag 4p3
34 Lu 5p1	56* Li 1s
35 La 5s	56* Se 3d
36 Mo 4p3	58 Au 5p3
36 Ce 5s	58 Lu 5s
36 Gd 5s	58 Fr 5d
37 Mo 4p1	59 Ti 3s
37 Sr 4s	60 Os 5p1
37 Hf 5p1	60* Co 3p
37 W 5p3	61 Nb 4s
37* V 3p	61 Er 5s
38 Pr 5s	61* Xe 4d5
38 Pm 5s	61* Ir 4f7
39 Tc 4p	61 Pt (N67O45O45)
39 Nd 5s	62 Ag 4p1
40 At 5d	63 Co 3p1
40 V 3p	63* Xe 4d3
40 Te 4d	63 Dy 5s
40 Ta 5p1	64 Mo 4s
40* Re 4f7	64* Ir 4f5
41 Sm 5s	64* Na 2s
41 As 3d	64 Hf 5s
41* Ne 2s	65 Hg 5p3
42 Cr 3p3	66 V 3s
42* Re 4f5	67* Ni 3p
42* As 3d	68 Cd 4p
43* Cr 3p	68 Ra 5d
44 Ca 3s	68 Tc 4s
45 Ru 4p	69* Br 3d
46 Y 4s	69 Ta 5s
46 Tb 5s	71* Au (N67O45O45)
47 W 5p1	71* Pt 4f7
48 Os 5p3	73* Al 2p
48 Rn 5d	74 Cr 3s
48* Mn 3p	74* Pt 4f5
49 Rh 4p	75* Hg (N7O45O45)
49* I 4d5	75 Cs 4d5
50* Mg 2p	75* Cu 3p3
51 Ho 5s	76 Tl 5p3
51 Po 5d	76 W 5s
51 Zr 4s	77* Cu 3p1
51* I 4d3	77 Ru 4s
51* Os 4f7	77* Cs 4d5
52 Pt 5p3	79 In 4p
53 Pd 4p	80* Cs 4d3
53 Ir 5p3	80 Ac 5d
53* Fe 3p	81 Hg (N6O45O45)
54 Se 3d	81 Re 5s
54 Tm 5s	83 Rh 4s
54* Os 4f5	83 Pb 5p3
55 Yb 5s	83 Mn 3s

84 Hg 5p1	120 Bi 5p1
84* Au 4f7	121* Nd 4d
86 Os 5s	122* Tl 4f5
86* Tl (N7O45O45)	122* Ge 3p3
87* Kr 3d	123 In 4s
87 Th 5d5	123 I 4p
87 Zn 3p3	123 Cu 3s
88 Tl (N6O45O45)	126* Ge 3p1
88 Pd 4s	127 Hg 5s
88* Au 4f5	127 Rn 5p3
89* Mg 2s	128* Eu 4d
89* Zn 3p3	129 Pm 4d
90* Ba 4d5	129* Sm 4d
91 Sn 4p	131* P 2p
91* Zn 3p1	132 Po 5p1
92 Fe 3s	133 Tl 5s
93* Ba 4d3	134* Sr 3d5
93 Pb (N7O45O45)	136* Sr 3d3
94 Bi 5p3	137 Sn 4s
94 Th 5d3	137* Pb 4f7
96* Pb (N6O45O45)	139 Xe 4p
98 Ag 4s	140 Fr 5p3
98 Ir 5s	140* Gd 4d
99* Si 2p	140 Zn 3s
100 Tl 5p1	141* As 3p3
100* Bi (N7O45O45)	142* Pb 4f5
101* Hg 4f7	146* As 3p1
101 La 4d5	146* Tb 4d
103* La 4d5	148 At 5p1
103 Co 3s	150 Pb 5s
104 Po 5p3	151* S (L23M23M23)
104* Ga 3p3	151* Si 2s
104 Bi (N6O45O45)	152* Dy 4d
104 Pt 5s	152 Th (N7O45O45)
105 Sb 4p	153 Sb 4s
105* Hg 4f5	153 Ra 5p3
106* La 4d3	156* Y 3d5
107* Ga 3p1	157* Bi 4f7
107 Pb 5p1	158* Y 3d3
109 Cd 4s	160* Ho 4d
109* Ce 4d5	160 Ga 3s
111 Au 5s	161 Bi 5s
111 Ni 3s	161 Cs 4p3
112* Rb 3d	162* Bi 4f5
112* Be 1s	163* Se 3p3
112* Ce 4d3	164* S 2p
114 Te 4p	164 Rn 5p1
115 At 5p3	167* Er 4d
115* Pr 4d	167 Ac 5p3
118* Tl 4f7	168* Nb (M45N23V)
118* Al 2s	169* Se 3p1

171 Te 4s	226 Th 5p1
173 Cs 4p1	228* S 2s
175* Tm 4d	228 Nd 4p3
177* B (KL23L23)	228* Mo 3d5
177 Po 5s	231 Ru (M45N23V)
177 Th 5p3	231* Mo 3d3
179* Zr 3d5	232 Se 3s
179 Ba 4p3	234 Cs 4s
181* Zr 3d3	234 Fr 5s
181 Ge 3s	234 Pr 4p1
182 Fr 5p1	238 Rn 4f
182* Yb 4d5	238* Ta 4d3
182* Br 3p3	240* Rb 3p3
183* Cl (L23M3M23)	242 Pm 4p3
184 Po 4f	242* Ar 2p3
187 I 4s	243* W 4d5
188* P 2s	244* Ar 2p1
188* Mo (M45N23V)	245 Nd 4p1
189* B 1s	246 Tc (M5N45N45)
189* Br 3p1	248* Th (N67O45V)
191* Yb 4d3	248* K (L3M23M23)
193 Ba 4p1	249* Rb 3p1
195 At 5s	250 Sm 4p3
196* Lu 4d5	253 Rh (M45N23V)
197 La 4p3	253 Tc 3d5
199* Cl 2p3	254 Ba 4s
200 Nb (M45N45N45)	254 Ra 5s
200 Ra 5p1	256 Br 3s
201* Cl 2p1	256* W 4d3
202* Nb 3d5	257 Tc 3d3
205 As 3s	260* Re 4d5
205* Nb 3d3	261 Eu 4p3
206* Lu 4d3	264 Pm 4p1
207 Xe 4s	264* C (KL23L23)
207 Ce 4p3	268 Fr 4f
207 Tc (M45N23V)	270* Sr 3p3
208* Kr 3p3	270 Gd 4p3
210 At 4f	271* Cl 2s
211* Hf 4d5	272 Ac 5s
213 La 4p1	274* Re 4d3
214 Rn 5s	275* Ru (M5N45N45)
215* Ar (L23M23M23)	275 La 4s
215 Ac 5p1	276 Pd (M45N23V)
216* Kr 3p1	279* Os 4d5
218 Pr 4p3	280* Ru 3d5
218 K (L3M1M23)	281* Sr 3p1
222* Hf 4d3	283* U (N67O45V)
223 Mo (M45N45N45)	283 Sm 4p1
223 Ce 4p1	284* Ru 3d3
226* Ta 4d5	285* Tb 4p3
226 K (L3M1M23)	285* C 1s

287 Kr 3s	353* Au 4d3
289 Eu 4p1	358 Ti (L3M1M23)
290 Ce 4s	358* Ag (M4N45N45)
290* Ca (L23M23M23)	360* Lu 4p3
293* Os 4d3	360 Sr 3s
294* K 2p3	361* Nb 3p3
294 Th 5s	361* Hg 4d5
296 Ag (M45N23V)	366 Eu 4s
297* K 2p1	368* Er 4p1
297* Ir 4d5	368* Ag 3d5
297* Dy 4p3	369 Sc (LM23M45)
299 Ra 4f	374* Ag 3d3
299* Y 3p3	376* Nb 3p1
301 Gd 4p1	377* Cd (M5N45N45)
302* Rh (M45N45N45)	377* U 4f7
305 Pr 4s	378 Gd 4s
307 Sc (L3M1M23)	380* K 2s
307* Rh 3d5	380* N (KL23L23)
309* Ho 4p3	380 Hf 4p3
311* Y 3p1	381* Hg 4d3
312* Ir 4d3	384* Cd (M4N45N45)
312* Rh 3d3	384* Tm 4p1
315* Pt 4d5	385* Tl 4d5
315 Sc (L3M1M23)	388* U 4f5
316 Cd (M45N23V)	389* Yb 4p1
319 Ac 4f	389 Ti (L23M23M23)
320 Nd 4s	394* Mo 3p3
320* Ar 2s	394 Y 3s
321* Er 4p3	396 Tb 4s
322* Tb 4p1	399* Sc 2p3
325 Rb 3s	400 V (L3M1M23)
328* Pd (M45N45N45)	400* N 1s
330* Zr 3p3	401 Ta 4p3
332* Pt 4d3	403* In (M5N45N45)
333* Th 4f7	404* Sc 2p1
333* Tm 4p3	405* Cd 3d5
335* Au 4d5	406* Tl 4d3
335* Pd 3d5	411* Mo 3p1
337 Pm 4s	411 V (L3M1M23)
337* Dy 4p1	411* In (M4N45N45)
338* Sc (L3M23M23)	412* Pb 4d5
338 Ti (L3M1M23)	412* Cd 3d3
340* Pd 3d3	413* Lu 4p1
341* Yb 4p3	417 Dy 4s
342* Th 4f5	419* Ti (L3M23M45)
344* Zr 3p1	424 W 4p3
347* Ca 2p3	425 Tc 3p3
349 Sm 4s	429* Sn (M5N45N45)
350* Ca 2p1	430 Zr 3s
352* Ag (M5N45N45)	434* Pb 4d3
353* Ho 4p1	435 Ho 4s

437 Hf 4p1	521* Rh 3p1
438* Sn (M4N45N45)	528* Cr (L3M23M45)
439 V (L23M23M23)	528* Sb 3d5
440* Ca 2s	531* O 1s
441* Bi 4d5	532* Xe (M5N45N45)
444* In 3d5	533* Pd 3p3
445 Tc 3p1	533 At 4d3
446 Re 4p3	534 Hf 4s
448 Cr (L3M1M23)	537* Sb 3d3
451 Er 4s	541 Rn 4d5
452* In 3d3	543 Mn (L23M23M23)
454* Ti 2p3	544 Tc 3s
455* Sb (M5N45N45)	545* Xe (M4N45N45)
460 Cr (L3M1M23)	547 Au 4p3
460* Ti 2p1	548 Os 4p1
462* Ru 3p3	549 Fe (L3M1M23)
463 Ta 4p1	555* Cs (M5N45N45)
465* Bi 4d3	560* Pd 3p1
465* Sb (M4N45N45)	561* Ti 2s
467 Nb 3s	563 Ta 4s
470 Tm 4s	564 Fe (L3M1M23)
471 Os 4p3	567 Rn 4d3
473* V (L3M23M45)	569* Cs (M4N45N45)
473 Po 4d5	570 Cr (L3M45M45)
474 O (KL1L1)	573* Te 3d5
482* Te (M5N45N45)	573* Ag 3p3
482 Yb 4s	574* Cr 2p3
484* Ru 3p1	577 Fr 4d5
485* Sn 3d5	578 Ir 4p1
488 O (KL1L23)	579 Hg 4p3
490 Cr (L23M23M23)	583* Te 3d3
491 W 4p1	583* Cr 2p1
492* Te (M4N45N45)	586 Ru 3s
493* Sn 3d3	587* Ba (M5N45N45)
495 Ir 4p3	587* Mn (L3M23M45)
497* Rh 3p3	594 W 4s
499* Sc 2s	599 Fe (L23M23M23)
500 Mn (L3M1M23)	601* Ba (M4N45N45)
500 Po 4d3	603 Fr 4d3
505* I (M5N45N45)	603 Ra 4d5
506 Mo 3s	604* Ag 3p1
507 At 4d5	607 Co (L3M1M23)
509* O (KL23L23)	609 F (KL1L1)
509 Lu 4s	609 Pt 4p1
510 V (L3M45M45)	610 Tl 4p3
512* V 2p3	619* Cd 3p3
514 Mn (L3M1M23)	619* I 3d5
516* I (M4N45N45)	620 Co (L3M1M23)
518 Re 4p1	620* La (M5N45N45)
520* V 2p1	625 Re 4s
520 Pt 4p3	626 V 2s

628 F (KL1L23)	740 At 4p3
629 Rh 3s	740* Cs 3d3
631* I 3d3	757* Sn 3p1
633* La (M4N45N45)	762 Pb 4p1
635 Mn (L3M45M45)	763 Au 4s
636 Ra 4d3	767* Sb 3p3
639* Mn 2p3	768 Cu (L3M23M23)
639 Ac 4d5	768 Rn 4p3
643 Au 4p1	769 Mn 2s
644 Pb 4p3	769 Zn (L3M1M23)
648 Fe (L3M23M45)	772 Cd 3s
649 Co (L3M23M23)	773 Pm (M45N45N45)
650* Mn 2p1	774* Co (L3M45M45)
653* Cd 3p1	775 Cu (L2M23M23)
654* Ce (M45N45N45)	775 Ni (L3M23M45;1P)
655* F (KL23L23)	778* Co 2p3
656 Co (L2M23M23)	779* U 4d3
658 Os 4s	781 Ni (L3M23M45;3P)
662 Ni (L3M1M23)	781* Ba 3d5
665* In 3p3	784 Zn (L3M1M23)
670* Xe 3d5	789 Co (L2M45M45)
671 Pd 3s	793* Co 2p1
675 Ni (L3M1M23)	796* Ba 3d3
675 Ac 4d3	805 Hg 4s
676* Th 4d5	805* Sm (M45N45N45)
679 Bi 4p3	806 Bi 4p1
682 Hg 4p1	810 Fr 4p3
683* Xe 3d3	813* Sb 3p1
685* F 1s	818* Ne (KL23L23)
690* Pr (M45N45N45)	820* Te 3p3
692 Ir 4s	827 Zn (L3M23M23)
696* Cr 2s	828 In 3s
703* Fe (L3M45M45)	831 Ga (L3M1M23)
703* In 3p1	835 Zn (L2M23M23)
705 Po 4p3	836* La 3d5
707* Fe 2p3	839 Cu (L3M23M45;1P)
709 Ni (L3M23M23)	845 Fe 2s
710 Co (L3M23M45;1P)	845 Ga (L3M1M23)
713* Th 4d3	846* Ni (L3M45M45)
715* Sn 3p3	847 Tl 4s
715 Ni (L2M23M23)	847 Cu (L3M23M45;3P)
716 Co (L3M23M45;3P)	850* Eu (M45N45N45)
718 Cu (L3M1M23)	851 Po 4p1
719 Ag 3s	853* La 3d3
720* Fe 2p1	853* Ni 2p3
720 Tl 4p1	859 Cu (L2M23M45)
725 Pt 4s	863 Ni (L2M45M45)
726* Cs 3d5	863* Ne 1s
729* Nd (M45N45N45)	870* Ni 2p1
731 Cu (L3M1M23)	871* Te 3p1
736* U 4d5	875 I 3p3

879 Ra 4p3	1022* Zn 2p3
884* Ce 3d5	1030 As (L2M23M23)
885 Sn 3s	1034* Pm 3d5
885* Gd (M45N45N45)	1043 Ge (L3M23M45;1P)
886 At 4p1	1045* Zn 2p1
888 Ga (L3M23M23)	1045 At 4s
890 Ge (L3M1M2)	1047 Er (M5N45N45)
893 Pb 4s	1054 Ge (L3M23M45;3P)
895 Ge (L3M1M3)	1058 Ra 4p1
898 Ga (L2M23M23)	1060* Pm 3d3
900 Ac 4p3	1064 Ba 3p3
902* Ce 3d3	1069* Ga (L3M45M45)
905 Zn (L3M23M45;1P)	1069 Cs 3p1
914 Zn (L3M23M45;3P)	1071 I 3s
919* Cu (L3M45M45)	1072* Na 1s
925 Co 2s	1075 Ge (L2M23M45)
926 Na (KL1L1)	1076 Tb (M45N45V)
928 Tb (M45N45N45)	1080 Ac 4p1
929 Rn 4p1	1081* Sm 3d5
930 I 3p1	1095 Ga (L2M45M45)
932* Pr 3d5	1097 Rn 4s
933* Cu 2p3	1097 Cu 2s
934 Xe 3p3	1106 Mg (KL1L1)
939 Cu (L2M45M45)	1108* Sm 3d3
940 Bi 4s	1116 As (L3M23M45;1P)
944 Sb 3s	1117* Ga 2p3
950 As (L3M1M23)	1119 Dy (M45N45V)
951 Na (KL1L23)	1126* Eu 3d5
952* Pr 3d3	1127 As (L3M23M45;3P)
953 Ge (L3M23M23)	1127 Se (L3M1M45)
953* Cu 2p1	1128 La 3p3
961* Dy (M45N45N45)	1138 Ba 3p1
962 Ge (L2M23M23)	1140 Mg (KL1L 23)
965 Th 4p3	1141 Xe 3s
966 As (L3M1M23)	1144* Ga 2p1
973 Ga (L3M23M45;1P)	1145* Ge (L3M45M45)
980 Fr 4p1	1151 As (L2M23M45)
981* Nd 3d5	1153 Fr 4s
983 Ga (L3M23M45;3P)	1156* Eu 3d3
992* Zn (L3M45M45)	1170 Th 4p1
994* Na (KL23L23)	1173 Ho (M45N45V)
995 Po 4s	1177 Ge (L2M45M45)
996 Xe 3p1	1184 Ce 3p3
999 Ho (M45N45N45)	1186* Gd 3d5
1000 Ga (L2M23M45)	1186* Mg (KL23L23)
1002* Nd 3d3	1188 Se (L3M2M45)
1002 Cs 3p3	1195 Zn 2s
1009 Te 3s	1200 Se (L3M23M45)
1009 Ni 2s	1208 Ra 4s
1015 Zn (L2M45M45)	1208 La 3p1
1020 As (L3M23M23)	1214 Er (M45N45V)

1216 Cs 3s	2116* S (KL23L23)
1217* Ge 2p3	2116 Ir 3d3
1218* Gd 3d3	2122 Pt 3d5
1225* As (L3M45M45)	2145 P 1s
1227* Tb (M5VV)	2194 Ta 3p3
1230 Se (L3M23M5)	2202 Pt 3d3
1241* Tb 3d5	2206 Au 3d5
1242 Pr 3p3	2264 Lu 3p1
1248* Ge 2p1	2281 W 3p3
1257 Tb (M4VV)	2291 Au 3d3
1261 As (L2M45M45)	2295 Hg 3d5
1269 Ac 4s	2365 Hf 3p1
1272 Ce 3p1	2367 Re 3p3
1276* Tb 3d3	2385 Hg 3d3
1292 Ba 3s	2389 Tl 3d5
1296* Dy 3d5	2457 Os 3p3
1301 Nd 3p3	2469 Ta 3p1
1301 Ga 2s	2472 S 1s
1303* Mg 1s	2484 Pb 3d5
1306* Se (L3M45M45)	2485 Tl 3d3
1324* As 2p3	2491 Lu 3s
1330 Th 4s	2551 Ir 3p3
1333* Dy 3d3	2575 W 3p1
1339 Pr 3p1	2580 Bi 3d5
1347 Se (L2M45M45)	2586 Pb 3d3
1359* As 2p1	2601 Hf 3s
1370* Ho (M4VV)	2645 Pt 3p3
1387 Al (KL23L23)	2682 Re 3p1
1387 Ho (M4VV)	2683 Po 3d5
1389* Er (M5VV)	2688 Bi 3d3
1431 Er (M4VV)	2708 Ta 3s
1560 Al 1s	2743 Au 3p3
1589 Lu 3d5	2787 At 3d5
1617* Si (KL23L23)	2792 Os 3p1
1639 Lu 3d3	2798 Po 3d3
1662 Hf 3d5	2820 W 3s
1675* Ta (M5N67N67)	2822 Cl 1s
1716 Hf 3d3	2847 Hg 3p3
1735 Ta 3d5	2892 Rn 3d5
1793 Ta 3d3	2909 Ir 3p1
1809 W 3d5	2909 At 3d3
1839 Si 1s	2932 Re 3s
1872 W 3d3	2957 Tl 3p3
1883 Re 3d5	3000 Fr 3d5
1949 Re 3d3	3004 Rh 2p3
1960 Os 3d5	3022 Rn 3d3
2016* Au (M5N7N7)	3027 Pt 3p1
2024 Lu 3p3	3049 Os 3s
2031 Os 3d3	3066 Pb 3p3
2040 Ir 3d5	3105 Fr 3d5
2108 Hf 3p3	3136 Fr 3d3

3146 Rh 2p1	4652 Fr 3s
3148 Au 3p1	4656 Ac 3p1
3174 Ir 3s	4822 Ra 3s
3173 Pd 2p3	4830 Th 3p1
3177 Bi 3p3	4966 Ti 1s
3206 Ar 1s	5001 Pa 3p1
3219 Ac 3d5	5002 Ac 3s
3248 Ra 3d3	5182 Th 3s
3279 Hg 3p1	5182 U 3p1
3296 Pt 3s	5367 Pa 3s
3302 Po 3p3	5548 U 3s
3330 Pd 2p1	5465 V 1s
3332 Th 3d5	5989 Cr 1s
3351 Ag 2p3	6539 Mn 1s
3370 Ac 3d3	7112 Fe 1s
3412 Rh 1s	7709 Co 1s
3416 Tl 3p1	8333 Ni 1s
3425 Au 3s	8979 Cu 1s
3426 At 3p3	9244 Lu 2p3
3442 Pa 3d5	9561 Hf 2p3
3491 Th 3d3	9659 Zn 1s
3524 Ag 2p1	9881 Ta 2p3
3552 U 3d5	10207 W 2p3
3554 Pb 3p1	10349 Lu 2p1
3562 Hg 3s	10367 Ga 1s
3538 Rn 3p3	10535 Re 2p3
3604 Pd 1s	10739 Hf 2p1
3608 K 1s	10870 Lu 2s
3611 Pa 3d3	10871 Os 2p3
3663 Fr 3p3	11103 Ge 1s
3696 Bi 3p1	11136 Ta 2p1
3792 Ra 3p3	11215 Ir 2p3
3704 Tl 3s	11271 Hf 2s
3728 U 3d3	11544 W 2p1
3806 Ag 1s	11564 Pt 2p3
3851 Pb 3s	11682 Ta 2s
3854 Po 3p1	11867 As 1s
3909 Ac 3p3	11919 Au 2p3
3999 Bi 3s	11959 Re 2p1
4008 At 3p1	12100 W 2s
4038 Ca 1s	12284 Hg 2p3
4046 Th 3p3	12385 Os 2p1
4149 Po 3s	12658 Se 1s
4159 Rn 3p1	12658 Tl 2p3
4174 Pa 3p3	12824 Ir 2p1
4303 U 3p3	12968 Os 2s
4317 At 3s	13035 Pb 2p3
4327 Fr 3p1	13273 Pt 2p1
4482 Rn 3s	13419 Ir 2s
4490 Ra 3p1	13419 Bi 2p3
4492 Sc 1s	13474 Br 1s

13734 Au 2p1	29200 Sn 1s
13814 Po 2p3	30491 Sb 1s
13880 Pt 2s	31814 Te 1s
14209 Hg 2p1	33169 I 1s
14214 At 2p3	34561 Xe 1s
14326 Kr 1s	35985 Cs 1s
14353 Au 2s	37441 Ba 1s
14619 Rn 2p3	38925 La 1s
14698 Tl 2p1	40443 Ce 1s
15031 Fr 2p3	41991 Pr 1s
15200 Rb 1s	43569 Nd 1s
15200 Pb 2p1	45184 Pm 1s
15347 Tl 2s	46834 Sm 1s
15444 Ra 2p3	48519 Eu 1s
15711 Bi 2p1	50239 Gd 1s
15861 Pb 2s	51996 Tb 1s
15871 Ac 2p3	53789 Dy 1s
16105 Sr 1s	55618 Ho 1s
16244 Po 2p1	57486 Er 1s
16300 Th 2p3	59390 Tm 1s
16388 Bi 2s	61332 Yb 1s
16733 Pa 2p3	63314 Lu 1s
16785 At 2p1	65351 Hf 1s
16939 Po 2s	67416 Ta 1s
17038 Y 1s	69525 W 1s
17166 U 2p3	71676 Re 1s
17337 Rn 2p1	73871 Os 1s
17493 At 2s	76111 Ir 1s
17907 Fr 2p1	78395 Pt 1s
17998 Zr 1s	80725 Au 1s
18049 Rn 2s	83102 Hg 1s
18484 Ra 2p1	85530 Tl 1s
18639 Fr 2s	88005 Pb 1s
18986 Nb 1s	90524 Bi 1s
19083 Ac 2p1	93105 Po 1s
19237 Ra 2s	95730 At 1s
19693 Th 2p1	98404 Rn 1s
19840 Ac 2s	101137 Fr 1s
20000 Mo 1s	103922 Ra 1s
20314 Pa 2p1	106755 Ac 1s
20472 Th 2s	109651 Th 1s
20948 U 2p1	112601 Pa 1s
21044 Te 1s	115606 U 1s
21105 Pa 2s	
21757 U 2s	Ag (M4N45N45).pos
22117 Ru 1s	
23220 Rh 1s	357.8 Ag
24350 Pd 1s	356.7 Ag2O
25514 Ag 1s	356.6 AgO
26711 Cd 1s	354.2 Ag2SO4
27940 In 1s	

Ag (M5N45N45).pos

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

Ag 3d5.pos

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

Al (KL23L23).pos

1393.3 Al
 1391.2 AlAs
 1389.0 AlN
 1388.2 Al₂O₃/alpha
 1387.9 Al₂O₃/sapphire
 1387.8 Al₂O₃/gamma
 1387.7 Al(OH)₃/bayerite
 1387.6 AlOOH
 1387.1 Mica/muscovite
 1386.9 Al₂SiO₅/sillimannite
 1386.9 Mol Sieve A
 1385.5 H Zeolon

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 2p.pos

241.5 Ar in graphite

As (L3M45M45).pos

1225.0 GaAs
 1224.0 As
 1222.9 AsI₃
 1222.1 As₂S₃
 1221.1 Ph₃As
 1219.5 Ph₃AsO
 1218.8 As₂O₃
 1218.1 AsBr₃
 1217.5 As₂O₅
 1213.8 KAsF₆

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 (M5N67N67).pos

2015.7 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

601.0 Ba
598.0 BaO
596.1 BaSO4
594.9 BaF2

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 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

1389.1 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 1s.pos

281.6 TiC
282.8 WC

283.9 Fe ₃ C	288.9 CaF ₂
283.9 K ₃ Fe(CN) ₆	
284.5 Graphite	Ca 2p₃.pos
284.6 PhNH ₂	
284.7 Benzene	345.9 Ca
285.0 -CH ₂ -	346.3 CaCrO ₄
285.5 C ₅ H ₅ N	346.5 CaS
285.6 C ₆ H ₅ F(C*H)	347.0 CaCO ₃
285.6 EtNH ₂	347.0 Ca ₃ Si ₃ O ₉
285.7 C ₆ H ₅ Cl(C*H)	347.3 CaO
285.7 (-C*H ₂ CFH-)n	347.9 CaF ₂
285.9 PVC(-C*H ₂ CHCl-)	348.0 CaSO ₄
286.1 KCN	348.3 CaCl ₂
286.3 CH ₃ C*H ₂ OH	
286.3 C*H ₃ CN	Cd (M₄N₄₅N₄₅).pos
286.4 (-C*H ₂ CF ₂ -)	
286.5 (CH ₃ C*H ₂) ₂ O	384.0 Cd
286.5 PVA(-CH ₂ C*HOH-)n	382.4 CdO
286.9 CH ₃ COOC*H ₂ CH ₃	382.4 CdTe
287.0 CS ₂	381.7 CdSe
287.0 PVC(-CH ₂ C*HCl-)	381.3 CdS
287.1 C ₆ H ₅ Cl(C*Cl)	381.2 CdI ₂
287.2 CH ₃ C*N	379.0 CdF ₂
287.8 C ₆ H ₅ F(C*F)	
287.9 (-CH ₂ C*FH-)n	Cd 3d₅.pos
287.9 CH ₃ C*OCH ₃	
288.0 Fe(CO) ₅	404.2 CdO
288.0 H ₂ NCSNH ₂	404.6 Hg _{0.8} Cd _{0.2} Te
288.2 CH ₃ C*OONa	405.0 CdSe
288.4 CH ₃ C*ONH ₂	405.1 Cd
288.7 H ₂ NCONH ₂	405.1 Cd(OH) ₂
289.3 CH ₃ C*OOH	405.1 CdCO ₃
289.4 Na ₂ CO ₃	405.2 CdTe
289.5 Cl ₃ C*COONa	405.3 CdS
289.6 CaCO ₃	405.4 CdI ₂
289.6 HCCl ₃	405.9 CdF ₂
290.0 NaHCO ₃	406.0 CdBr ₂
290.9 (-CH ₂ C*F ₂ -)n	406.1 CdCl ₂
291.9 CO ₂	
292.2 Teflon(-CF ₂ CF ₂ -)n	Ce 3d₅.pos
292.4 CCl ₄	
292.9 C*F ₃ COOEt	881.9 CeO ₂
294.7 HCF ₃	883.5 CeAl ₂
296.7 CF ₄	883.6 CeCu ₂ Si ₂
	883.9 Ce
Ca (L₂₃M₂₃M₂₃).pos	884.3 CePd ₃
	884.3 CeSe
298.2 Ca	886.0 CeH ₃
292.5 CaO	
291.9 CaCO ₃	Cl 2p₃.pos
291.9 CaCl ₂	

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

773.0 Co
 766.8 K₃Co(CN)₆
 768.6 Co(NH₃)₆Cl₃
 768.3 CoSiF₆

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

527.2 Cr

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

568.7 CsOH
 568.4 Cs₂SO₄

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 (L3M45M45).pos

918.6 Cu
 918.6 Cu₆₄Zn₃₆
 918.1 CuO
 917.9 CuS
 916.6 Cu₂O
 916.2 Cu(OH)₂
 915.6 CuSO₄
 915.3 CuCl
 915.3 CuCl₂
 915.1 CuF₂
 914.5 CuCN
 914.4 Cu₂S

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 3d5.pos

1295.5 Dy
 1298.9 Dy₂O₃

Dy 4d.pos

152.4 Dy
 167.7 Dy₂O₃

Er 4d.pos

167.3 Er
 168.7 Er₂O₃

Eu 3d5.pos

1125.6 Eu

Eu 4d.pos

128.2 Eu
 135.9 Eu₂O₃

F (KL23L23).pos

656.2 CuF₂
 656.0 CdF₂
 655.4 CaF₂
 655.0 NaF
 654.7 LiF
 654.4 MgF₂
 654.1 Na₃AlF₆
 653.8 CsF
 653.0 Na₂SiF₆
 652.8 NaBF₄
 652.4 (-CF₂-CF₂-)_n

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

702.9 FeB
 702.4 Fe

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 (L3M45M45).pos

1068.1 Ga
 1066.3 GaAs
 1065.6 GaP
 1064.5 GaN
 1062.4 Ga₂O₃

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 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

1145.2 Ge
 1143.7 GeS
 1142.9 GeSe
 1137.7 GeO₂
 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 4f7.pos

14.2 Hf
 16.7 HfO₂

Hg 4f7.pos

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

Ho 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

I (M5N45N45).pos

507.0 CdI
 506.8 AgI

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

410.4 In
 408.9 In₂Te₃
 408.6 CuInSe₂
 408.0 InP
 408.0 In₂Se₃
 407.3 In₂S₃
 496.4 In₂O₃
 405.8 InI₃
 405.0 In(OH)₃
 404.8 InBr₃
 404.6 InCl₃
 403.7 InF₃
 401.6 InSb

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 4f7.pos

60.8 Ir
 62.0 IrO₂
 62.7 IrCl₃
 63.5 K₂IrCl₆

K (L2M23M23).pos

250.7 KBr
 250.1 KF
 249.3 KSbF₆

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 3d.pos

87.0 Kr in graphite

La 3d5.pos

834.8 La₂O₃
 835.8 La
 838.8 LaH₃

La 4d5.pos

101.3 La₂O₃
 103.9 La

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 4d5.pos

196.5 Lu₂O₃
 196.6 Lu
 198.5 Lu₂(SO₄)₃

Lu 4f7.pos

6.3 Lu

Mg (KL23L23).pos

1185.6 Mg
 1180.4 MgO
 1178.8 MgSO₄·7H₂O
 1178.2 MgF₂

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

586.4 Mn

585.7 MnO₂
584.8 MnS
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 (L3M35M45).pos

2039.0 MoSi₂
2038.8 Mo
2032.2 MoO_x

Mo 3d5.pos

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

N (KVV).pos

396.6 Gd(NO₃)₃·5H₂O
385.0 GaN
379.2 BN
376.6 NH₃

N 1s.pos

397.0 GaN

397.7 Si₃N₄
398.0 K₄Fe(CN)₆
398.1 BN
398.5 Na(N*NN*)
398.7 NH₃
398.8 C₅H₅N/Pyridine
398.9 EtNH₂
399.2 PhCN
399.5 H₂NCONH₂
399.4 C₆H₁₂N₄/Urotropin
399.8 KCN
400.2 C₄H₅N/Pyrrrole
401.3 (NH₄)₂SO₄
401.4 Et₄NCl
401.7 NH₄Cl
402.2 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

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 1s.pos

1070.8 NaN₃
1070.8 Na₂C₂O₄
1071.1 Na₃PO₄
1071.1 NaOAc
1071.2 NaF

1071.2 Na ₂ SO ₄	863.4 Ne in Fe
1071.4 NaNO ₃	
1071.5 Na ₂ CO ₃	Ni (L3M45M45).pos
1071.5 Na ₂ HPO ₄	
1071.6 NaI	846.2 Ni
1071.6 NaPO ₃	842.4 Ni(acac) ₂
1071.6 NaCl	842.4 NiF ₂
1071.7 Na ₂ SiF ₆	
1071.7 NaBr	Ni 2p3.pos
1071.8 Na	
1072.0 NaH ₂ PO ₄	852.7 Ni
1072.5 Na ₂ O	852.8 NiS
1072.7 NaBF ₄	854.4 NiO
Nb (M45N23V).pos	855.7 Ni(acac) ₂
	855.9 Ni(OH) ₂
167.8 Nb	856.0 Ni ₂ O ₃
165.6 NbH _x	856.7 NiCl ₂
161.6 Nb ₂ O ₅	856.8 NiSO ₄
	857.1 Ni(NO ₃) ₂
Nb 3d5.pos	857.5 NiF ₂ ·4H ₂ O
	861.0 K ₂ NiF ₆
202.4 Nb	O (KL23L23).pos
203.2 NbH _x	
203.7 NbO	515.1 PbO ₂
203.8 NbN	513.1 PbO
206.5 KNbO ₃	510.8 ZrO ₂
207.1 NbBr ₅	509.7 CaCO ₃
207.6 Nb ₂ O ₅	509.3 CaO
207.7 NbS ₂	508.8 CaSiO ₃
208.0 NbCl ₅	508.7 CaSO ₄
Nd 3d5.pos	508.6 Al(OH) ₃
	508.5 Al ₂ O ₃
980.8 Nd	507.9 NaPO ₃
982.0 Nd ₂ O ₃	507.7 H ₂ O
984.9 Nd ₂ (SO ₄) ₃	507.7 NaAlSi ₃ O ₈
	506.8 SiO ₂
Nd 4d.pos	O 1s.pos
120.8 Nd ₂ O ₃	529.3 CrO ₂
122.5 Nd ₂ (SO ₄) ₃	529.5 NiO
Ne (KL23L23).pos	529.6 Fe ₂ O ₃
	529.8 FeO
818.0 Ne in Fe	529.9 Co ₂ O ₃
	530.0 Fe ₃ O ₄
Ne 1s.pos	530.1 K ₄ P ₂ O ₇
	530.2 Co ₃ O ₄
861.6 Ne in Au	530.2 CrO ₃
863.1 Ne in graphite	530.2 CoO
	530.4 K ₃ PO ₄

530.6 Na₂SiO₃·3H₂O
 531.0 Al₂O₃/sapphire
 531.2 Ni(OH)₂
 531.4 Al(OH)₃
 531.4 CaCO₃
 531.5 Cr₂O₃
 531.6 Na₂CO₃
 531.7 BeO
 531.7 R-O-CO*-Ph
 531.8 Ni₂O₃
 532.1 NiSO₄
 532.2 KClO₄
 532.2 p-Benzoquinone
 532.2 PhCONH₂
 532.2 R-O-CO*-(CH₂)_n-
 532.3 KClO₃
 532.5 Na₂SiO₃·H₂O*
 532.9 -(CH₂)_n-OH
 533.0 B₂O₃
 533.0 Ba(NO₃)₂
 533.0 SiO₂
 533.1 R-O*-CO-Ph
 533.1 H₂O
 533.5 Hydroquinone
 533.6 R-O*-CO-(CH₂)_n-

Os 4f7.pos

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

P (KL23L23),pos

1848.6 NaPO₃
 1857.3 GaP
 1858.4 InP
 1856.1 P/red
 1850.5 Na₃PO₄
 1845.2 NH₄PF₆
 1848.0 P₄O₁₀
 1853.2 P₄S₁₀
 1849.9 Na₄P₂O₇

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

96.3 Pb
 95.5 PbTe
 94.8 PbSe
 94.6 PbS
 93.4 PbI₂
 93.1 PbO₂
 92.9 PbO
 92.6 PbBr₂
 92.1 PbCl₂
 92.0 Pb(OH)₂
 91.7 Pb(NO₃)₂
 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 PbSO ₄	72.5 Pt ₂ Si
Pd (M4N45N45).pos	72.6 I ₂ Pt(Me ₃ P) ₂ /cis
323.1 K ₂ PdCl ₄	72.6 K ₂ PtBr ₄
327.8 Pd	72.6 Pt(OH) ₂
	72.7 I ₂ Pt(Me ₃ P) ₂ /trans
Pd 3d5.pos	73.0 PtSi
335.1 Pd	73.0 Cl ₂ Pt(Ph ₃ P) ₂ /cis
336.3 PdO	73.4 K ₂ PtCl ₄
336.4 PdI ₂	73.4 K ₂ PtI ₆
336.6 Pd ₂ (Ph ₃ P) ₂	73.4 Pt(NH ₃) ₄ Cl ₂
337.1 PdBr ₂	73.6 PtCl ₂
337.7 K ₂ PdBr ₄	74.2 PtO
337.8 PdCl ₂	74.6 K ₂ PtBr ₆
337.9 PdO ₂	75.0 PtO ₂
337.9 K ₂ PdCl ₄	75.4 K ₂ PtCl ₆
338.6 Pd(OAc) ₂	75.5 PtCl ₄
338.8 K ₂ Pd(NO ₂) ₄	75.9 Cl ₄ Pt(Et ₃ P) ₂
340.3 K ₂ PdCl ₆	76.3 Pt(NH ₃) ₆ Cl ₄
	77.6 K ₂ PtF ₆
Pm 3d5.pos	Rb 3d5.pos
1033..5 PmCl ₃	109.8 RbF
	109.9 RbCl
Pr 3d5.pos	110.0 Rb ₃ PO ₄
931.8 Pr	110.0 RbBr
933.6 Pr ₂ O ₃	110.4 RbI
935.3 PrO ₂	111.5 Rb
Pr 4d.pos	Re 4f7.pos
116.1 Pr ₂ O ₃	40.5 Re
116.2 PrO ₂	43.2 ReO ₂
	43.9 Cl ₃ ReO(Ph ₃ P) ₂
Pt (M4N67N67).pos	44.0 K ₂ ReCl ₆
2040.5 Pt	46.8 ReO ₃
2035.2 K ₂ PtCl ₄	
Pt (M5N67N67).pos	Rh 3d5.pos
1960.7 Pt	307.2 Rh
	307.4 ClRh(Ph ₃ P) ₃
Pt 4f7.pos	308.5 KRhO ₂
71.2 Pt	308.6 RhI ₃
71.4 Pt(Ph ₃ P) ₃	308.7 Rh ₂ O ₃
71.4 Pt(Ph ₃ P) ₄	308.8 CaRh ₂ O ₄
	309.4 Rh ₂ WO ₆
	309.8 K ₃ RhCl ₆
	310.0 RhCl ₃ ·3H ₂ O
	310.1 RhCl ₃
	310.5 K ₃ Rh(NO ₂) 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

2116.1 NiS
 2115.8 FeS₂/Pyrite
 2115.6 WS₂
 2113.5 ZnS
 2113.4 S
 2111.8 Na₂S*SO₃
 2108.0 CuSO₄
 2107.6 Na₂SS*O₃
 2107.3 Na₂SO₃
 2106.2 SO₂
 2105.9 Na₂SO₄
 2100.5 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 Na₂SO₄169.7 CaSO₄174.4 SF₆**Sb (M4N45N45).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

Se (L3M45M45).pos

1307.0 Se
 1304.0 Ph₂Se
 1304.3 Ph₂Se₂
 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

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 3d5.pos

1081.1 Sm
 1083.2 Sm₂O₃
 1083.4 Sm₂(SO₄)₃

Sn (M4N45N45).pos

437.3 Sn
 435.7 SnS
 432.6 SnO₂
 431.7 Na₂SnO₃
 430.8 NaSnF₃

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

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 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

492.1 Te
 490.8 CdTe
 488.5 Ph2Te2
 487.3 TeBr4
 487.1 TeO2
 486.4 (NH4)2TeCl6
 486.3 Cl2TePh2
 486.1 TeCl4
 485.5 TeO3
 485.5 Na2TeO4
 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 4d5.pos

675.2 Th
 675.5 ThO2

Th 4f7.pos

333.1 Th
 334.4 ThO2
 336.5 ThF4

Ti (L3M23M45).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 4d.pos

175.4 Tm
176.6 Tm₂O₃
178.3 Tm₂(SO₄)₃

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

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

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
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

124.3 Y
123.3 YH_x
117.8 Y₂O₃

Y 3d5.pos

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

Yb 4d5.pos

182.4 Yb
185.4 Yb₂O₃
187.3 Yb₂(SO₄)₃

Zn (L3M45M45).pos

992.1 Zn
991.3 ZnTe
989.7 ZnS
989.4 ZnCl₂
988.7 ZnI₂
987.7 Zn(acac)₂
987.7 ZnO
987.3 ZnBr₂
986.2 ZnSO₄
986.2 ZnF₂
989.5 ZnSe

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

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 directory Unifit_2016_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 NbH_x

Ne 1s + Ne (KL23L23).aup

1681.4=863.4+818.0 Ne in Fe

Ni 2p₃ + Ni (L3M45M45).aup

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

O 1s + O(KL23L23).aup

1043.8=528.7+515.1 PbO₂
1042.1=529.0+513.1 PbO
1041.7=530.9+510.8 ZrO₂
1041.0=531.3+509.7 CaCO₃
1040.8=533.1+507.7 H₂O
1040.7=532.0+508.7 CaSO₄
1040.6=531.3+509.3 CaO
1040.2=531.4+508.8 CaSiO₃
1040.1=531.5+508.6 Al(OH)₃
1039.9=532.0+507.9 NaPO₃

1039.6=532.8+506.8 SiO₂
1039.6=531.9+507.7 NaAlSi₃O₈
1039.1=530.6+508.5 Al₂O₃

P 2p + P (KL23L23).aup

1987.3=128.9+1858.4 InP
1986.8=130.7+1856.1 P/red
1986.7=129.4+1857.3 GaP
1986.5=133.3+1853.2 P₄S₁₀
1983.8=135.8+1848.0 P₄O₁₀
1983.5=133.6+1849.9 Na₄P₂O₇
1983.3=132.8+1850.5 Na₃PO₄
1983.3=134.7+1848.6 NaPO₃
1982.9=137.7+1845.2 NH₄PF₆

Pb 4f₇ + Pb (N6O45O45).aup

233.1=136.8+96.3 Pb
232.7=137.3+95.4 PbTe
232.4=137.6+94.8 PbSe
232.1=137.5+94.6 PbS
231.7=138.4+93.3 PbI₂
231.4=138.8+92.6 PbBr₂
231.0=138.9+92.1 PbCl₂
230.5=137.4+93.1 PbO₂
230.2=138.5+91.7 Pb(NO₃)₂
230.1=137.3+92.8 PbO
230.1=140.0+90.1 PbSO₄
229.9=138.0+91.9 Pb(OH)₂
229.1=138.5+90.6 PbF₂

Pd 3d₅ + Pd (M4N45N45).aup

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

Pt 4f₇ + Pt (M4N67N67).aup

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

S 2p + S (KL23L23).aup

2278.9=162.8+2116.1 NiS
2278.8=163.0+2115.8 FeS₂/Pyrite
2278.4=162.8+2115.6 WS₂
2277.2=163.8+2113.4 S
2277.1=169.1+2108.0 CuSO₄
2276.2=168.6+2107.6 Na₂SS*O₃
2275.8=162.3+2113.5 ZnS

2275.3=169.4+2105.9 Na₂SO₄
 2274.9=167.6+2107.3 Na₂SO₃
 2274.9=174.4+2100.5 SF₆
 2274.6=162.8+2111.8 Na₂S*SO₃
 2273.6=167.4+2106.1 SO₂

Sb 3d₅ + Sb (M4N45N45).aup

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

Se 3d₅ + Se (L3M45M45).aup

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

Si 2p + Si (KL23L23).aup

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

Sn 3d₅ + Sn (M4N45N45).aup

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

Ta 4f₇ + Ta (M5N67N67).aup

1696.6=21.9+1674.7 Ta

Te 3d₅ + Te (M4N45N45).aup

1065.0=572.9+492.1 Te

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

Ti 2p₃ + Ti (L3M23M45).aup

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

V 2p₃ + V (L3M23M45).aup

984.2=512.2+472.0 V

W 4f₇ + W (M5N67N67).aup

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

Xe 3d₅ + Xe (M4N45N45).aup

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

Y 3d₅ + Y (M45N23V).aup

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

Zn 2p₃ + Zn (L3M45M45).aup

2013.8=1021.7+992.1 Zn
 2012.9=1021.6+991.3 ZnTe
 2011.5=1022.0+989.5 ZnSe
 2011.3=1021.6+989.7 ZnS
 2011.3=1021.9+989.4 ZnCl₂
 2011.2=1022.5+988.7 ZnI₂
 2010.7=1023.4+987.3 ZnBr₂
 2009.8=1022.1+987.7 ZnO
 2009.2=1023.0+986.2 ZnSO₄

2009.1=1021.4+987.7 Zn(acac)₂

2008.0=1021.8+986.2 ZnF₂

Zr 3d5 + Zr (M45N23V).aup

327.6=179.0+148.6 Zr

325.2=183.3+141.9 ZrO₂

324.9=179.6+145.3 ZrH_x

3 Experimental Files

3.1 XPS Data

3.1.1 VG ESCALAB 220i-XL (*.TAP;*.TXT)

Comment:

- All necessary acquisition parameters are available
- Example: multiregion measurement with 8 spectra
- Folder: Install-CD:\XPS_Measurement_Reference_Data\01-ESCALAB Eclipses(.TAP)\ESCALAB-MultiReg-Ver1-with-lense-name.TAP

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

Spectrum: 1

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

INSTRUMENT INFO:

Model: EscaLab 220-IXL

Transmission function coefficients:

1: 4.06581

2: -0.151464

3: 0.0432657

4: -0.0691272

Abscissa label: Kinetic Energy

Abscissa units: eV

Abscissa start: 1401.6

Abscissa end: 1419.6

Abscissa increment: 0.04

Ordinate label:

Ordinate units: Counts

Ordinate data: 451 values

Ordinate minimum, maximum: 1173.25 2435.98

1480.8

1463.72

1483.72

...

1249.83

1238.93

Spectrum: 2

Name (Spectrum): C 1s

Label: St EK neu

Data Version: 1

Technique: XPS

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

ANALYSER:

Mode: CAE

Value: 10

Magnification: 1

Work function: 4.55

Width x: 0

Width y: 0

Source azimuth: 0

Polar angle: 0

Target bias: 0

Lens mode ID: 8

Lens name: Large Area XL

SOURCE:

Type: AL KALPHA

Non-Monochromated

Energy: 1486.6

Voltage: 0

Current: 0

Width x: 0

Width y: 0

Polar angle: 0

Azimuth: 0

Atomic number: 0

Atoms: 0

Charge: 0

Name: Al K-alpha

SIGNAL:

Time: 0.1 seconds

Scans: 12

Correction: 0

SAMPLE:

Charging: 0

Polar angle: 0

Azimuth: 0

Rotation: 0

PROFILE INFO:

None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
1: 4.06581
2: -0.151464
3: 0.0432657
4: -0.0691272
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 1181.6
Abscissa end: 1206.6
Abscissa increment: 0.04
Ordinate label:
Ordinate units: Counts
Ordinate data: 626 values
Ordinate minimum, maximum: 1659.28 4300.5
1910.85
1975.97
...
1704.28
1690.68

Spectrum: 3

Name (Spectrum): Fe 2p
Label: St EK
Data Version: 1
Technique: XPS
Acquired at 14:56:33 on Monday 8-12-1997
ANALYSER:
Mode: CAE
Value: 10
Magnification: 1
Work function: 4.55
Width x: 0
Width y: 0
Source azimuth: 0
Polar angle: 0
Target bias: 0
Lens mode ID: 8
Lens name: Large Area XL
SOURCE:
Type: AL KALPHA
Non-Monochromated
Energy: 1486.6
Voltage: 0
Current: 0
Width x: 0
Width y: 0
Polar angle: 0
Azimuth: 0
Atomic number: 0
Atoms: 0
Charge: 0
Name: Al K-alpha
SIGNAL:
Time: 0.1 seconds
Scans: 12
Correction: 0
SAMPLE:
Charging: 0
Polar angle: 0
Azimuth: 0
Rotation: 0
PROFILE INFO:

None

INSTRUMENT INFO:

Model: EscaLab 220-IXL

Transmission function coefficients:

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

Abscissa label: Kinetic Energy

Abscissa units: eV

Abscissa start: 748.6

Abscissa end: 783.6

Abscissa increment: 0.04

Ordinate label:

Ordinate units: Counts

Ordinate data: 876 values

Ordinate minimum, maximum: 3318.28 10694.6

9387.9

9342.67

9209.9

...

3343.3

3409.8

Spectrum: 4

Name (Spectrum): Na 1s

Label: St EK neu

Data Version: 1

Technique: XPS

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

ANALYSER:

Mode: CAE

Value: 10

Magnification: 1

Work function: 4.55

Width x: 0

Width y: 0

Source azimuth: 0

Polar angle: 0

Target bias: 0

Lens mode ID: 8

Lens name: Large Area XL

SOURCE:

Type: AL KALPHA

Non-Monochromated

Energy: 1486.6

Voltage: 0

Current: 0

Width x: 0

Width y: 0

Polar angle: 0

Azimuth: 0

Atomic number: 0

Atoms: 0

Charge: 0

Name: Al K-alpha

SIGNAL:

Time: 0.1 seconds

Scans: 8

Correction: 0

SAMPLE:

Charging: 0

Polar angle: 0

Azimuth: 0

Rotation: 0

PROFILE INFO:
None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
 1: 4.06581
 2: -0.151464
 3: 0.0432657
 4: -0.0691272
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 403.6
Abscissa end: 419.6
Abscissa increment: 0.04
Ordinate label:
Ordinate units: Counts
Ordinate data: 401 values
Ordinate minimum, maximum: 13493.5 19037.6
13689
13877.8
13782.6
...
13847.3
13846.7
13683.1

Spectrum: 5

Name (Spectrum): O 1s
Label: St EK neu
Data Version: 1
Technique: XPS
Acquired at 14:56:33 on Monday 8-12-1997
ANALYSER:
Mode: CAE
Value: 10
Magnification: 1
Work function: 4.55
Width x: 0
Width y: 0
Source azimuth: 0
Polar angle: 0
Target bias: 0
Lens mode ID: 8
Lens name: Large Area XL
SOURCE:
Type: AL KALPHA
Non-Monochromated
Energy: 1486.6
Voltage: 0
Current: 0
Width x: 0
Width y: 0
Polar angle: 0
Azimuth: 0
Atomic number: 0
Atoms: 0
Charge: 0
Name: Al K-alpha
SIGNAL:
Time: 0.1 seconds
Scans: 7
Correction: 0
SAMPLE:
Charging: 0
Polar angle: 0

Azimuth: 0
Rotation: 0
PROFILE INFO:
None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
 1: 4.06581
 2: -0.151464
 3: 0.0432657
 4: -0.0691272
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 942.6
Abscissa end: 960.6
Abscissa increment: 0.04
Ordinate label:
Ordinate units: Counts
Ordinate data: 451 values
Ordinate minimum, maximum: 1226.07 10376.7
2004.45
1971.05
1981.03
...
1281.15
1294.15

Spectrum: 6

Name (Spectrum): Si 2p
Label: St EK neu
Data Version: 1
Technique: XPS
Acquired at 14:56:34 on Monday 8-12-1997
ANALYSER:
Mode: CAE
Value: 10
Magnification: 1
Work function: 4.55
Width x: 0
Width y: 0
Source azimuth: 0
Polar angle: 0
Target bias: 0
Lens mode ID: 8
Lens name: Large Area XL
SOURCE:
Type: AL KALPHA
Non-Monochromated
Energy: 1486.6
Voltage: 0
Current: 0
Width x: 0
Width y: 0
Polar angle: 0
Azimuth: 0
Atomic number: 0
Atoms: 0
Charge: 0
Name: Al K-alpha
SIGNAL:
Time: 0.1 seconds
Scans: 20
Correction: 0
SAMPLE:
Charging: 0

Polar angle: 0
Azimuth: 0
Rotation: 0
PROFILE INFO:
None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
1: 4.06581
2: -0.151464
3: 0.0432657
4: -0.0691272
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 1373.6
Abscissa end: 1388.6
Abscissa increment: 0.04
Ordinate label:
Ordinate units: Counts
Ordinate data: 376 values
Ordinate minimum, maximum: 2281.43 2833.18
2501.45
2450.4
2489.18
...
2556.43
2568.73

Spectrum: 7

Name (Spectrum): Si 2p
Label: St EK neu
Data Version: 1
Technique: XPS
Acquired at 16:25:43 on Monday 8-12-1997
ANALYSER:
Mode: CAE
Value: 10
Magnification: 1
Work function: 4.55
Width x: 0
Width y: 0
Source azimuth: 0
Polar angle: 0
Target bias: 0
Lens mode ID: 8
Lens name: Large Area XL
SOURCE:
Type: AL KALPHA
Non-Monochromated
Energy: 1486.6
Voltage: 0
Current: 0
Width x: 0
Width y: 0
Polar angle: 0
Azimuth: 0
Atomic number: 0
Atoms: 0
Charge: 0
Name: Al K-alpha
SIGNAL:
Time: 0.1 seconds
Scans: 20
Correction: 0
SAMPLE:

Charging: 0
Polar angle: 0
Azimuth: 0
Rotation: 0
PROFILE INFO:
None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
 1: 4.06581
 2: -0.151464
 3: 0.0432657
 4: -0.0691272
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 1373.6
Abscissa end: 1394.6
Abscissa increment: 0.04
Ordinate label:
Ordinate units: Counts
Ordinate data: 526 values
Ordinate minimum, maximum: 2279 2917.02
2433.98
2443.35
2441.97
...
2815.25
2884.63
2861.65

Spectrum: 8

Name (Spectrum): Survey
Label: St EK neu
Data Version: 1
Technique: XPS
Acquired at 14:47:17 on Monday 8-12-1997
ANALYSER:
Mode: CAE
Value: 70
Magnification: 1
Work function: 4.55
Width x: 0
Width y: 0
Source azimuth: 0
Polar angle: 0
Target bias: 0
Lens mode ID: 8
Lens name: Large Area XL
SOURCE:
Type: AL KALPHA
Non-Monochromated
Energy: 1486.6
Voltage: 0
Current: 0
Width x: 0
Width y: 0
Polar angle: 0
Azimuth: 0
Atomic number: 0
Atoms: 0
Charge: 0
Name: Al K-alpha
SIGNAL:
Time: 0.1 seconds
Scans: 1

```

Correction: 0
SAMPLE:
Charging: 0
Polar angle: 0
Azimuth: 0
Rotation: 0
PROFILE INFO:
None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
    1: 4.06581
    2: -0.151464
    3: 0.0432657
    4: -0.0691272
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 136.6
Abscissa end: 1486.6
Abscissa increment: 0.5
Ordinate label:
Ordinate units: Counts
Ordinate data: 2701 values
Ordinate minimum, maximum: 300.64 29010.5
23993.9
23681.5
23669.4
...
490.024
449.588
300.486

```

3.1.2 ESCALB Avantage (*.AVG)

Comment:

- All necessary acquisition parameters are available
- Single spectrum, profile of one region, line scan of one region, multipoint (area) scan of one region are saved
- Example: profile measurement with 5 Zn2p_{3/2} spectra
- Folder: Install-CD:\XPS_Measurement_Reference_Data\02-Avanatge(.AVG)\Avantage-Profile-Zn2p3.AVG

```

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

```

```

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

```

```

$FORMAT=3

```

```

;Summary Properties present:

```

```

$PROPERTIES=SUM
DS_EXT_SUPROPID_TITLE           : VT_BSTR = 'Zn2p3'
DS_EXT_SUPROPID_SUBJECT        : VT_BSTR = 'VG Scientific acquisition datafile'
DS_EXT_SUPROPID_AUTHOR         : VT_BSTR = 'vgengineer'
DS_EXT_SUPROPID_COMMENTS       : VT_BSTR = ''
DS_EXT_SUPROPID_CREATED        : VT_DATE  = 11/5/2006   13:35:36

```

DS_EXT_SUPROPID_SAVED : VT_DATE = 11/5/2006 14:31:53

;Standard Properties present:

\$PROPERTIES=STD

```

DS_GEPROPID_TECHNIQUE           : VT_I4   = 17
DS_GEPROPID_INSTRUMENT         : VT_BSTR = 'ESCALab250'
DS_GEPROPID_SOURCE_TYPE       : VT_I4   = 1
DS_GEPROPID_GUID               : VT_BSTR = '{823B2E65-8BB2-4D75-
8518-536FEE14F4F7}'
DS_GEPROPID_SOURCE_GUID       : VT_BSTR = '{823B2E65-8BB2-4D75-
8518-536FEE14F4F7}'
DS_GEPROPID_EXPT_RUN_GUID     : VT_BSTR = '{007F1444-1B99-4164-
893C-A1522841C235}'
DS_GEPROPID_VALUE_TYPE        : VT_I4   = 11
DS_GEPROPID_VALUE_LABEL       : VT_BSTR = 'Counts'
DS_GEPROPID_VALUE_SYMBOL      : VT_BSTR = 'C'
DS_GEPROPID_VALUE_UNIT        : VT_BSTR = ''
DS_DATASTOREID_DATA_STORAGE_METHOD : VT_I4   = 0
DS_SOPROPID_ENERGY            : VT_R4   = 1253.599976
DS_SOPROPID_GUN                : VT_I2   = -1
DS_STPROPID_POS_X              : VT_I4   = 0
DS_STPROPID_POS_Y              : VT_I4   = 0
DS_STPROPID_POS_Z              : VT_I4   = 0
DS_STPROPID_POS_TILT           : VT_I4   = 0
DS_STPROPID_POS_AZIM           : VT_I4   = 0
DS_ACPROPID_START_TIME        : VT_DATE = 11/5/2006 13:36:22
DS_ACPROPID_END_TIME          : VT_DATE = 11/5/2006 14:31:53
DS_ACPROPID_ACQ_TIME          : VT_R4   = 0.099960
DS_ACPROPID_PERIODS           : VT_I4   = 6
DS_ACPROPID_CORRECTION        : VT_R4   = 0.000000
DS_ACPROPID_MODE               : VT_I2   = 0
DS_ACPROPID_DIRECTION         : VT_I2   = 1
DS_ACPROPID_SIG_COMP          : VT_BOOL  = False
DS_ACPROPID_EV_SCALE          : VT_I2   = 1
DS_DEPTHPROFILE_IONGUNPROPID_CURRENT : VT_R4   = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_ENERGY : VT_R4   = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_RASTER_WIDTH : VT_R4   = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_RASTER_HEIGHT : VT_R4   = 0.000000
DS_DEPTHPROFILE_IONGUNPROPID_ANGLETOSURFACE : VT_R4   = 45.000000
DS_DEPTHPROFILE_IONGUNPROPID_IONTYPE : VT_BSTR = 'Ar+'
DS_DEPTHPROFILE_IONGUNPROPID_DESCRIPTION : VT_BSTR = ''
DS_DEPTHPROFILE_PROPS_ROTATION : VT_I4   = 0
DS_ANPROPID_MODE               : VT_I2   = 1
DS_ANPROPID_PASS               : VT_R4   = 50.000000
DS_ANPROPID_WORK_FTN           : VT_R4   = 4.444000
DS_ANPROPID_LENS_MODE_NAME     : VT_BSTR = 'LargeAreaXL'
DS_ANPROPID_TXFN_COEFFS       : VT_I4   = 1
; Property list for DS_ANPROPID_TXFN_COEFF (expecting 1) follows:
DS_ANPROPID_TXFN_COEFF[0]     : VT_R4   = 1.000000

```

;Extended Properties present:

\$PROPERTIES=EXT

; NONE found

=====

;DataSpace has 2 data axes as follows:

; #= start, end, numSpaceAxes

\$DATAAXES=2,#empty#

```

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

```

=====

;DataSpace has 3 space axes as follows:


```

;   #=      start,      width,      numPoints,  axisType,  linear,
symbol,    unit,      label
$SPACEAXES=3
0=      223.600000,      0.200000,      76,  ENERGY,  LINEAR,  'E',
'eV',    'Energy'
1=      0.000000,      600.840000,      6,  ETCHTIME,  NON-LINEAR,
'EtchTime', 's', 'Etch Time'
2=      0.000000,      1.000000,      6,  ETCHLEVEL,  LINEAR,
'EtchLevel', '', 'Etch Level'

;=====

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

```

3.1.3 VG ESCA3 (*.TAP)

Comment:

- First row: ** + region name
- Second row: 8 characters number of steps, 8 characters start energy, 8 characters empty, 8 characters step width, 8 characters pass energy, 8 characters excitation energy, 8 characters number of scans, 8 characters time per step
- Third row to start of next region: 15 characters intensity ten times per row
- Example: multiregion measurement, 1 survey, 4 single regions (S 2p, C 1s, N 1s, O 1s)
- Folder: Install-CD:\Measurement_Reference_Data\03-Esca3(.TAP)\Esca3-MultiReg2.TAP

```

**US
1200****1500*****.8*****50*****1486.6**1*****.4*****
280          207          201          243          204          206
226          221          233          218
252          277          266          247          239          258
279          284          271          279
...
9848          9888          9938          9983          9846          9817
9869          9913          10023         10003
**S2p
200****1330*****.1*****20*****1486.6**3*****1*****
2374          2334          2383          2299          2177          2179
2191          2189          2193          2105
2035          2061          1949          1985          2008          1931
1950          1970          1933          1863
...
2871          2866          2783          2885          2887          2899
2893          2823          2999          2890
2884          2949          2982          2956          2950          2971
2989          2952          2934          3068
**C1s
200****1210*****.1*****20*****1486.6**3*****1*****
8371          8274          8204          8384          8307          8060
8024          7841          7911          7799
7712          7745          7245          7029          7024          6879
6858          6749          6535          6485
...
9292          9421          9408          9170          9259          9228
9306          9257          9263          9196
9233          9129          9274          9045          9234          9198
9166          9241          9191          9562
**N1s
200****1093*****.1*****20*****1486.6**5*****1*****
18327          18075          18128          18163          18351          17911
18006          17780          18030          18093
17978          18101          17998          18011          17880          18067
18060          17946          17995          17680
...
18193          18522          18462          18410          18675          18442
18566          18438          18578          18508
18285          18592          18553          18612          18546          18356
18771          18669          18597          18595
**O1s
200****962*****.1*****20*****1486.6**3*****1*****
12530          12412          12270          12341          12263          12323
12218          12219          12046          12048
12036          12036          11769          12169          11998          12001
12059          11893          11735          11841
...
13163          13029          13096          12800          12906          13365
13075          13071          13097          13024

```

13222	12930	13149	13103	13047	13139
13246	13015	13219	13291		

3.1.4 BESSY (*.*)

Comment:

- 1. – 14. row: acquisition parameters
- from row 15: column1: kinetic energy, column 2: intensity, column 3: flux
- Excitation energy not available
- Intensities are divided by flux (only flux <> 0)
- One single regions is saved
- Example: single region, Cu 2p
- Folder: Install-CD:\XPS_Measurement_Reference_Data\04-BESSY(.TXT)\BESSY-SingleReg-Cu2p-EP=1486.6.TXT

```

komm_row   : Cu 2p
prob_row   : xpsrew Cu Ar+5keV/5mA 5min A112/20
date       :
time       :
source     :
MessMode   : EDC
max_energy : 561.62557
min_energy : 511.60555
pass_energy : 20
step_w     : 0.06100
anz_scans  : 3
count_time : 100
num_of_data : 821
E_kin;resCh;secCh
511.60555;8202;1.0000
511.66655;9032;1.0000
511.72755;9055;1.0000
511.78855;8922;1.0000
511.84955;9028;1.0000
...
561.50355;5248;1.0000
561.56455;5183;1.0000
561.62555;5123;1.00001

```

3.1.5 VSI (*.GPH)

Comment:

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

```

%%%%% 001 # General data
2.10 0.40 HSA FFFFE1F # 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 FFFF529
CHANNELT 2000.0000000000 6 1 1.0000000000 0.0000000000 FFFF651
##### 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
100000.0000000000 # warning level
##### 007 # Ramp Mode Parameter
1 # mode
5.000 # parameter FRR
5.000 # parameter FAT
0 # kinetic energy mode
2 # MCD
0 # adjustable magnification
0.000000 # XPS-Gain
0 # polarity
##### 008 # Timedata
0.1999999285 # Meas time
5.3999977112 # startTime
0.0099999998 # sleepTime
##### 009 # Graphicoptionen
880.000000 882.000000# X-Zoom
20000.000000 30000.000000# Y-Zoom

```

```

##### 011 # Transformation
-1 # Length of Differentiation
-1 # Length of Smoothing
##### 012 # Background Correction
0 # Active
0.000000 # LeftX
0.000000 # LeftY
0.000000 # RightX
0.000000 # RightY
##### 020 # Measure Global
12-05-1997 10:51:01 # Startzeit
12-05-1997 10:59:53 # Endzeit
3 # Averageanzahl
000 # Scanindex
10000 # Kanäle
##### 021 # Measure Segment
1 # Number of Segments
501 0.0099999998 865.000000000 890.000000000 0.0500000007
0.1999999285 # Segmentsize wait start stop inc meastime
0.000000 # MCD Correction
##### 022 # Measure Data
COUNTER
S 0000 865.000000
M 0000 552.333313
S 0001 865.049988
M 0001 567.000000
S 0002 865.099976
M 0002 557.333374
S 0003 865.149963
M 0003 574.333313
...
S 0500 889.993896
M 0500 294.000000
##### ENDE # end of file

```

3.1.6 HHUD (*.DAT)

Comment:

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

XPS 2: XE2425.DAT

Thu Mar 25 16:55:39 1999
nach wartung
au stand nach 4min 4kevar+ mg
Magnesium

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

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

3.1.7 CAF (*.CAF)

Comment:

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

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

3.1.8 KRATOS (*.CIL)

Comment:

- Acquisition parameters are not saved
- 1. column: xywe, 2. column: binding energy BE, 3. column: intensities
- Manual input of all acquisition parameters
- Excitation energy E_P , initial E_I and final energy E_F must give the BE values of the first and last saved energy value
- For the example: Name: K 2p, $E_P = 1486.6$ eV, $E_I = 1173.6$ eV ($1486.6 - 1173.6 = 313$), $E_F = 1198.4$ eV ($1486.6 - 1198.4 = 288.2$), step width = 0.2 eV, dwell time = 1, accumulations = 1
- Example: single region K 2p
- Folder: Install-CD:\XPS_Measurement_Reference_Data\05-Kratos(.CLI)\Kratos-SingleReg-K2p.CIL

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

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

Comment:

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

File (*.INF)

IDENTIFICATION: identification information

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

3709	Number of points per line
210.000000	Acquisition time entered
96.900009	Actual acquisition time
0.000000	SIMS time to sputter before acquisition
0.000000	Linear gating (percent)
3676	SIMS resolution
1486.599976	ESCA anode reference energy
NO	Image registration
CYCLE	Registration type
596	Register:every Nth cycle,region etc.

SEQUENCE CONTROL: acquisition sequence control parameters

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

ELECTRON GUN: electron gun control information

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

ION GUN: ion gun control information

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

X-RAY: x-ray control settings

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

ANGLES: angle information


```

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

```

SIMS ANALYZER: SIMS analyzer information

```

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

```

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

```

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

```

REGION INFORMATION: acquisition control block

```

5                     Number of acb_region structures stored

```

Region acquisition control block structure

```

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

```

```

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

```

```

Region acquisition control block structure
C1           Element name
100         Old time per step
5           Number of sweeps
292.000000  Energy upper limit
10.000000   Energy range
292.000000  Analysis upper limit
10.000000   Analysis range
0.100000    Volts per step
101         Steps per sweep
5           Number of diff points
0.000000    Window width for test acq
1           Flag, acquire data
0           Flag, triggered acquisition
2           Resolution
1           Calculation type
0           Gate trigger
0           Ion polarity
1           Transition
0.000000    Trigger relative rise %
0.000000    Trigger relative fall %
1558        Minimum counts
2794        Maximum counts
2147483647  Peak to peak minimum
0           Peak to peak maximum
0.000000    Actual sputter time
35.750000   Pass energy
35.750000   Retard ratio
2           Number of mcd channels
0.000000    Trigger fracture beam gating
0.000000    Trigger time beam gating
0.000000    Retard energy
0.000000    Ion energy
0.000000    Focus voltage
100.000008  Acceleration voltage
500         Signal to noise limit
100.000000  Time per step

```

```

Region acquisition control block structure
O1           Element name
100         Old time per step
4           Number of sweeps
538.000000  Energy upper limit
12.000000   Energy range
538.000000  Analysis upper limit
12.000000   Analysis range
0.100000    Volts per step
121         Steps per sweep
5           Number of diff points
0.000000    Window width for test acq
1           Flag, acquire data
0           Flag, triggered acquisition
2           Resolution
1           Calculation type
0           Gate trigger
0           Ion polarity
1           Transition
0.000000    Trigger relative rise %
0.000000    Trigger relative fall %

```

1832	Minimum counts
2281	Maximum counts
2147483647	Peak to peak minimum
0	Peak to peak maximum
0.000000	Actual sputter time
35.750000	Pass energy
35.750000	Retard ratio
2	Number of mcd channels
0.000000	Trigger fracture beam gating
0.000000	Trigger time beam gating
0.000000	Retard energy
0.000000	Ion energy
0.000000	Focus voltage
0.000000	Acceleration voltage
500	Signal to noise limit
100.000000	Time per step

Region acquisition control block structure

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

Region acquisition control block structure

S2	Element name
100	Old time per step
16	Number of sweeps
240.000000	Energy upper limit
20.000000	Energy range
240.000000	Analysis upper limit
20.000000	Analysis range
0.100000	Volts per step
201	Steps per sweep
5	Number of diff points

```

0.000000      Window width for test acq
1             Flag, acquire data
0             Flag, triggered acquisition
2             Resolution
1             Calculation type
0             Gate trigger
0             Ion polarity
1             Transition
0.000000      Trigger relative rise %
0.000000      Trigger relative fall %
6087          Minimum counts
8912          Maximum counts
2147483647    Peak to peak minimum
0             Peak to peak maximum
0.000000      Actual sputter time
35.750000     Pass energy
35.750000     Retard ratio
2             Number of mcd channels
0.000000      Trigger fracture beam gating
0.000000      Trigger time beam gating
0.000000      Retard energy
0.000000      Ion energy
0.000000      Focus voltage
0.000000      Acceleration voltage
50            Signal to noise limit
100.000000    Time per step

```

File (*.ASC)

```

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

```

3.1.10 PHI-545/590

3.1.10.1 Single Region (*.TXT)

Comment:

- Acquisition parameters are saved in first row
- First column: binding energies, second column: intensities in counts
- Example: survey
- Folder: Install-CD:\XPS_Measurement_Reference_Data\07-PHI545-590 (.TXT)\PHI545-SingleReg.TXT

Element ; Region 1 of 1; Depth Cycle 1 of 1; Time Per Step 50; Sweeps 5; Anode Mg; Photon Energy 1253.6; XPS;

```

1000  66517
999   66561
998   66742
997   66295
...
5     6557
4     4785
3     2797
2     1563

```

1 1058

3.1.10.2 Multiregion (*.TXT)

Comment:

- Acquisition parameters are saved in first row of each region
- First row: number of regions, excitation energy
- First column: binding energies, second column: intensities in counts
- Example: multiregion C 1s, C KVV, O 1s
- Folder: Install-CD:\XPS_Measurement_Reference_Data\07-PHI545-590 (.TXT)\PHI545-MultiReg.TXT

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

C 1s CKVV O 1s

86.9897 0.000192393 13.0101

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

Anode Mg; Photon Energy 1253.6; XPS;

340 2775

339.95 2789

339.9 2845

...

275.15 1707

275.1 1723

275.05 1630

275 1876

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

Anode Mg; Photon Energy 1253.6; XPS;

1037 14170

1036.9 14298

1036.8 14560

...

957.3 8263

957.2 8116

957.1 8344

957 8109

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

Anode Mg; Photon Energy 1253.6; XPS;

540 3435

539.9 3362

539.8 3460

...

525.3 3153

525.2 3271

525.1 3867

525 3282

3.1.10.3 Profile (*.TXT)

Comment:

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

Depth Cycles 3; Regions 3; SputterTime Interval 180; Photon Energy 1253.6; XPS
 NumberOfPreSputterCycles 1;

Cycle	C 1s	CKVV	O 1s
0	64.9423	14.9515	6.00912
1	64.751	13.63	8.49895
2	69.822	12.6472	6.28457

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

340	2775
339.95	2789
339.9	2845
...	
275.15	1707
275.1	1723
275.05	1630
275	1876

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

1037	14170
1036.9	14298
1036.8	14560
...	
957.3	8263
957.2	8116
957.1	8344
957	8109

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

540	3435
539.9	3362
539.8	3460
...	
525.3	3153
525.2	3271
525.1	3867
525	3282

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

340	2775
339.95	2789
339.9	2845
...	
275.15	1707
275.1	1723
275.05	1630
275	1876

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

1037	14170
1036.9	14298
1036.8	14560
...	
957.3	8263
957.2	8116
957.1	8344
957	8109

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

540	3435
539.9	3362
539.8	3460

```

...
525.3      3153
525.2      3271
525.1      3867
525        3282

```

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

```

340        2775
339.95     2789
339.9      2845

```

```

...
275.15     1707
275.1      1723
275.05     1630
275        1876

```

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

```

1037       14170
1036.9     14298
1036.8     14560

```

```

...
957.3      8263
957.2      8116
957.1      8344
957        8109

```

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

```

540        3435
539.9      3362
539.8      3460

```

```

...
525.2      3271
525.1      3867
525        3282

```

3.1.11 PHI-1600/1600C

3.1.11.1 Standard Format, Version 1 (*.csv)

Comment:

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

```

[ID INFO]
App,PHI SCA XPS
Technique,XPS
Type,MULTIPLEX
Mode,7FAT
Version,1.00
Comment,
[VACUUM INFO]
Vacuum(Pa),0.00
[TRANSMISSION FUNCTION INFO]
A,24.500
B,0.207

```

```
[CONTROL INFO]
NumberOfRegions,3
NumberOfAreas,1
NumberOfAngles,1
NumberOfCycles,16
[INPUT LENS INFO]
LensType,Omnii2
Aperture,4
LensMode,MINIMUM
[SCA CONTROL INFO]
SCAControlType,Model_80_365_B
MinimumEnergyStep,0.025
[X RAY INFO]
Source,Conventional
Anode#,2
WorkFunction(eV),3.50
HighVoltage(kV),15.0
AnodeName,Al
SourceEnergy(eV),1486.6
Power(W),400
[ION GUN INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
SputterRate(nm/min),1.00
BeamVoltage(kV),3.0
GridSupply(V),200
Emission(mA),25.00
Float(V),0
Condenser(%),80.0
Objective(%),65.0
Bend(%),0.0
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
SputterTime(sec),30
[ION GUN NEUTRALIZE INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
BeamVoltage(kV),0.5
GridSupply(V),120
Emission(mA),25.00
Float(V),450
Condenser(%),80.0
Objective(%),65.0
Bend(%),5.0
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
FilamentStatus,OFF
[NEUTRALIZER INFO]
EmissionCurrent(mA),0.000
BiasVoltage(V),0.0
Extractor(V),0.0
XSteering(%),0.0
YSteering(%),0.0
FilamentStatus,OFF
[STAGE INFO]
X(mm),0
Y(mm),0
Z(mm),0
Rotate(deg),0
Tilt(deg),45
DirectionOfRotation,CCW
[DETECTOR INFO]
```



```

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

```

3.1.11.2 Standard Format, Version 2 (*.csv)

Comment:

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

- Folder: Install-CD:\XPS_Measurement_Reference_Data\08-PHI-16001600C (.CSV)\PHI1600-MultiReg-Ver2-AuAg.CSV

Area1

Ag3d

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

Area1

Au4d3

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

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

Comment:

- All acquisition parameters saved in header
- Example: sputter depth profile, 5 regions (C 1s, O 1s, Pt 4f, Cu 2p_{3/2}, Si 2p), 35 sputter cycles
- Folder: Install-CD:\XPS_Measurement_Reference_Data\08-PHI-16001600C (.CSV)\PHI1600-Profile.CSV

```
[ID INFO]
App,PHI_SCA_XPS_V1.3
Technique,XPS
Type,DEPTHPROFILE
Mode,FAT
Version,1.30
Comment,SiO2_3
[VACUUM INFO]
Vacuum(Pa),0.00
[TRANSMISSION FUNCTION INFO]
A,24.500
B,0.207
[CONTROL INFO]
NumberOfRegions,5
NumberOfAreas,1
NumberOfAngles,1
NumberOfCycles,35
[INPUT LENS INFO]
LensType,Omnis3
Aperture,5
LensMode,MINIMUM
[SCA CONTROL INFO]
SCAControlType,Model_80_365
MinimumEnergyStep,0.025
[X RAY INFO]
Source,Monochromated
Anode#,1
```

```
WorkFunction(eV),3.70
HighVoltage(kV),13.0
AnodeName,Al
SourceEnergy(eV),1486.7
Power(W),300
[ION GUN INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
SputterRate(nm/min),1.00
BeamVoltage(kV),3.0
GridSupply(V),200
Emission(mA),25.00
Float(V),0
Condenser(%),80.0
Objective(%),65.0
Bend(%),0.0
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
SputterTime(sec),30
Pressure(mPa),0.000
[ION GUN NEUTRALIZE INFO]
GasSpecies,Ar
IonCurrent(uA),1.000
BeamVoltage(kV),0.5
GridSupply(V),120
Emission(mA),25.00
Float(V),450
Condenser(%),80.0
Objective(%),65.0
Bend(%),5.0
XRaster(%),0.0
YRaster(%),0.0
XOffset(mm),0.00
YOffset(mm),0.00
FilamentStatus,OFF
[NEUTRALIZER INFO]
EmissionCurrent(mA),20.000
BiasVoltage(V),3.0
Extractor(V),0.0
XSteering(%),0.0
YSteering(%),0.0
FilamentStatus,ON
[STAGE INFO]
X(mm),0
Y(mm),0
Z(mm),0
Rotate(deg),0
Tilt(deg),0
DirectionOfRotation,CCW
[DETECTOR INFO]
MultiplierOffset(V),200
MultiplierVoltage(V),1900
[ENERGY SCAN INFO]
EnergyScanMode,Scanned
[PEAK DATA INFO]
PeakDataMode,Height
[SPUTTER INFO]
SputterType,Alternate
ZalarRotation,notused
DirectionOfRotation,CW
XrayWhileSputtering,Off
SputterTime(min),33.00
IntervalTime(min),1.00
DelayTime(sec),15
```

```

[IMAGE INFO]
ImageSize(mm),2.000
FileName,
[REGION INFO]
RegionNumber,RegionName,Lower(eV),Range(eV),PassEnergy(eV),EnergyStep(eV),Time/S
tep(ms),Repeats
1,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
 vgeengineer

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
 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
238.6599999999962
239.6399999999449
233.7399999999547
245.1799999999964
...
193.0999999999989
200.5400000000061
Region 3
sample id
2007
7
11
11
37
34
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
0
C1s

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



```
0
10000
2948.54000000032
2975.699999999348
3025.55999999944
3080.799999999792
...
3039.599999999812
3074.74000000033
3136.04000000021
Region 4
sample id
2007
7
11
12
26
15
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
0
Ga2p3

-1
kinetic energy
eV
356.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
401
0
10000
8753.79999999996
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
321
0
10000
113.819999999877
99.2999999998113
103.619999999768
...
43.7999999998772
35.3000000000432
40.7799999999868
Region 6
sample id
2007
7
11
11
54
25
0
0
XPS
```

```
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
01s

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

```
0
0
0
0
0
Survey
-1
kinetic energy
eV
86.59999999999999
0.5
1
counts per channel
d
pulse counting
0.3
2
0
0
0
0
0
2801
0
10000
113668.31
113261.39
111981.53
111248.01
...
444.8499999999974
197.1399999999988
68.0399999999922
Region 8
sample id
2007
7
11
12
33
29
0
0
XPS
Al
1486.6
1.0E37
1.0E37
1.0E37
1.0E37
1.0E37
FAT
10
1
4.444
0
0
0
0
0
VB
-1
kinetic energy
eV
```

```
1476.6
0.05
1
counts per channel
d
pulse counting
0.3
5
0
0
0
0
0
241
0
10000
37.2599999999985
30.5399999999924
35.53999999999286
...
4.14000000000136
2.259999999999409
2.18000000000005
end of experiment
```

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

Comment:

- SDP' in 7. row means profile (e.g. sputter depth profile, angle resolved measurement)
- Example consists of 21 spectra, i.e. 3 regions (O 1s, C 1s, Si 2p) with 7 steps (sputter time, angle etc.)
- Folder: Install-CD:\XPS_Measurement_Reference_Data\10-Vamas (.VMS)\Vamas-Profile-Si_C_O_20-Parasteps_KE-increasing_Counts_without_Cor_Par.VMS

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

1998
12
21
9
47
2
255
0
XPS
0
```

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

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

1998
12
21
10
33
19
255
0
XPS

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

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

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

18
1
1
1486.6
0
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
01s
01s
-1
Kinetic Energy
eV
947.6
0.1
1

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

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


```
1
1
1486.6
0
0
0
0
0
0
FAT
20
1E+37
4.61
0
0
0
0
0
01s
01s
-1
Kinetic Energy
eV
947.6
0.1
1

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

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

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

Counts
pulse counting
0.3
3
0
0
1
1
1
1
0
0
Cyclic
0
0
0
0
131
1785.06
18039.9
...
1837.52
1842.62
...
Region 2

1998
12
21
10
25
37
255
0
XPS
300
Al K-alpha
18
1
1
1486.6
0
```

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

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

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

```

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

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

```

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

Comment:

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

```

VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4
Not Specified
Kratos Axis Ultra
Not Specified
/C=/data/Hirsch/test_RH_Matrix.dset

```

```
0
MAP
REGULAR
4
41
32768
32768
1
Etch Time
s
0
0
0
0
211
0 1s/2
Not Specified
2013
9
23
11
28
51
0
3
      XPS      Spectrum
Acqn. Time(s): 65           Sweeps: 2           Anode:Mono (Al (Mono)) (150 W)
Step(meV): 100.0
      Dwell Time(ms): 180       Charge Neutraliser :On   Acquired On :13/09/23
11:28:51
XPS
51.31
1.241
0
Mono (Al (Mono))
1486.69
150
1E+37
1E+37
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
0
1s
-1
Kinetic Energy
eV
946.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
```

2
0
1E+37
1E+37
1E+37
0
362
1127
2334
0.709544
0.712206
1127
0.709544
1140
0.709558
1163
0.709573
1141
0.709588
1156
0.709603
...
1281
0.712162
1316
0.712177
1330
0.712192
1333
0.712206
Ag 3d/3
Not Specified

2013

9
23
11
28
51
0
3

XPS Spectrum

Acqn. Time(s): 65

Sweeps: 2

Anode: Mono (Al (Mono)) (150 W)

Step (meV): 100.0

Dwell Time (ms): 180

Charge Neutraliser : On

Acquired On : 13/09/23

11:28:51

XPS

51.31

1.241

0

Mono (Al (Mono))

1486.69

150

1E+37

1E+37

6000

6000

1E+37

1E+37

FAT

80

1E+37

-4.479

0

1E+37

1E+37

1E+37

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

Sweeps: 3 Anode:Mono(Al (Mono)) (150 W)
Charge Neutraliser :On Acquired On :13/09/23

1E+37
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
Bi
4f
-1
Kinetic Energy
eV
1317.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
3
0
1E+37
1E+37
1E+37
0
362
427
912
0.783451
0.786926
517
0.783451
574
0.783462
516
0.783473
...
603
0.786891
592
0.786926
0 1s/7
Not Specified
2013
9
23
11
35
24
0
3

XPS Spectrum
Acqn. Time(s): 65
Step(meV) : 100.0
Dwell Time(ms): 180
11:35:24
XPS

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

51.61
1.241
0
Mono (Al (Mono))
1486.69
150
1E+37
1E+37
6000
6000
1E+37
1E+37
FAT
80
1E+37
-4.479
0
1E+37
1E+37
1E+37
1E+37
0
1s
-1
Kinetic Energy
eV
946.69
0.1
2
Intensity
d
Transmission
d
pulse counting
0.18
2
0
1E+37
1E+37
1E+37
0
362
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 4f_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
```

```
dwel1: 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: "0 1s_2"
ManipulationProtocol:
{
  mp_nstrings = 0;
  mp_strings = {
  }
}
measure_date: 13 09 2005 11 14
filename: "050913_Au_Mg_13"
visible: 0
depth: 1
sputter_def: 0
data: 351 long 2081
10501
10265
10450
...
9563
10156
9816
enddata
background: 351 double 3463
10413.160
10413.160
10413.121
...
9768.989
9806.995
9845.000
endbackground
original: 351 long 2081
10501
```



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

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

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

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

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

3.1.16 VSW-Tübingen (*.dat)

Comment:

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

```
PCF
EISCA
5. 6.2003
```

```
Goetz, 2, Ag3d, Au4f
frei
Referenz Au 123ø mm 474
Gesamtsignal
50.84 Prozent Totzeit
*
2
XPS
FAT
2
X-Ray
1
1.0000000000E+01
1.0000000000E+04
*
486
860.001
884.977
50.0
0.051
0.200
*
486
1144.999
1169.975
50.0
0.051
0.200
*
105890.000000
106290.000000
107775.000000
...
94910.000000
93670.000000
93560.000000
*
72170.000000
```


0.25 1208

3.1.18 ScientaSES-Signals (*.txt)

Comment::

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

[Info]

Number of Regions=2
Version=1.2.2

[Region 1]

Region Name=014

Dimension 1 name=Kinetic Energy [eV]

Dimension 1 size=451

Dimension 1 scale=1060.00000 1060.10000 1060.20000 1060.30000 1060.40000
1060.50000 1060.60000 1060.70000 1060.80000 1060.90000 1061.00000 1061.10000
1061.20000 1061.30000 1061.40000 1061.50000 1061.60000 1061.70000 1061.80000
1061.90000 1062.00000 1062.10000 1062.20000 1062.30000 1062.40000 1062.50000
1062.60000 1062.70000 1062.80000 1062.90000 1063.00000 1063.10000 1063.20000

...

1101.10000 1101.20000 1101.30000 1101.40000 1101.50000 1101.60000 1101.70000
1101.80000 1101.90000 1102.00000 1102.10000 1102.20000 1102.30000 1102.40000
1102.50000 1102.60000 1102.70000 1102.80000 1102.90000 1103.00000 1103.10000
1103.20000 1103.30000 1103.40000 1103.50000 1103.60000 1103.70000 1103.80000
1103.90000 1104.00000 1104.10000 1104.20000 1104.30000 1104.40000 1104.50000
1104.60000 1104.70000 1104.80000 1104.90000 1105.00000

[Info 1]

Instrument=SES 2002-2MS201

Location=WERA

User=CP

Sample=WERA20

Comments=La0.9Ce0.1CoO3

xsl=-240 50/50 size=5 slit=2.5

Date=8/15/2007

Time=5:32:08 PM

Region Name=VB_1100

Excitation Energy=0

Energy Scale=Kinetic

Acquisition Mode=Swept

Center Energy=9

Low Energy=1060

High Energy=1105

Energy Step=0.1

Step Time=100

Detector First X-Channel=1

Detector Last X-Channel=471

Detector First Y-Channel=127

Detector Last Y-Channel=536

Number of Slices=1

Lens Mode=Transmission

Pass Energy=100

Number of Sweeps=3

Time per Spectrum Channel=24.3

[User Interface Information 1]

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

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

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

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

Date=8/15/2007
Time=5:32:08 PM
Region Name=Ce_La_Co_1100
Excitation Energy=0
Energy Scale=Kinetic
Acquisition Mode=Swept
Center Energy=9
Low Energy=120
High Energy=340
Energy Step=0.1
Step Time=100
Detector First X-Channel=1
Detector Last X-Channel=471
Detector First Y-Channel=127
Detector Last Y-Channel=536
Number of Slices=1
Lens Mode=Transmission
Pass Energy=100
Number of Sweeps=3
Time per Spectrum Channel=24.3

[User Interface Information 2]
Monochromator Energy= 0.0000


```
[Manipulator]
Z=-0.313
Phi=-0.203
Ph. energy=1099.995
XSL=-239.962
```

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

3.1.19 ScientaSES-Spectra (*.txt)

Comment:

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

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

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

```
[Info 1]
Instrument=R3000-6MS014
Location=Scienta
User=Scienta
Sample=transmission
Comments=
Date=5/14/2009
Time=11:41:49 AM
Region Name=Ag 3d5
Excitation Energy=1486.6
Energy Scale=Binding
Acquisition Mode=Swept
Center Energy=9
Low Energy=1111.6
High Energy=1121.6
Energy Step=0.05
Step Time=200
Detector First X-Channel=19
Detector Last X-Channel=784
Detector First Y-Channel=210
Detector Last Y-Channel=609
```

Number of Slices=100
 Lens Mode=Transmission
 Pass Energy=50
 Number of Sweeps=4
 Time per Spectrum Channel=87.2

[User Interface Information 1]

R1=0.000

R2=0.000

[Data 1]

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

3.1.20 PHI Spectrometer

Comment:

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

3.1.20.1 Multiregion Measurements (*.spe)

Software Version 1: SS 2.1.0.1

- Example of 2 regions: Te 3d_{5/2}, Bi 4f
- Folder: Install-CD:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V1-SS 2.1.0.1.SPE

SOFH

Platform: PC

Technique: XPS

FileType: SPECTRUM

FileDesc: Bi2Te3

SoftwareVersion: SS 2.1.0.1

InstrumentModel: PHI VersaProbe II

AcqFilename: C:\ZCH\120685\120685.11.BST 307 TP.spe

FileDate: 2012 8 16

AcqFileDate: 2012 8 16

Institution: PHI

Operator:

ExperimentID: 120685

EnergyReference: none 0.0

AnalyserWorkFcn: 4.218 eV

AnalyserRetardGain: 1.000207

PlatenID:

PhotoFilename: 120685.7.Low Mag.pho

SXIFilename:

SourceAnalyserAngle: 45.0 d

AnalyserSolidAngle: 20.0 sr

IntensityRecal: no

IntensityCalCoeff: 100.000 0.330

EnergyRecal: no

ScanDeflectionSpan: 50 70

ScanDeflectionOffset: 0 -20

SCAMultiplierVoltage: 1650.0 V

```
NarrowAcceptanceAngle: no
PeakToNoiseRatioState: no
DelayBeforeAcquire: 5 seconds
C60IonGun: None
BiasBoxMode: 0
SemFieldOfView: 0.0000000
EBeamCurrent: 0.0 nA
ImageSizeXY: 0.0000 0.0000
IonGunMode: Standby
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 2.000 kV
FloatVolt: 0.0 V
FloatEnable: no
GridVolt: 150.0
CondensorVolt: 1420.00
ObjectiveVolt: 1344.00
BendVolt: 26.00
SputterRaster: 3.00 3.00 mm
SputterRasterOffset: -0.690 -0.300 mm
TargetSputterTime: 2.0 min
SputterEmission: 15.00 mA
DeflectionBias: 0.0 V
XpsScanMode: scanned
AnalyserMode: FAT
SurvNumCycles: 15
SurvTimePerStep: 50.000000
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2197 3136
PhotoOffsetInPixel: 1519 200
PhotoSizeInMm: 35.000 50.000
PhotoOffsetInMm: 0.008 0.008
NoSpectralRegFull: 5
SpectralRegDefFull: 1 1 Te3d5 52 301 -0.1000 597.0000 567.0000 596.0000 568.0000
0.000000 5.85 AREA
SpectralRegDef2Full: 1 30.0 1 0 8 1
SpectralRegBackgroundFull: 1 0.0 582.0 0.0
SpectralRegHeroFull: 1 582.0 0.0 0.0 0.00
SpectralRegDefFull: 2 0 Sb3d5 51 201 -0.1000 545.0000 525.0000 544.0000 526.0000
0.000000 5.85 AREA
SpectralRegDef2Full: 2 20.0 1 0 8 1
SpectralRegBackgroundFull: 2 0.0 535.0 0.0
SpectralRegHeroFull: 2 535.0 0.0 0.0 0.00
SpectralRegDefFull: 3 1 Bi4f 83 201 -0.1000 172.0000 152.0000 171.0000 153.0000
0.000000 5.85 AREA
SpectralRegDef2Full: 3 20.0 1 0 8 1
SpectralRegBackgroundFull: 3 0.0 162.0 0.0
SpectralRegHeroFull: 3 162.0 0.0 0.0 0.00
SpectralRegDefFull: 4 0 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 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 1 1 (-279.7 -8247.6 18557.9 45.0 -90.1)
SpatialAreaDesc: 1 Bi2Te3
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 0
XrayPower: 25.61 W
XrayBeamDiameter: 100.0 um
XrayBeamVoltage: 15000.0 V
XrayCondenserLensVoltage: 8230.0 V
XrayObjectiveCoilCurrent: 0.748 A
XrayBlankingVoltage: 325.0 V
XrayFilamentCurrent: 1.576 A
XrayStigmator: 0.0 0.0
XrayHighPower: no
EgunNeutMode: Off
NeutralizerCurrent: 0.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 30.0 V
EgunNeutXSteering: 0.0
EgunNeutYSteering: 0.0
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 1458.6 eV
SxiPassEnergy: 376 eV
SxiLens2: 476 V
SxiLens3: 406 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 350.0 V
SxiDisplayMode: 2
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.698
Channel Info: 2 1 1.467
Channel Info: 3 1 1.392
Channel Info: 4 1 1.320
Channel Info: 5 1 1.251
Channel Info: 6 1 1.103
Channel Info: 7 1 1.074
Channel Info: 8 1 1.026
Channel Info: 9 1 1.001
Channel Info: 10 1 0.941
Channel Info: 11 1 0.824
Channel Info: 12 1 0.819
Channel Info: 13 1 0.750
Channel Info: 14 1 0.650
Channel Info: 15 1 0.674
Channel Info: 16 1 1.266
StagePosition: 8.0986 0.7914 18.5579 45.0062 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 1
DefectPosComment: Bi2Te3
DefectPosU: -0.2797
DefectPosV: 8.2476
DefectPosX: 8.0986

```

DefectPosY: 0.7914
DefectPosZ: 18.5579
DefectPosTilt: 45.0063
DefectPosRotation: -90.0500
DefectPosAligment: None
DefectPosReferenceImage: 120685.7.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH

```

```

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

```

Software Version 2: XPS V1.00

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

```

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

```

```

SpectralRegDef: 2 2 Ag3d 47 201 -0.100 382.000 362.000 382.000 362.000 2.560
11.75 none
SpectralRegDef: 3 3 Au4f 79 201 -0.100 99.000 79.000 99.000 79.000 2.560 11.75
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
      L      +
f8 È+ 0      1      y|      chn      sar      c/s
c/s      f8 H- ø,      L      É      chn      sar
sar      c/s      f8 H- @3      çhR'ç81A-
4±Mò AØÅ »0¹ A»hèfàr AM|G¹¾ Až.²%|Ð A¹ %ÚPÌ AÂèR¹fY A¹ púýM AØEÎ¹O? AíçnÐù¹
...

```

Software Version 3: XPS V1.20

- Example of 9 regions: Cu 2p, Ag 3p_{1/2}, Ag 3d, Au 4f, C 1s, Au 3p, Au 4d_{3/2}, Au 4d_{5/2}, C 1s
- Folder: Install-CD:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V3-XPS V1.20.SPE

```

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

```

```

SpectralRegDef: 3 3 Ag3d 47 161 -0.100 378.000 362.000 378.000 362.000 1.250
23.50 none
SpectralRegDef: 4 4 Au4f 79 181 -0.100 97.000 79.000 97.000 79.000 1.250 23.50
none
SpectralRegDef: 5 5 C1s 6 201 -0.100 300.000 280.000 300.000 280.000 1.250 23.50
none
SpectralRegDef: 6 6 Cu3p 29 502 -0.100 109.100 59.000 109.100 59.000 1.250 23.50
none
SpectralRegDef: 7 7 Au4d3 79 201 -0.100 364.000 344.000 364.000 344.000 1.250
23.50 none
SpectralRegDef: 8 8 Au4d5 79 201 -0.100 345.000 325.000 345.000 325.000 1.250
23.50 none
SpectralRegDef: 9 9 O1s 8 201 -0.100 543.000 523.000 543.000 523.000 1.250 23.50
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDesc: 1
EOFH
      \L +
      -          chn      sar          c/s
f8 ø
      pL
      1@ÿø†µ/† 1@ ó" /k†@DUTÑ...8†@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 µm
NeutralizerEnergy: 1.0 eV
NeutralizerCurrent: 20.0 mA
SourceAnalyzerAngle: 90.0 d
AnalyzerSolidAngle: 7 sr
AnalyzerMode: FAT
AnalyzerWorkFcn: 3.7 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA

```

```

SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 5
SpectralRegDef: 1 1 Sc2p3 21 171 -0.100 412.000 395.000 412.000 395.000 0.740
11.75 none
SpectralRegDef: 2 2 Ge3d 32 681 -0.025 40.000 23.000 40.000 23.000 2.220 5.85
none
SpectralRegDef: 3 3 Gd3d 64 1001 -0.100 1275.000 1175.000 1275.000 1175.000
2.220 11.75 none
SpectralRegDef: 4 4 O1s 8 361 -0.050 541.000 523.000 541.000 523.000 0.740 11.75
none
SpectralRegDef: 5 5 C1s 6 151 -0.100 293.000 278.000 293.000 278.000 1.480 11.75
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
| à †
f8 X| ð
c/s f8 H† H•
sar c/s f8 H f8 H
chn sar c/s f8 H f8 H
ø; chn sar | c/s | f8 H chn sar c/s
f8 ,† G ñ†d ~|°@-dÃóît~@ÀE@o
...

```

Software Version 5: XPS V2.0

- Example of 1 regions: survey
- Folder: Install-CD:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V5-XPS V2.0.SPE

```

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

```



```

SputterEnergy: 4.000 keV
SputterCurrent: 15.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 4.2 A/s
NoSpectralReg: 1
SpectralRegDef: 1 1 1su 111 1351 -1.0000 1345.0 -5.0 1345.0 -5.0 1.760000
117.40 AREA
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (22045.7 4351.8 24560.0 45.0 -0.3)
SpatialAreaDesc: 1 Nr1 Bahn sauber1
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH

```

```

      +          G|          pnt 7777sar 7777 77777777c/s 7777777
77777f8 78* p          1*          Δ>リ@          *  リ@          ・・リ@
λeリ@          Δvリ@          瑾リ@          phリ@          ・{`リ@          夕87リ@          夕h湍@          ・・華@          1Hリ@          ~曖@          @7
↓リ@          夕ネリ@          @j.リ@          `DZリ@          >リ@          !@リ@
・@リ@          N@リ@          @:葦@          瑜@          ・鯨@          `・@          `リ祖@          @z  5@          3・@          聡@
・vリ@          潦@          ・+1@          ・3
...

```

Software Version 6: XPS V3.5s

- Example of 1 region: survey
- Folder: Install-CD:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V6-XPS V3.5S.SPE

```

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

```

```

PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 1
SpectralRegDef: 1 1 C1 6 401 -0.050 275.400 255.400 275.400 255.400 0.250 5.85
none
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (127.0, 127.0, 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
      +
2005\06c\s05\XPS2.PCS f8 e^ p          chn e~1\sar ni~2
è³@   ø²@   ,´@   T´@   ì³@   "²@   ³@   ¬³@   $´@   ²@
³@   ü³@   ð³@   ø³@   ð³@   Ð³@   ´@   (´@   ´@   ô³@
...

```

Software Version 7: EIS V2.1

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

```

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

```

Software Version 8: Compass V7.2.2

- Example of 6 regions: Ni 2p, Al 2p, Al 2s, O 1s, C 1s, VB
- Folder: Install-CD:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V8-Compass V7.2.2.SPE

```

SOFH
Platform: PC
Technique: XPS
FileType: SPECTRUM
FileDesc: Xu Sample-A
SoftwareVersion: Compass V7.2.2
InstrumentModel: PHI Quantera SXM
Institution: PHI
FileDate: 2006 7 3

```

```

AcqFileDate: 2006 7 3
AcqFilename: Xu-A_060703-02.spe
Operator:
ExperimentID: Ota
PlatenID: Platen 1
PlatenDesc: Xu_A-C
StagePosition: 21.4967 37.2531 24.0190 45.0000 -0.0066
PhotoFilename: Xu-A_060703-02.pho
ActualPhotoFilename: /C=/Program
Files/PHI/Compass7.2.1/datafiles/photos/3_1151890988.pho
SXIFilename: none
ActualSXIFilename:
XraySource: Al 1486.6 mono
XrayPower: 25.10 W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 0.0 V
NeutralizerCurrent: 0.0 uA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 4.125 eV
IntensityRecal: no
IntensityCalCoeff: 82.402 0.235
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 2.000 keV
SputterCurrent: 25.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0.2 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 Ni2p 28 401 -0.1250 890.0 840.0 890.0 844.0 12.000000
69.00 AREA
SpectralRegDef: 2 2 Al2p 13 241 -0.1250 85.0 55.0 75.0 68.0 12.000000
69.00 AREA
SpectralRegDef: 3 3 Al2s 13 321 -0.1250 130.0 90.0 110.0 90.0 12.000000
69.00 AREA
SpectralRegDef: 4 4 O1s 8 241 -0.1250 550.0 520.0 540.0 527.0 1.200000
69.00 AREA
SpectralRegDef: 5 5 C1s 6 241 -0.1250 300.0 270.0 300.0 275.0 1.200000
69.00 AREA
SpectralRegDef: 6 6 V11s 112 401 -0.1250 30.0 -20.0 30.0 -20.0 1.200000
69.00 AREA
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (21339.2 37232.7 24019.0 45.0 0.0)
SpatialAreaDesc: 1 sample-A
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH
      -   @1   +
i c/s Té↑  j   Äçrÿf8  ^
... P1          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
      +
È c/s Tèl  j   iÂrøf8 h" p          Mj          pnt °·oøsar j          *køh
     e^lâe   @çäe   àûäe   @øåe   ÀRå   ø"   e åe   íåe   -äe   @ûäe
...

```

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
  J      e      +
  J      f4      L      .
  ...
  E      pnt      sar      p↑      c/s      +
  E      pnt      sar      p↑

```

Software Version 11: XPS 3.3

- Example of 5 region: C 1s, O 1s, Au 4f, N 1s, Si 2p
- Folder: Install-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@      e†Éf8      (L      ð
...

```

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 0.0
NoSpectralReg: 3
SpectralRegDef: 1 1 Fls 9 101 -0.2000 699.0000 679.0000 698.0000 680.0000
0.200000 46.95 AREA
SpectralRegDef2: 1 20.0 1 0 4 1 0.00
SpectralRegBackground: 1 0.0 689.0 0.0
SpectralRegHero: 1 689.0 0.0 0.0 0.0
SpectralRegDef: 2 1 Ols 8 101 -0.2000 543.0000 523.0000 542.0000 524.0000
0.200000 46.95 AREA
SpectralRegDef2: 2 20.0 1 0 4 1 0.00
SpectralRegBackground: 2 0.0 533.0 0.0
SpectralRegHero: 2 533.0 0.0 0.0 0.0
SpectralRegDef: 3 1 La3d5 57 126 -0.2000 850.0000 825.0000 849.0000 826.0000
0.200000 46.95 AREA
SpectralRegDef2: 3 25.0 1 0 4 1 0.00
SpectralRegBackground: 3 0.0 837.5 0.0
SpectralRegHero: 3 837.5 0.0 0.0 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 1 1 (10354.5 2256.9 18760.0 45.0 -90.0)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 0
XrayPower: 25.61 W
XrayBeamDiameter: 100.0 um
XrayBeamVoltage: 15000.0 V
XrayCondenserLensVoltage: 8230.0 V
XrayObjectiveCoilCurrent: 0.748 A
XrayBlankingVoltage: 325.0 V
XrayFilamentCurrent: 1.577 A
XrayStigmator: 0.0 0.0
XrayHighPower: no
EgunNeutMode: Neutralize
NeutralizerCurrent: 0.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 40.0 V
EgunNeutXSteering: 1.0
EgunNeutYSteering: 4.0
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 694.0 eV
SxiPassEnergy: 188 eV
SxiLens2: -591 V
SxiLens3: -560 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 349.9 V
SxiDisplayMode: 1
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.698
Channel Info: 2 1 1.467
Channel Info: 3 1 1.392
Channel Info: 4 1 1.320
Channel Info: 5 1 1.251
Channel Info: 6 1 1.103
Channel Info: 7 1 1.074
Channel Info: 8 1 1.026
Channel Info: 9 1 1.001


```

Channel Info: 10 1 0.941
Channel Info: 11 1 0.824
Channel Info: 12 1 0.819
Channel Info: 13 1 0.750
Channel Info: 14 1 0.650
Channel Info: 15 1 0.674
Channel Info: 16 1 1.266
StagePosition: -2.6672 -9.4501 18.7598 45.0094 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 1
DefectPosComment:
DefectPosU: 10.3546
DefectPosV: -2.2577
DefectPosX: -2.6672
DefectPosY: -9.4501
DefectPosZ: 18.7598
DefectPosTilt: 45.0094
DefectPosRotation: -90.0500
DefectPosAlignment: None
DefectPosReferenceImage: 120530.20.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
|      à  †      e  †      pnt      cyc      c/s
ñDnw|  □  f4 5$!  δ      1      1      e  †      pnt      cyc
...

```

Software Version 4: XPS V1.30

- Example. sputter depth profile with 41 sputter steps (sputter time: 30 s, -30 ... 1170) and 6 regions: C 1s, O 1s, Ni 2p_{3/2}, Fe 2p_{3/2}, Cr 2p_{3/2}, Mo 3d,
- Folder: Install-CD:\XPS_Measurement_Reference_Data\19-PHI-Profile(.PRO)\PHI-Profile-V4-XPS V1.30.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
Comment: Nr 3 TP
SoftwareVersion: XPS V1.30
InstrumentModel: PHI Model 1600/3057
Institution:
FileDate: 2009 07 05
AcqFileDate: 2009 07 05
AcqFilename: C:\XPS_Data\Besmehn\19650018.pdt
Operator:
ExperimentID:
PlatenID:
PlatenDesc: Nr 3 TP
StagePosition: 0.0 0.0 0.0 0.0 0.0
SampleID:
SampleDesc:
PhotoFilename: none
SXIFilename: none
XraySource: Al 1486.7 mono
XrayPower: 300 W
XrayBeamDiameter: 0.0 um
NeutralizerEnergy: 1.0 eV
NeutralizerCurrent: 20.0 mA
SourceAnalyzerAngle: 90.0 d
AnalyzerSolidAngle: 7 sr
AnalyzerMode: FAT
AnalyzerWorkFcn: 3.7 eV
IntensityRecal: no

```

```

IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: Ar
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 C1s 6 261 -0.050 291.000 278.000 291.000 278.000 0.200 11.75
HEIGHT
SpectralRegDef: 2 2 O1s 8 261 -0.050 539.000 526.000 539.000 526.000 0.200 11.75
HEIGHT
SpectralRegDef: 3 3 Ni2p3 28 441 -0.050 871.000 849.000 871.000 849.000 0.200
11.75 HEIGHT
SpectralRegDef: 4 4 Fe2p3 26 401 -0.050 723.000 703.000 723.000 703.000 0.300
11.75 HEIGHT
SpectralRegDef: 5 5 Cr2p3 24 361 -0.050 588.000 570.000 588.000 570.000 0.200
11.75 HEIGHT
SpectralRegDef: 6 6 Mo3d 42 361 -0.050 240.000 222.000 240.000 222.000 0.300
11.75 HEIGHT
NoDPDataCyc: 41
NoPreSputterCyc: 2
SputterInterval: 30.000 s
SputterMode: alt
SampleRotation: off
DepthRecal: no
NoSpatialArea: 1
SpatialAreaDef: 1 Area1 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDescription: 1
EOFH
  ▣      L  +                ▣  )  -      cyc      reg
...

```

Software Version 5: XPS V2.0

- Example. sputter depth profile with 11 steps and 6 regions: C 1s, O 1s, Cu 2p, N 1s, Ag 3d, S 2p
- Folder: Install-CD:\XPS_Measurement_Reference_Data\19-PHI-Profile(.PRO)\PHI-Profile-V5-XPS V2.0.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
FileDesc: none
SoftwareVersion: XPS V2.0
InstrumentModel: PHI Quantum 2000
Institution: PHI
FileDate: 2006 1 30
AcqFileDate: 2006 1 30
AcqFilename: Profilschleifer001.pro
Operator: ro
ExperimentID: 2006-0067
PlatenID: 0067b
PlatenDesc: none
StagePosition: 7.4316 38.0950 8.6000 45.0000 -0.0207
PhotoFilename: Profilschleifer001.pProfilschleifer001.sxi
ActualPhotoFilename: /D=/Compass6.1.1/datafiles/photos/1_1138109828.pho
SXIFilename: Profilschleifer001.sxi
ActualSXIFilename: /D=/Compass6.1.1/datafiles/SXIs/1_1138176141.sxi
XraySource: Al 1486.6 mono
XrayPower: 19.47 W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 2.5 V
NeutralizerCurrent: 5.0 uA

```

```

SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 3.9 eV
IntensityRecal: no
IntensityCalCoeff: 23.460 0.183
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 1.000 keV
SputterCurrent: 15.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0.4 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 Cu2p 29 161 -0.0500 936.0 928.0 936.0 928.0 13.199999
23.50 AREA
SpectralRegDef: 2 2 C1s 6 201 -0.0500 290.0 280.0 290.0 280.0 15.840002 23.50
AREA
SpectralRegDef: 3 3 O1s 8 201 -0.0500 537.0 527.0 537.0 527.0 26.399998 23.50
AREA
SpectralRegDef: 4 4 N1s 7 161 -0.0500 403.0 395.0 403.0 395.0 13.199999 23.50
AREA
SpectralRegDef: 5 5 Ag3d 47 301 -0.0500 379.0 364.0 375.0 364.0 10.559999
23.50 AREA
SpectralRegDef: 6 6 S2p 16 201 -0.0500 166.0 156.0 166.0 158.0 26.399998 23.50
AREA
NoDPDataCyc: 11
NoPreSputterCyc: 1
SputterMode: alt
SampleRotation: off
DepthRecal: no
NoDepthReg: 10
DepthCalDef: 1 Layer1 2 0.4000
DepthCalDef: 2 Layer2 3 0.4000
DepthCalDef: 3 Layer3 4 0.4000
DepthCalDef: 4 Layer4 5 0.4000
DepthCalDef: 5 Layer5 6 0.4000
DepthCalDef: 6 Layer6 7 0.4000
DepthCalDef: 7 Layer7 8 0.4000
DepthCalDef: 8 Layer8 9 0.4000
DepthCalDef: 9 Layer9 10 0.4000
DepthCalDef: 10 Layer10 11 0.4000
LayerRegionFlags: Cycle 1 0 0 0 0 0 0
LayerRegionFlags: Cycle 2 0 0 0 0 0 0
LayerRegionFlags: Cycle 3 0 0 0 0 0 0
LayerRegionFlags: Cycle 4 0 0 0 0 0 0
LayerRegionFlags: Cycle 5 0 0 0 0 0 0
LayerRegionFlags: Cycle 6 0 0 0 0 0 0
LayerRegionFlags: Cycle 7 0 0 0 0 0 0
LayerRegionFlags: Cycle 8 0 0 0 0 0 0
LayerRegionFlags: Cycle 9 0 0 0 0 0 0
LayerRegionFlags: Cycle 10 0 0 0 0 0 0
LayerRegionFlags: Cycle 11 0 0 0 0 0 0
NoSpatialArea: 1
SpatialAreaDef: 1 Point1 1 (6185.8 36097.0 8600.0 45.0 -0.3)
SpatialAreaDesc: 1 Nr1 Schleifer Stelle1
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH
  ▣      L  +      ▣
  -      cyc 7777reg 7777 7777777s 7777777777777f8 7+1  +L  1      1
  ...

```

Software Version 10: Without software specification

- Example. sputter depth profile with 20 sputter steps (step width: 3, from -3 to 54) and 12 regions: C 1s, O 1s, F 1s, Na 1s, Si 2p, Cr 2p, Fe 2p, Ni 2p, N 1s, Mo 3d, Cu 2p, Mn 2p
- Folder: Install-CD:\XPS_Measurement_Reference_Data\19-PHI-Profile(.PRO)\PHI-Profile-V10-without_software_specification.PRO

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
FileDesc: 1) ASF III Lu Einbau 2005 IV
FileDate: 108 7 21
AcqFileDate: 108 7 21
AcqFilename: ham26_2.pro
ScanMode: scan
StagePosition: 0.0 0.0 0.0 45.0 0.0
XraySource: Al 1486.6 mono
XrayPower: 300.00 W
NeutralizerEnergy: 0.0 eV
NeutralizerCurrent: 0.0 mA
SourceAnalyserAngle: 90.0 d
AnalyserMode: FAT
AnalyserWorkFcn: 4.5 eV
IntensityRecal: no
IntensityCalCoeff: 24.500 0.207
EnergyRecal: no
EnergyReference: none 0.0
SputterIon: 3He
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 10.0 0.0 um
PreAcqSputterTime: 6 s
PreAcqSputterRate: 1.0 A/s
NoSpectralReg: 12
SpectralRegDef: 1 1 C1 6 200 -0.1000 295.0 275.0 295.0 280.0 0.100000 23.50 none
SpectralRegDef: 2 2 O1 8 200 -0.1000 540.0 520.0 540.0 525.0 0.100000 23.50 none
SpectralRegDef: 3 3 F1 9 200 -0.1000 695.0 675.0 695.0 680.0 0.100000 23.50 none
SpectralRegDef: 4 4 Na1 11 200 -0.1000 1081.0 1061.0 1081.0 1066.0 0.100000
23.50 none
SpectralRegDef: 5 5 Si1 14 200 -0.1000 110.0 90.0 110.0 95.0 0.100000 23.50 none
SpectralRegDef: 6 6 Cr1 24 400 -0.1000 605.0 565.0 605.0 567.0 0.100000 23.50
none
SpectralRegDef: 7 7 Fe1 26 400 -0.1000 735.0 695.0 735.0 700.0 0.100000 23.50
none
SpectralRegDef: 8 8 Ni1 28 500 -0.1000 890.0 840.0 890.0 844.0 0.100000 23.50
none
SpectralRegDef: 9 9 N1 7 200 -0.1000 410.0 390.0 410.0 394.0 0.100000 23.50 none
SpectralRegDef: 10 10 Mo1 42 200 -0.1000 240.0 220.0 240.0 223.0 0.100000 23.50
none
SpectralRegDef: 11 11 Cu1 29 500 -0.1000 970.0 920.0 970.0 924.0 0.100000 23.50
none
SpectralRegDef: 12 12 Mn1 25 400 -0.1000 670.0 630.0 670.0 632.0 0.100000 23.50
none
NoDPDataCyc: 20
NoPreSputterCyc: 2
SputterInterval: 3.000 s
SputterMode: alt
SampleRotation: off
DepthRecal: no
NoSpatialArea: 1
SpatialAreaDef: 1 Full 1 (0.0 0.0 0.0 0.0 0.0)
EOFH
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Software Version 11: XPS V1.3.6

- Example. sputter depth profile with 7 sputter steps (step width: 60 s, from 0 to 360) and 5 regions: Cu 2p, Ni 2p, Ti 2p, O 1s, Si 2p
- Folder: Install-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

```

      •      °  †
f8 ↑      °  †      □ • |      cyc      reg      s
c/s * eV      f8 ↑  EL | • |      cyc      reg      chn
...

```

Software Version 12: SS 2.5.0.9

- Example of 1 regions: survey
- Folder: Install-CD:\XPS_Measurement_Reference_Data\18-PHI-NORM(.SPE)\PHI-MultiReg-V1-SS 2.5.0.9.SPE

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 0.0
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 0.0
SpectralRegIR: 1 0 0.000 0.000 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 13 4 (8215.5 5905.4 19312.7 46.0 -90.1) (9615.5 5905.4 19312.7
46.0 -90.1) (9615.5 6105.4 19312.7 46.0 -90.1) (8215.5 6105.4 19312.7 46.0 -
90.1)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 1
XrayPower: 92.65 W
XrayBeamDiameter: 100.0 um
XrayBeamVoltage: 20000.0 V
XrayCondenserLensVoltage: 9250.0 V
XrayObjectiveCoilCurrent: 0.929 A
XrayBlankingVoltage: 400.0 V
XrayFilamentCurrent: 1.621 A
XrayStigmator: 0.0 0.0
XrayHighPower: yes
EgunNeutMode: Neutralize
NeutralizerCurrent: 20.0 uA
NeutralizerEnergy: 1.01 V
EgunNeutExtractor: 50.0 V
EgunNeutXSteering: 2.0
EgunNeutYSteering: 4.1
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 534.0 eV
SxiPassEnergy: 188 eV
SxiLens2: -711 V
SxiLens3: -673 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 342.0 V
SxiDisplayMode: 1
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.661
Channel Info: 2 1 1.490
Channel Info: 3 1 1.499
Channel Info: 4 1 1.268
Channel Info: 5 1 1.149

```

Channel Info: 6 1 1.100
Channel Info: 7 1 1.148
Channel Info: 8 1 1.079
Channel Info: 9 1 1.118
Channel Info: 10 1 1.021
Channel Info: 11 1 0.942
Channel Info: 12 1 0.803
Channel Info: 13 1 0.730
Channel Info: 14 1 0.627
Channel Info: 15 1 0.634
Channel Info: 16 1 1.028
StagePosition: -5.8668 -8.6215 19.3127 46.0031 -90.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 13
DefectPosComment:
DefectPosU: 8.9165
DefectPosV: -6.0062
DefectPosX: -5.8668
DefectPosY: -8.6215
DefectPosZ: 19.3127
DefectPosTilt: 46.0031
DefectPosRotation: -90.0500
DefectPosAlignment: None
DefectPosReferenceImage: 140420.1.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
XRaySetting: 100u100W20kV_HP
EOFH
...

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

Comment:

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

Software Version 1: SS 2.1.0.1

- Example. angle resolved measurement with 15 angles (angle steps: 5°, 15°...85°) and 6 regions: Si 2p, Ti 2p, O 1s, Hf 4f, Ni 2p_{3/2}, Al 2p
- Folder: Install-CD:\XPS_Measurement_Reference_Data\19-PHI-Profile(.ANG)\PHI-Profile-V1-SS 2.1.0.1.ANG

```

SOFH
Platform: PC
Technique: XPS
FileType: ANGLEPRO
FileDesc:
SoftwareVersion: SS 2.1.0.1
InstrumentModel: PHI VersaProbe II
AcqFilename: C:\ZCH\120749\Temp120749.23.AN20120601C01_1_1.ang
FileDate: 2012 11 14
AcqFileDate: 2012 11 14
Institution: PHI
Operator:
ExperimentID: 120749
EnergyReference: none 0.0
AnalyserWorkFcn: 4.218 eV
AnalyserRetardGain: 1.000207
PlatenID:
PhotoFilename: 120749.17.Low Mag.pho
SXIFilename:

```



```
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
IntensityRecal: no
IntensityCalCoeff: 100.000 0.204
EnergyRecal: no
ScanDeflectionSpan: 50 70
ScanDeflectionOffset: 0 -20
SCAMultiplierVoltage: 1650.0 V
NarrowAcceptanceAngle: yes
PeakToNoiseRatioState: no
DelayBeforeAcquire: 5 seconds
C60IonGun: None
BiasBoxMode: 0
SemFieldOfView: 0.0000000
EBeamCurrent: 0.0 nA
ImageSizeXY: 0.0000 0.0000
IonGunMode: Off
SputterIon: Ar+
SputterCurrent: 0.000 uA
SputterRate: 0.000 A/min
SputterEnergy: 4.000 kV
FloatVolt: 0.0 V
FloatEnable: no
GridVolt: 150.0
CondensorVolt: 2780.00
ObjectiveVolt: 2688.00
BendVolt: 52.00
SputterRaster: 3.00 3.00 mm
SputterRasterOffset: -0.810 -0.310 mm
TargetSputterTime: 2.0 min
SputterEmission: 0.00 mA
DeflectionBias: 0.0 V
XpsScanMode: scanned
AnalyserMode: FAT
SurvNumCycles: 15
SurvTimePerStep: 50.000000
NoPolarAngles: 15
PolarAngles: 15.0 20.0 25.0 30.0 35.0 40.0 45.0 50.0 55.0 60.0 65.0 70.0 75.0
80.0 85.0
PolarAngleCycles: 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
PhotoZoomMode: Low Magnification
PhotoSizeInPixel: 2197 3136
PhotoOffsetInPixel: 1519 200
PhotoSizeInMm: 35.000 50.000
PhotoOffsetInMm: 0.008 0.008
NoSpectralRegFull: 7
SpectralRegDefFull: 1 1 Si2p 14 76 -0.2000 110.0000 95.0000 109.0000 96.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 1 15.0 20 0 6 1
SpectralRegBackgroundFull: 1 0.0 102.5 0.0
SpectralRegHeroFull: 1 102.5 0.0 0.0 0.00
SpectralRegDefFull: 2 1 Ti2p 22 101 -0.2000 468.0000 448.0000 467.0000 449.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 2 20.0 25 0 6 1
SpectralRegBackgroundFull: 2 0.0 458.0 0.0
SpectralRegHeroFull: 2 458.0 0.0 0.0 0.00
SpectralRegDefFull: 3 1 O1s 8 61 -0.2000 539.0000 527.0000 538.0000 528.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 3 12.0 10 0 6 1
SpectralRegBackgroundFull: 3 0.0 533.0 0.0
SpectralRegHeroFull: 3 533.0 0.0 0.0 0.00
SpectralRegDefFull: 4 0 N1s 7 61 -0.2000 405.0000 393.0000 404.0000 394.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 4 12.0 20 0 6 1
SpectralRegBackgroundFull: 4 0.0 399.0 0.0
SpectralRegHeroFull: 4 399.0 0.0 0.0 0.00
```

SpectralRegDefFull: 5 1 Hf4f 72 86 -0.2000 26.0000 9.0000 25.0000 10.0000
0.000000 23.50 AREA
SpectralRegDef2Full: 5 17.0 25 0 6 1
SpectralRegBackgroundFull: 5 0.0 17.5 0.0
SpectralRegHeroFull: 5 17.5 0.0 0.0 0.0
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 0.0
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 0.0
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 0.0
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 0.0
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 0.0
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 0.0
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 0.0
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 0.0
NoSpatialArea: 1
SpatialAreaDef: 1 2 1 (-7006.4 -3844.4 12719.4 45.0 -0.1)
SpatialAreaDesc: 1
SpatialHRPhotoCor: 1 (0.0 0.0)
XraySource: Al 1486.6 mono
XrayAnodePosition: 0
XrayPower: 25.61 W
XrayBeamDiameter: 100.0 um
XRayBeamVoltage: 15000.0 V
XRayCondenserLensVoltage: 8230.0 V
XRayObjectiveCoilCurrent: 0.748 A
XRayBlankingVoltage: 325.0 V
XRayFilamentCurrent: 1.575 A
XRayStigmator: 0.0 0.0
XRayHighPower: no
EgunNeutMode: Off
NeutralizerCurrent: 0.0 uA
NeutralizerEnergy: 1.00 V
EgunNeutExtractor: 30.0 V
EgunNeutXSteering: 0.0

```

EgunNeutYSteering: 0.0
EgunNeutFilament: 0.00 A
EgunNeutPulseLength: 10.0 msec
SxiPersistence: 1 V
SxiSecPerDisplay: 1.0
SxiAutoContrast: yes
SxiAutoContrastLow: 0.30
SxiAutoContrastHigh: 0.30
SxiBindingEnergy: 534.0 eV
SxiPassEnergy: 188 eV
SxiLens2: -711 V
SxiLens3: -673 V
SxiLensBias: 0 V
SxiShutterBias: yes
SxiShutterBiasVoltage: 350.0 V
SxiDisplayMode: 2
Detector Acq Time: 20.0 (min)
Number Of Channels: 16
Channel Info: 1 1 1.698
Channel Info: 2 1 1.467
Channel Info: 3 1 1.392
Channel Info: 4 1 1.320
Channel Info: 5 1 1.251
Channel Info: 6 1 1.103
Channel Info: 7 1 1.074
Channel Info: 8 1 1.026
Channel Info: 9 1 1.001
Channel Info: 10 1 0.941
Channel Info: 11 1 0.824
Channel Info: 12 1 0.819
Channel Info: 13 1 0.750
Channel Info: 14 1 0.650
Channel Info: 15 1 0.674
Channel Info: 16 1 1.266
StagePosition: -7.6122 3.8962 12.7194 45.0062 -0.0500
StageCurrentRotationSpeed: 0.6700
DefectPosID: 2
DefectPosComment:
DefectPosU: -7.0063
DefectPosV: 3.8434
DefectPosX: -7.6114
DefectPosY: 3.8962
DefectPosZ: 12.7194
DefectPosTilt: 45.0094
DefectPosRotation: -0.0500
DefectPosAlignment: None
DefectPosReferenceImage: 120749.17.Low Mag.pho
Deconvolution: no
DeconvolutionPassEnergy: 2.95 eV
DeconvolutionPeakToNoise: 100
EOFH
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  ▣  f4 ;D◀  +L
...

```

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 Cls 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  ÐL  1      1      1      L      □      ang      reg
...

```

- 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  +          □  '  L          ang  reg          sin
  ...

```

Software Version 5: XPS V2.0

- Example. angle resolved measurement with 5 angles and 6 regions: Cu 2p, C 1s, O 1s, N 1s, Ag 3d, S 2p

- Folder: Install-CD:\XPS_Measurement_Reference_Data\19-PHI-Profile(.ANG)\PHI-Profile-V5-XPS V2.0.ANG

```

SOFH
Platform: PC
Technique: XPS
FileType: ANGLEPRO
FileDesc: none
SoftwareVersion: XPS V2.0
InstrumentModel: PHI Quantum 2000
Institution: PHI
FileDate: 2006 1 25
AcqFileDate: 2006 1 25
AcqFilename: Winkelschleifer003.ang
Operator: ng
ExperimentID: 2006-0067
PlatenID: 0067b
PlatenDesc: none
StagePosition: 60.5992 38.3998 8.3400 45.0000 -0.0207
PhotoFilename: Winkelschleifer003.pWinkelschleifer003.sxi
ActualPhotoFilename: /D=/Compass6.1.1/datafiles/photos/1_1138109828.pho
SXIFilename: Winkelschleifer003.sxi
ActualSXIFilename: /D=/Compass6.1.1/datafiles/SXIs/1_1138176890.sxi
XraySource: Al 1486.6 mono
XrayPower: 19.47 W
XrayBeamDiameter: 100.0 um
NeutralizerEnergy: 2.5 V
NeutralizerCurrent: 5.0 uA
SourceAnalyserAngle: 45.0 d
AnalyserSolidAngle: 20.0 sr
AnalyserMode: FAT
AnalyserWorkFcn: 3.9 eV
IntensityRecal: no
IntensityCalCoeff: 23.460 0.183
EnergyRecal: no
SputterIon: Ar+
SputterEnergy: 1.000 keV
SputterCurrent: 15.0 nA
SputterRaster: 0.0 0.0 um
PreAcqSputterTime: 0 s
PreAcqSputterRate: 0.4 A/s
NoSpectralReg: 6
SpectralRegDef: 1 1 Cu2p 29 461 -0.0500 950.0 927.0 940.0 927.0 5.760000
23.50 AREA
SpectralRegDef: 2 2 C1s 6 301 -0.0500 295.0 280.0 295.0 280.0 5.760000 23.50
AREA
SpectralRegDef: 3 3 O1s 8 261 -0.0500 540.0 527.0 539.0 527.0 7.200000 23.50
AREA
SpectralRegDef: 4 4 N1s 7 241 -0.0500 406.0 394.0 404.0 394.0 5.760000 23.50
AREA
SpectralRegDef: 5 5 Ag3d 47 401 -0.0500 380.0 360.0 380.0 364.0 7.200000
23.50 AREA
SpectralRegDef: 6 6 S2p 16 301 -0.0500 170.0 155.0 170.0 158.0 10.800000 23.50
AREA
NoPolarAngles: 5
NoSpatialArea: 1
SpatialAreaDef: 1 Point3 1 (59385.6 36657.7 8340.0 45.0 -0.3)
SpatialAreaDesc: 1 Nr3 Schleifer Stelle1
SpatialHRPhotoCor: 1 (0.0 0.0)
EOFH
  ▣      L  +
  ïïïïïïïf8 ïg  +L  1      1  |  -      ang ïïïïreg ïïïï ïïïïïïïdeg ïïïï
  ïïïïïïïc/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 "
...
```

3.1.21 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_Sils.cexp
ScriptFile=E3-110222N004.cexp
SampleTemperature=300
SamplePressure=1.0E-9
ThetaManipulatorNormal=0.0
PhiManipulatorReference=0.0
CalculatedInitialManipulatorAngles=No
ThetaManipulatorInitial=0.0
PhiManipulatorInitial=0.0
PhotonSource=MXPS Al Ka
PhotonEnergy=1486.600
RegionName=O1s_20
EnergyScale=Binding
AnalyserMode=FAT/CAE
PassEnergy=20.000
DwellTime=0.1

```

```

AutoSupplyRange=Yes
EnergyHigh=524.235
EnergyLow=540.785
WorkFunction=4.200
EnergyFirst=525.000
EnergyLast=540.000
NumberOfEnergies=301
EnergyStep=-0.050
NumberOfSweeps=15
LensMode=Mono Range
KIris=19.0
RIris=10.0
MeasurementType=Energy spectrum
StartDate=22.02.2011
StartTime=17:37:42
EndDate=22.02.2011
EndTime=17:47:25
InternalDimensions=EnergySetpoint

```

[Detector]

```

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

```

[Data]

```

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

```

3.1.23 SSI-XPS (*.MRS)

Comment:

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

```

file_version=2
type=0 (node)
head_count=1
data=Multiple RegionS
regions=1
file_path=C:\ESC\NID\2DMPD35R

```

```
file_name=2DMPD35R
file_type=MRS
pause_flag=0
oper=nid
aperture=0
fgeV=0.
lo_be=275.
up_be=295.
res=2.
spot=2
time_limit=251.
pump_extra_min=0
time_stamp=Thu Sep 29 16:34:24 2011
desc=4-10-2-20 1500cycles 185C
desc2=Ru3d
!
type=0 (node)
data=Region node
head_count=0
!
sub_data_file=1.REG
file_version=2
type=0 (node)
head_count=2
data=Spectrum
region=1
scan_limit=5
tech=scanned
count_limit=0.
time_limit=251.
det_ms=100
fgeV=0.
spot=2
spot_type=3
res=2
res_ev=20.41
aperture=0
sensitivity_exponent=0.5
xrays=0
xrays_ev=0.
start=Thu Sep 29 16:31:24 2011
scan_total=5
delta_ev=0.
detw_ev=8.3
pass_ev=67.38
ref_ev=1486.6
finis=Thu Sep 29 16:34:24 2011
time_total=142.
!
type=0 (node)
head_count=3
data=Data node
!
type=12 (int array)
data=Data Array
lo_be=275.
up_be=295.
array_size=201
!
403
371
...
75
73
!
type=12 (int array)
```

```

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

```

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

```
lo_be=-50.
model_area=1.064
fwhm=23.554
!
0.000
0.000
...
0.000
0.000
!
type=14 (float array)
array_size=102
data=Model
model_num=4
peak_type=100
model_limit=50
up_be=51.
lo_be=-50.
model_area=1.064
fwhm=23.554
!
0.000
0.000
...
0.000
0.000
!
type=0 (node)
data=Peaks
head_count=4
!
type=14 (float array)
array_size=37
data=Peak
peak_num=1
long_desc=# 1: 279.86 eV    0.86 eV    10838.74 cts    19.94%
area_fit=10838.74
up_be=281.6
lo_be=278.
displayed=1
!
256.358
253.726
...
79.117
79.100
!
type=14 (float array)
array_size=83
data=Peak
peak_num=2
long_desc=# 2: 284.13 eV    1.91 eV    20494.73 cts    37.70%
area_fit=20494.732
up_be=288.2
lo_be=280.
displayed=1
!
440.793
440.311
...
167.432
156.168
!
type=14 (float array)
array_size=81
data=Peak
```

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

3.1.24 SPECS Phoibos225 (*.XY)

Comment:

- Measurement data format generated via converter using the SPECSLab Software

- example has six regions:
 1. Survey, Scans 1, Pass 40 eV
 2. VB, Scans 5, Pass 20
 3. Sb2p3/2 Sb2p1/2, Scans 2, Pass 40
 4. Survey, Scans 1, Pass 40
 5. VB, Scans 5, Pass 20
 6. Sb3/2 Sb1/2, Scans 1, Pass 40
- the header of the region includes all important recording parameters
- Data: KE, two space characters, intensities (cps)
- the intensities are saved after the two lines: # ColumnLabels and #
- Example: multi region high energy measurement, excitation energy: 5900 eV, 6 regions: survey, VB, Sb 2p, survey 1, VB 1, Sb 2p
- Folder: Install-CD:\XPS_Measurement_Reference_Data\23-SPECS-Phoibos(.XY)\SPECS-Phoibos-MultiReg-HEXPS-Separatescans.XY

```
# Created by:          SpecsLab2, Version 2.60-r21162
#
# XY-Serializer Export Settings: as follows
# Comment Prefix:      #
# Counts Per Second:   yes
# Kinetic Energy Axis: yes
# Separate Scan Data:  yes
# Separate Channel Data: no
# External Channel Data: no
# Transmission Function: no
# Asymmetry Recalculation: no
# ErrorBar:            no
#
# Group:               MS24
#
# values in kinetic energy
# Region:              Survey
# Analysis Method:     UPS
# Analyzer:            PHOIBOS HSA15000 DLD 225 R6-HV[HWTtype 31:60, 32:63, 33:64,
542:511] DLD
# Analyzer Lens:       SmallArea:3.5kV
# Analyzer Slit:       4:3x20\2:open
# Scan Mode:           FixedAnalyzerTransmission
# Number of Scans:     1
# Curves/Scan:         1
# Values/Curve:        2008
# Dwell Time:          0.3
# Excitation Energy:   5900
# Kinetic Energy:      4900
# Pass Energy:         40
# Bias Voltage:        50
# Detector Voltage:    2650
# Eff. Workfunction:   4.658
# Source:              UVDummy
# Comment:
#
# Cycle: 0
#
# Cycle: 0, Curve: 0, Scan: 0
#
# ColumnLabels: energy counts/s
#
4900 1090
4900.5 1063.3333
...
5903 0
```



```
5903.5  0

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

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

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

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

# Cycle: 0, Curve: 0, Scan: 4
```

```
#
# ColumnLabels: energy counts/s
#
5890 25
5890.05 26
...
5903.95 2
5904 2.5

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

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

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

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

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

3.1.25 Energy-Intensity (*.dat)

Comment:

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

Version 1: BE decreasing

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

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

Version 2: BE increasing

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

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

Version 3: KE decreasing

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

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

Version 4: KE increasing

- Example: single region

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

```
BE  Int
1458.61    583
1458.64    595
1458.67    598
...
1465.54    240
1465.57    252
1465.6     217
```

3.2 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

```

4 Files Created Using UNIFIT

4.1 Exported Files

4.1.1 Call: [File – Export] (*.DAT)

4.1.1.1 Standard Windows

Comment:

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

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

4.1.1.2 3D-Waterfall 0°

Comment:

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

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

4.1.1.3 3D-Waterfall 0° Plus

Comment:

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

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

```

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

```

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

Comment:

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

```

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

```

4.1.1.5 Parameter Plot

Comment:

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

```

Energy      0      1      2      3      ...      9      10
Parameter C1s Peak1  O1s Peak1  O1s Peak2  Si2p Peak1  Si2p Peak2  Si2p Peak3
0  199.99999999999994  1.000000000000031  999.9999999999999  998.985316335666  ...
1  799.9999999999998  99.9999999999998  899.9999999999997  367.7999999999992  ...
2  799.9999999999998  199.9999999999995  799.9999999999996  135.2999999999989  ...
...
8  199.9999999999994  799.9999999999996  199.9999999999998  0  ...

```

```

9      799.999999999998  899.999999999996  99.9999999999967  0      ...
10     799.999999999998  999.999999999999  0.999999999999153  0      ...

```

4.1.1.6 Wagner Plot

Comment:

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

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

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

Comment:

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

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

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

Comments:

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

```

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

```

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

Comment:

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

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

decimal character - comma, delimiter - Tab

Product function, absolute parameters; all parameters exported

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

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

decimal character - dot, delimiter - semicolon

Product function, absolute parameters; all parameters exported

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

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

Comment:

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

C:\UNIFIT31\BEISPIEL.TAP

Fenster: ;Komponente;Peakname: Fläche (cps*eV);Empf.-Fa.;Korr.Fläche;Atomproz.

1;1;S2p;10614.9235;0.54;19657.2659;10.7111497012371;

2;1;C1s;32946.5733;0.25;131786.293;71.8097178740435;

3;1;N1s;4058.77430;0.42;9663.74834;5.26573001823287;

4;1;O1s;14793.3872;0.66;22414.2230;12.2134024064866;

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_2016_User_Files\examples\Calibration_Intensity_Cu.ufp
- Example of 3 lines (Cu 2p, Cu 3p and survey), Cu 2p3 and Cu 3p fitted, project comment, quantification
- Data structure: ,space'+,Auger parameter'+,='+,position photoelectron peaks as BE'+,+'+,position Auger peak as KE'+,space'+,space'+,name of Auger parameter'

3

0 2016

1

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-1

-1

-1

300

21

30

1

0

0

0

frei

frei

Calibration of intensity scale

Acquisition conditions:

Twin, LAX, 50eV pass

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119857.939026664
206
411
C:\Users\rhesse\Documents\Unifit_2016_User_Files\examples\Calibration_Intensity_
Cu\CUATLX19.VMS
1
12
Cu2p3_0
Cu2p3_0
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411
523.6
564.6
0.1
10
1486.6
3
0.3
FAT
3-5-2004
23295.2

23118.5
23312.2
23248.2
23248.7
23117.2
23163.2
23192.3
23189.6
23266.4
23005.6
23149.6
23308.6
23062.1
23132.7
23313.4
23224.6
23148.4
23299.8
23196.4
23320.4
23257.7
23245.1
23085.6
22983.8
22991.1
23133
23289.4
22981
23021.3
23436
23574.4
23281.3
23008
23165.2
23235.9
23274.1
23239.7
23035.9
23117.4
23382.1
23295.1
23317.4
23107
23131.4
23378.1
23157.3
23291
23342.7
23496.7
23283.8
23293.5
23202.3
23407.7
23197.6
23488.6
23543.2
23404.1
23467.4
23524.9
23547.2
23637.8
23658.7
23696.1
23820.7
23963.7
23885.2

23954.7
23766.4
23897
23861.9
24046.7
24224.2
24388.4
24151.8
24394.1
24360.3
24674.3
24769.5
25155.8
25233
25275
25615.9
25914.5
25779.3
26122.9
26406.9
27010.9
27557.3
27907
28325.1
29123
29725.3
30550.9
31617.5
32442.9
33900.1
35115.9
36240.81
37541.56
39214.8
40514.53
41926.83
42850.79
43348.7
43499.78
43151.8
42549.82
41377.66
40165.61
38949.07
37109.99
35305.93
33991.7
32672.62
31341.24
29783.09
28875.94
28069.84
27470.46
26884.02
26251.74
25656.53
25260.46
24901.9
24810.52
24324.52
24001.17
23689.34
23505.6
23353.8
23218.05
22950.42

22825.78
22745.92
22581.12
22449.29
22657.66
22204.4
22173.21
22065.13
21914.06
21942.75
22095.5
21742.55
21706.65
21628.56
21695.16
21646.55
21643.82
21615.08
21506.93
21495.3
21495.96
21719.95
21569.77
21335.37
21319.21
21531.32
21398.7
21481.54
21566.87
21480.9
21318.7
21282.54
21229.77
21515.82
21332.38
21187.48
21276.89
21146.46
21296.37
21182.42
21295.99
21321.67
21106.66
20939.26
20774.97
20772.64
20596.18
20705.98
20749.7
20649.88
20526.21
20715.48
20632.67
20757.62
20778.88
20508.4
20360.98
20650.1
20593.82
20810.71
20494.26
20411.72
20576.7
20672.29
20360.02
20396.75

20390.28
20217.81
20217.11
20111.32
20164.06
20082.28
20098.19
20017.45
19762.31
19621.78
19692.46
19692.26
19822.1
19640.15
19479.47
19634.65
19331.9
19347.1
19519.33
19523.74
19237.21
19442.21
19323.07
19313.81
19207.46
19197.67
19552.18
19468.57
19244.42
19371.44
19589.64
19351.05
19273.28
19244.02
19350.23
19158.76
19151.71
19308.89
19145.13
19061.44
19006.4
18894.16
18962.45
19062.44
19160.37
19119.1
18962.64
18967.57
19079.17
19234.77
19184.65
19138.99
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19130.44
18947.6
19202.16
19402.21
19307.85
19411.75
19446.73
19448.99
19445.29
19373.09
19654.06
19655.6
19492.2

19456.58
19582.33
19424.45
19572.69
19667.12
19670.57
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20035.31
19785.14
20034.05
20096.47
20054.08
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20358.27
20650.79
20792.02
20990.4
21447.51
21815.65
22267.91
22660.87
23428.17
24236.18
24974.63
26001.11
27274.42
28875.28
31090.46
33183.28
36260.9
39772.87
44242.29
49367.75
55288.75
61094.58
66596.37
71574.03
74958.34
76770.7
75914.42
72974.4
67573.32
60873.16
54680.98
48012.27
42280.18
37596.21
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30533.52
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26111.47
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23095.16
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20972.94
20222.29
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19118.95
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17075.17
17012.25
16687.97
16624.58

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15111.28
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15072.79
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14893.29
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14740.37
14700.98
14836.13
14806.11
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14749.37
14644.92
14814
14638.55
14712.89
14678.45
14593.33
14540.01
14316.33
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14514.75
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14294.94
14282.89
14119.48
14020.39
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14233.44
14294.22
14133.62
14082.83
14008.21
14015.65
14042.06
14069.44
14295.46
14133.02
14115.04
13960.35
14101.75
14000.64
14029.81
13986.87
14119.73
14090.24
14086.83
14204.63

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14094.55
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13725.84
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13542.67
13536
13570.76
13712.63
13853.88
13892.22
13808.54
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943
922
21
Binding Energy / eV
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14803425
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12303291
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9671571
8289918
6974058
8453888
16776960
16744703
16711680
33023
4227327
4227200
8421631
8454143
8454016
8453888
16777088
16744448

12615935
12615935
16744703
4227327
8421376
16744576
8388863
33023
12632256
0
5066061
0
90
1
1
1
1
0
16777215
15263976
0
90
1
1
1
1
1
8454143
65535
4227327
0
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Wahr
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Wahr
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8421631
8454143
8454016
8453888

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16777088
16744448
12615935
12615935
16744703
4227327
8421376
16744576
8388863
33023
12632256
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0
5
Kurve 1
Kurve 2
Kurve 3
Kurve 4
Kurve 5
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1
1
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-1
-1
-1
300
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0
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frei
frei
Calibration of intensity scale
Acquisition conditions:
Twin, LAX, 50eV pass
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512
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512
348
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4
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Doublet
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12377.7387706924
1
401
C:\Users\rhesse\Documents\Unifit_2016_User_Files\examples\Calibration_Intensity_
Cu\CUATLX19.VMS
1
12
Cu3p_0
Cu3p_0
0
401
1391.6
1431.6
0.1
10
1486.6
3
0.3
FAT
3-5-2004
1184.84
1206.17
1197.49
1200.52
1184.73
```


1189.21
1200.13
1215.37
1185.15
1204.03
1222.89
1178.49
1189.05
1193.54
1169.85
1098.47
1130.98
1168.7
1180.86
1158.11
1149.82
1192.34
1170.82
1115.21
1142.45
1060.73
1075.01
1114.02
1136.36
1136.07
1133.86
1169.87
1161.87
1133.71
1096.39
1134.99
1143.06
1096.99
1127.12
1146.74
1132.25
1146.33
1104.88
1108.31
1139.04
1116.31
1050.14
1083.29
1152.12
1122.91
1126.48
1099.77
1102.3
1086.27
1044.65
1096.24
1099.27
1152.47
1110.47
1122.82
1128.63
1127
1102.84
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4.3 Fit-Parameter File (*.PAR)

Comment:

- first row: single peak or doublet
- second row:
 - a) number with three digits: background was fitted, second and third digit = number of peaks
 - b) number with two digits: background subtracted, number = number of peaks
- Parameters
- XPS: for fitted background: last six rows = background parameters: constante parameter, linear parameter, square parameter, cubic parameter, Shirley parameter, Tougaard parameter
- XAS: for fitted background: next five rows = background parameters: constante parameter, linear parameter, square parameter, cubic parameter, Shirley parameter, number of steps, per step: hight, E-A mixing, position, FWHM

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4.4 Annotation/Design File (*.DSG)

Remark:

- saved in Unifit_2016_User_Files\design\GaAs-survey.dsg

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Ga 3d
0.956521739130435
0.866583541147132
As 3d
0.939393939393939
0.822942643391521
As (L3M45M45)
0.792322215229704
0.594219653179191
C 1s
0.769433465085639
0.713216957605985
Ga (L3M45M45)
0.679043423536816
0.530635838150289
O 1s
0.608558842039018
0.438150289017341

O (KL23L23)
0.272087568412823
0.66383701188455
Ga 2p3
0.206851119894598
0.251870324189526
Ga 2p1
0.13965744400527
0.397755610972569
As 2p3
0.0632411067193676
0.0236907730673317
As 2p1
-0.00592885375494071
0.0511221945137157
C (KL23L23)
0.0691699604743083
0.665835411471322
|
0.794210195091252
0.757225433526012
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GaAs_Ozone
0.262429200755192
0.0751445086705202
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```
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_2016_User_Files\cross section*.cro
- example: estimated inelastic electron scattering cross section of SiO₂

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

5 Data Banks Integrated in UNIFIT

5.1 Auger Parameter (*.AUP)

Comment:

- Saved in Unifit_2016_User_Files\auger parameters
- Example of Ag 3d5 and Ag (M4N45N45)
- Data structure: ,space'+,Auger parameter'+,='+,position photoelectron peak as BE'+,+'+,position Auger line as KE'+,space'+,space'+,name of the Auger parameter'

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

5.2 Peaks Positions of Photoelectron Lines (*.POS)

Comment:

- Saved in Unifit_2012_User_Files\lines
- Example of the Ag 3d5 peak
- Data structure: ,space'+,position as BE'+,space'+,space'+,name of compound'

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

5.3 Sensitivity Factors (*.SEN)

Comment:

- 1. row ,Sensitivity Factors'
- from row 2: line, comma, sensitivity factor, line...
- number of data pairs as many as you needed
- saved in Unifit2012_User_Files\sensitivity factors
- Example: Wagner factors

Sensitivity Factors

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

5.4 Satellite File (satellit.set)

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

Comment:

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

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

Magnesiumsatelliten 1

8.4
0.08
0
0
0
0
0
0

...

0

0

0

Aluminiumsatelliten 5

69.7
0.0055
0
0
0
0
0
0
0
0

Magnesiumsatelliten 5

48.5
0.005
0
0
0
0
0
0
0
0

5.5 Doublet File (doublet.dda)

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

Comment:

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

Dublett Werte

Ag3p, 0.5, 30.8, Ag3d, 0.666, 6.00, Al2p, 0.5, 0.4, Ar2p, 0.5, 2.2, As3d, 0.5, 0.7, Au4d, 0.666, 18.1, Au4f, 0.75, 3.65
Ba3d, 0.666, 15.4, Ba4d, 0.666, 2.6, Bi4d, 0.666, 23.9, Bi4f, 0.75, 5.39, Bi5d, 0.666, 3.1, Br3p, 0.5, 7.0, Br3d, 0.666, 1.0
Ca2p, 0.5, 3.5, Cd3p, 0.5, 34.1, Cd3d, 0.666, 6.76, Cd4d, 0.666, 0.6, Ce3d, 0.666, 18.3, Ce4d, 0.666, 4.0, Cl2p, 0.5, 1.6, Co2p, 0.5, 15.05
Co3p, 0.5, 2.0, Cr2p, 0.5, 9.3, Cr3p, 0.5, 1.0, Cs3d, 0.666, 13.9, Cs4d, 0.666, 2.3
Cu2p, 0.5, 19.8, Cu3p, 0.5, 2.4, Dy4d, 0.666, 0.0, Dy4p, 0.5, 40.3, Er4p, 0.5, 45.8, Er4d, 0.666, 0.0, Eu3d, 0.666, 31.1
Eu4d, 0.666, 0.0, Fe2p, 0.5, 13.2, Fe3p, 0.5, 1.0, Ga2p, 0.5, 26.8, Ga3p, 0.5, 3.0, Ga3d, 0.666, 0.4, Gd4d, 0.666, 0.0
Ge2p, 0.5, 31.1, Ge3p, 0.5, 4.1, Hf4d, 0.666, 8.5, Hf4f, 0.75, 1.55, Hg4d, 0.666, 19.4, Hg4f, 0.75, 4.1, Ho4d, 0.666, 0.0
Ho4p, 0.5, 36.8, I3d, 0.666, 11.52, I4d, 0.666, 2.0, In3p, 0.5, 37.9, In3d, 0.666, 7.6, In4d, 0.666, 0.9, Ir4d, 0.666, 15.6, Ir4f, 0.75, 2.95
K2p, 0.5, 2.8, Kr3p, 0.5, 7.8, La3d, 0.666, 16.8, La4d, 0.666, 2.8, Lu4p, 0.5, 53.2, Lu4d, 0.666, 9.8, Mg2p, 0.5, 0.4
Mn2p, 0.5, 11.25, Mn3p, 0.5, 1.0, Mo3p, 0.5, 16.6, Mo3d, 0.666, 3.15, Nb3p, 0.5, 15.5, Nb3d, 0.666, 2.8, Nd4d, 0.666, 0.0

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

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