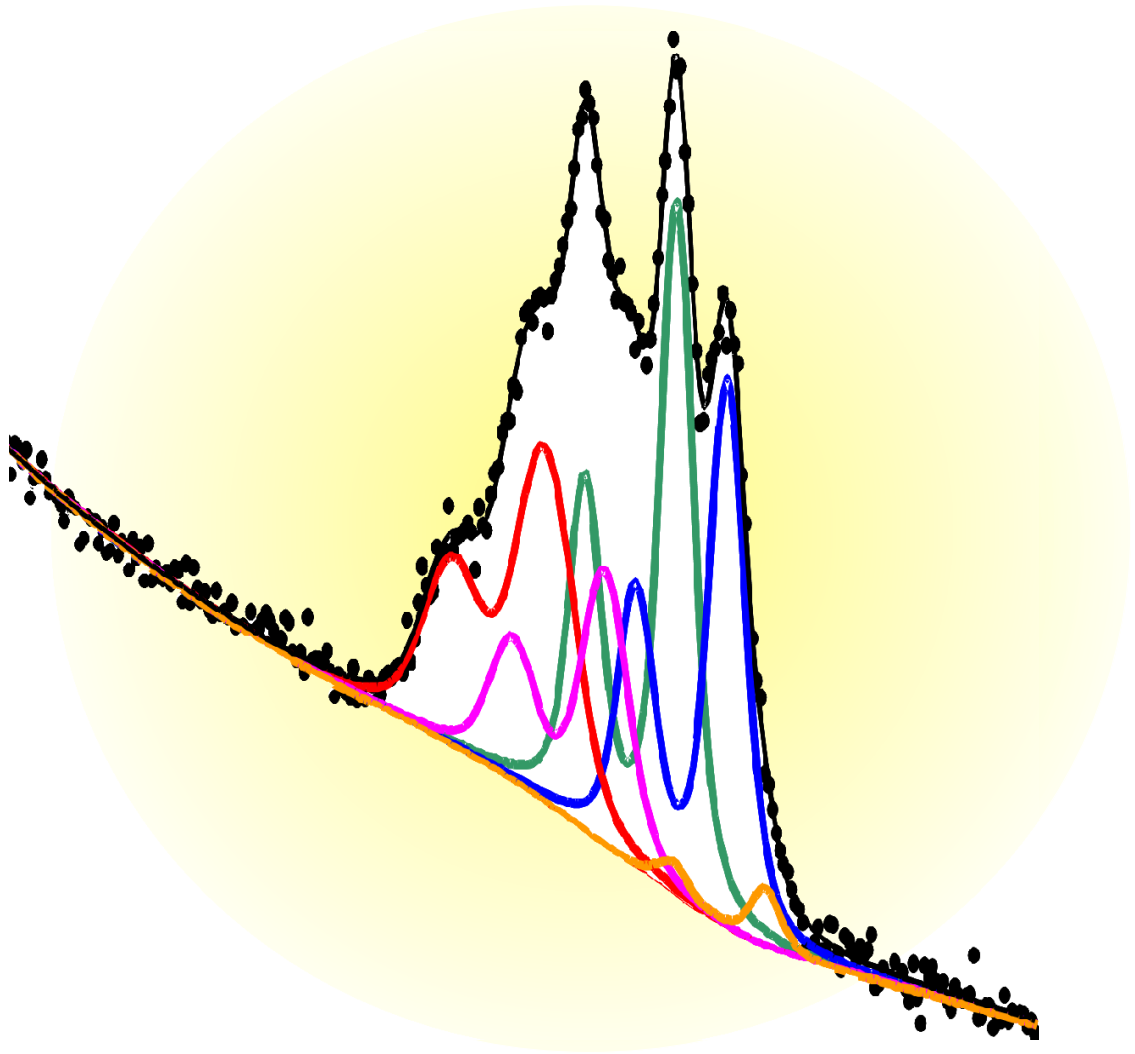


unifit FOR WINDOWS



Line Positions and Data Formats

Version 2012

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Unifit for Windows

Data Formats

Version 2012

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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_2012_User_Files\lines. The second part gives the chemical shifts of some compounds.

line positions.pos

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

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

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

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

279* Os 4d5	340* Pd 3d3
280* Ru 3d5	341* Yb 4p3
281* Sr 3p1	342* Th 4f5
283* U (N67O45V)	344* Zr 3p1
283 Sm 4p1	347* Ca 2p3
284* Ru 3d3	349 Sm 4s
285* Tb 4p3	350* Ca 2p1
285* C 1s	352* Ag (M5N45N45)
287 Kr 3s	353* Ho 4p1
289 Eu 4p1	353* Au 4d3
290 Ce 4s	358 Ti (L3M1M23)
290* Ca (L23M23M23)	358* Ag (M4N45N45)
293* Os 4d3	360* Lu 4p3
294* K 2p3	360 Sr 3s
294 Th 5s	361* Nb 3p3
296 Ag (M45N23V)	361* Hg 4d5
297* K 2p1	366 Eu 4s
297* Ir 4d5	368* Er 4p1
297* Dy 4p3	368* Ag 3d5
299 Ra 4f	369 Sc (LM23M45)
299* Y 3p3	374* Ag 3d3
301 Gd 4p1	376* Nb 3p1
302* Rh (M45N45N45)	377* Cd (M5N45N45)
305 Pr 4s	377* U 4f7
307 Sc (L3M1M23)	378 Gd 4s
307* Rh 3d5	380* K 2s
309* Ho 4p3	380* N (KL23L23)
311* Y 3p1	380 Hf 4p3
312* Ir 4d3	381* Hg 4d3
312* Rh 3d3	384* Cd (M4N45N45)
315* Pt 4d5	384* Tm 4p1
315 Sc (L3M1M23)	385* Tl 4d5
316 Cd (M45N23V)	388* U 4f5
319 Ac 4f	389* Yb 4p1
320 Nd 4s	389 Ti (L23M23M23)
320* Ar 2s	394* Mo 3p3
321* Er 4p3	394 Y 3s
322* Tb 4p1	396 Tb 4s
325 Rb 3s	399* Sc 2p3
328* Pd (M45N45N45)	400 V (L3M1M23)
330* Zr 3p3	400* N 1s
332* Pt 4d3	401 Ta 4p3
333* Th 4f7	403* In (M5N45N45)
333* Tm 4p3	404* Sc 2p1
335* Au 4d5	405* Cd 3d5
335* Pd 3d5	406* Tl 4d3
337 Pm 4s	411* Mo 3p1
337* Dy 4p1	411 V (L3M1M23)
338* Sc (L3M23M23)	411* In (M4N45N45)
338 Ti (L3M1M23)	412* Pb 4d5

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

603 Ra 4d5	713* Th 4d3
604* Ag 3p1	715* Sn 3p3
607 Co (L3M1M23)	715 Ni (L2M23M23)
609 F (KL1L1)	716 Co (L3M23M45;3P)
609 Pt 4p1	718 Cu (L3M1M23)
610 Tl 4p3	719 Ag 3s
619* Cd 3p3	720* Fe 2p1
619* I 3d5	720 Tl 4p1
620 Co (L3M1M23)	725 Pt 4s
620* La (M5N45N45)	726* Cs 3d5
625 Re 4s	729* Nd (M45N45N45)
626 V 2s	731 Cu (L3M1M23)
628 F (KL1L23)	736* U 4d5
629 Rh 3s	740 At 4p3
631* I 3d3	740* Cs 3d3
633* La (M4N45N45)	757* Sn 3p1
635 Mn (L3M45M45)	762 Pb 4p1
636 Ra 4d3	763 Au 4s
639* Mn 2p3	767* Sb 3p3
639 Ac 4d5	768 Cu (L3M23M23)
643 Au 4p1	768 Rn 4p3
644 Pb 4p3	769 Mn 2s
648 Fe (L3M23M45)	769 Zn (L3M1M23)
649 Co (L3M23M23)	772 Cd 3s
650* Mn 2p1	773 Pm (M45N45N45)
653* Cd 3p1	774* Co (L3M45M45)
654* Ce (M45N45N45)	775 Cu (L2M23M23)
655* F (KL23L23)	775 Ni (L3M23M45;1P)
656 Co (L2M23M23)	778* Co 2p3
658 Os 4s	779* U 4d3
662 Ni (L3M1M23)	781 Ni (L3M23M45;3P)
665* In 3p3	781* Ba 3d5
670* Xe 3d5	784 Zn (L3M1M23)
671 Pd 3s	789 Co (L2M45M45)
675 Ni (L3M1M23)	793* Co 2p1
675 Ac 4d3	796* Ba 3d3
676* Th 4d5	805 Hg 4s
679 Bi 4p3	805* Sm (M45N45N45)
682 Hg 4p1	806 Bi 4p1
683* Xe 3d3	810 Fr 4p3
685* F 1s	813* Sb 3p1
690* Pr (M45N45N45)	818* Ne (KL23L23)
692 Ir 4s	820* Te 3p3
696* Cr 2s	827 Zn (L3M23M23)
703* Fe (L3M45M45)	828 In 3s
703* In 3p1	831 Ga (L3M1M23)
705 Po 4p3	835 Zn (L2M23M23)
707* Fe 2p3	836* La 3d5
709 Ni (L3M23M23)	839 Cu (L3M23M45;1P)
710 Co (L3M23M45;1P)	845 Fe 2s

845 Ga (L3M1M23)	980 Fr 4p1
846* Ni (L3M45M45)	981* Nd 3d5
847 Tl 4s	983 Ga (L3M23M45;3P)
847 Cu (L3M23M45;3P)	992* Zn (L3M45M45)
850* Eu (M45N45N45)	994* Na (KL23L23)
851 Po 4p1	995 Po 4s
853* La 3d3	996 Xe 3p1
853* Ni 2p3	999 Ho (M45N45N45)
859 Cu (L2M23M45)	1000 Ga (L2M23M45)
863 Ni (L2M45M45)	1002* Nd 3d3
863* Ne 1s	1002 Cs 3p3
870* Ni 2p1	1009 Te 3s
871* Te 3p1	1009 Ni 2s
875 I 3p3	1015 Zn (L2M45M45)
879 Ra 4p3	1020 As (L3M23M23)
884* Ce 3d5	1022* Zn 2p3
885 Sn 3s	1030 As (L2M23M23)
885* Gd (M45N45N45)	1034* Pm 3d5
886 At 4p1	1043 Ge (L3M23M45;1P)
888 Ga (L3M23M23)	1045* Zn 2p1
890 Ge (L3M1M2)	1045 At 4s
893 Pb 4s	1047 Er (M5N45N45)
895 Ge (L3M1M3)	1054 Ge (L3M23M45;3P)
898 Ga (L2M23M23)	1058 Ra 4p1
900 Ac 4p3	1060* Pm 3d3
902* Ce 3d3	1064 Ba 3p3
905 Zn (L3M23M45;1P)	1069* Ga (L3M45M45)
914 Zn (L3M23M45;3P)	1069 Cs 3p1
919* Cu (L3M45M45)	1071 I 3s
925 Co 2s	1072* Na 1s
926 Na (KL1L1)	1075 Ge (L2M23M45)
928 Tb (M45N45N45)	1076 Tb (M45N45V)
929 Rn 4p1	1080 Ac 4p1
930 I 3p1	1081* Sm 3d5
932* Pr 3d5	1095 Ga (L2M45M45)
933* Cu 2p3	1097 Rn 4s
934 Xe 3p3	1097 Cu 2s
939 Cu (L2M45M45)	1106 Mg (KL1L1)
940 Bi 4s	1108* Sm 3d3
944 Sb 3s	1116 As (L3M23M45;1P)
950 As (L3M1M23)	1117* Ga 2p3
951 Na (KL1L23)	1119 Dy (M45N45V)
952* Pr 3d3	1126* Eu 3d5
953 Ge (L3M23M23)	1127 As (L3M23M45;3P)
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)

1151 As (L2M23M45)	1735 Ta 3d5
1153 Fr 4s	1793 Ta 3d3
1156* Eu 3d3	1809 W 3d5
1170 Th 4p1	1839 Si 1s
1173 Ho (M45N45V)	1872 W 3d3
1177 Ge (L2M45M45)	1883 Re 3d5
1184 Ce 3p3	1949 Re 3d3
1186* Gd 3d5	1960 Os 3d5
1186* Mg (KL23L23)	2016* Au (M5N7N7)
1195 Zn 2s	2024 Lu 3p3
1208 Ra 4s	2031 Os 3d3
1208 La 3p1	2040 Ir 3d5
1214 Er (M45N45V)	2108 Hf 3p3
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
1241* Tb 3d5	2202 Pt 3d3
1242 Pr 3p3	2206 Au 3d5
1248* Ge 2p1	2264 Lu 3p1
1257 Tb (M4VV)	2281 W 3p3
1261 As (L2M45M45)	2291 Au 3d3
1269 Ac 4s	2295 Hg 3d5
1272 Ce 3p1	2365 Hf 3p1
1276* Tb 3d3	2367 Re 3p3
1292 Ba 3s	2385 Hg 3d3
1296* Dy 3d5	2389 Tl 3d5
1301 Nd 3p3	2457 Os 3p3
1301 Ga 2s	2469 Ta 3p1
1303* Mg 1s	2472 S 1s
1306* Se (L3M45M45)	2484 Pb 3d5
1324* As 2p3	2485 Tl 3d3
1330 Th 4s	2491 Lu 3s
1333* Dy 3d3	2551 Ir 3p3
1339 Pr 3p1	2575 W 3p1
1347 Se (L2M45M45)	2580 Bi 3d5
1359* As 2p1	2586 Pb 3d3
1370* Ho (M4VV)	2601 Hf 3s
1387 Al (KL23L23)	2645 Pt 3p3
1387 Ho (M4VV)	2682 Re 3p1
1389* Er (M5VV)	2683 Po 3d5
1431 Er (M4VV)	2688 Bi 3d3
1560 Al 1s	2708 Ta 3s
1589 Lu 3d5	2743 Au 3p3
1617* Si (KL23L23)	2787 At 3d5
1639 Lu 3d3	2792 Os 3p1
1662 Hf 3d5	2798 Po 3d3
1675* Ta (M5N67N67)	2820 W 3s
1716 Hf 3d3	2822 Cl 1s

2847 Hg 3p3	3854 Po 3p1
2892 Rn 3d5	3909 Ac 3p3
2909 Ir 3p1	3999 Bi 3s
2909 At 3d3	4008 At 3p1
2932 Re 3s	4038 Ca 1s
2957 Tl 3p3	4046 Th 3p3
3000 Fr 3d5	4149 Po 3s
3004 Rh 2p3	4159 Rn 3p1
3022 Rn 3d3	4174 Pa 3p3
3027 Pt 3p1	4303 U 3p3
3049 Os 3s	4317 At 3s
3066 Pb 3p3	4327 Fr 3p1
3105 Fr 3d5	4482 Rn 3s
3136 Fr 3d3	4490 Ra 3p1
3146 Rh 2p1	4492 Sc 1s
3148 Au 3p1	4652 Fr 3s
3174 Ir 3s	4656 Ac 3p1
3173 Pd 2p3	4822 Ra 3s
3177 Bi 3p3	4830 Th 3p1
3206 Ar 1s	4966 Ti 1s
3219 Ac 3d5	5001 Pa 3p1
3248 Ra 3d3	5002 Ac 3s
3279 Hg 3p1	5182 Th 3s
3296 Pt 3s	5182 U 3p1
3302 Po 3p3	5367 Pa 3s
3330 Pd 2p1	5548 U 3s
3332 Th 3d5	5465 V 1s
3351 Ag 2p3	5989 Cr 1s
3370 Ac 3d3	6539 Mn 1s
3412 Rh 1s	7112 Fe 1s
3416 Tl 3p1	7709 Co 1s
3425 Au 3s	8333 Ni 1s
3426 At 3p3	8979 Cu 1s
3442 Pa 3d5	9244 Lu 2p3
3491 Th 3d3	9561 Hf 2p3
3524 Ag 2p1	9659 Zn 1s
3552 U 3d5	9881 Ta 2p3
3554 Pb 3p1	10207 W 2p3
3562 Hg 3s	10349 Lu 2p1
3538 Rn 3p3	10367 Ga 1s
3604 Pd 1s	10535 Re 2p3
3608 K 1s	10739 Hf 2p1
3611 Pa 3d3	10870 Lu 2s
3663 Fr 3p3	10871 Os 2p3
3696 Bi 3p1	11103 Ge 1s
3792 Ra 3p3	11136 Ta 2p1
3704 Tl 3s	11215 Ir 2p3
3728 U 3d3	11271 Hf 2s
3806 Ag 1s	11544 W 2p1
3851 Pb 3s	11564 Pt 2p3

11682 Ta 2s	19083 Ac 2p1
11867 As 1s	19237 Ra 2s
11919 Au 2p3	19693 Th 2p1
11959 Re 2p1	19840 Ac 2s
12100 W 2s	20000 Mo 1s
12284 Hg 2p3	20314 Pa 2p1
12385 Os 2p1	20472 Th 2s
12658 Se 1s	20948 U 2p1
12658 Tl 2p3	21044 Te 1s
12824 Ir 2p1	21105 Pa 2s
12968 Os 2s	21757 U 2s
13035 Pb 2p3	22117 Ru 1s
13273 Pt 2p1	23220 Rh 1s
13419 Ir 2s	24350 Pd 1s
13419 Bi 2p3	25514 Ag 1s
13474 Br 1s	26711 Cd 1s
13734 Au 2p1	27940 In 1s
13814 Po 2p3	29200 Sn 1s
13880 Pt 2s	30491 Sb 1s
14209 Hg 2p1	31814 Te 1s
14214 At 2p3	33169 I 1s
14326 Kr 1s	34561 Xe 1s
14353 Au 2s	35985 Cs 1s
14619 Rn 2p3	37441 Ba 1s
14698 Tl 2p1	38925 La 1s
15031 Fr 2p3	40443 Ce 1s
15200 Rb 1s	41991 Pr 1s
15200 Pb 2p1	43569 Nd 1s
15347 Tl 2s	45184 Pm 1s
15444 Ra 2p3	46834 Sm 1s
15711 Bi 2p1	48519 Eu 1s
15861 Pb 2s	50239 Gd 1s
15871 Ac 2p3	51996 Tb 1s
16105 Sr 1s	53789 Dy 1s
16244 Po 2p1	55618 Ho 1s
16300 Th 2p3	57486 Er 1s
16388 Bi 2s	59390 Tm 1s
16733 Pa 2p3	61332 Yb 1s
16785 At 2p1	63314 Lu 1s
16939 Po 2s	65351 Hf 1s
17038 Y 1s	67416 Ta 1s
17166 U 2p3	69525 W 1s
17337 Rn 2p1	71676 Re 1s
17493 At 2s	73871 Os 1s
17907 Fr 2p1	76111 Ir 1s
17998 Zr 1s	78395 Pt 1s
18049 Rn 2s	80725 Au 1s
18484 Ra 2p1	83102 Hg 1s
18639 Fr 2s	85530 Tl 1s
18986 Nb 1s	88005 Pb 1s

90524 Bi 1s
 93105 Po 1s
 95730 At 1s
 98404 Rn 1s
 101137 Fr 1s
 103922 Ra 1s
 106755 Ac 1s
 109651 Th 1s
 112601 Pa 1s
 115606 U 1s

Ag (M4N45N45).pos

357.8 Ag
 356.7 Ag₂O
 356.6 AgO
 354.2 Ag₂SO₄

Ag (M5N45N45).pos

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 AgOOCFF₃
 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 Fe3C
283.9 K3Fe(CN)6
284.5 Graphite
284.6 PhNH2
284.7 Benzene
285.0 -CH2-
285.5 C5H5N
285.6 C6H5F(C*H)
285.6 EtNH2
285.7 C6H5Cl(C*H)
285.7 (-C*H2CFH-)n
285.9 PVC(-C*H2CHCl-)
286.1 KCN
286.3 CH3C*H2OH
286.3 C*H3CN
286.4 (-C*H2CF2-)
286.5 (CH3C*H2)2O
286.5 PVA(-CH2C*HOH-)n
286.9 CH3COOC*H2CH3
287.0 CS2
287.0 PVC(-CH2C*HCl-)
287.1 C6H5Cl(C*Cl)
287.2 CH3C*N
287.8 C6H5F(C*F)
287.9 (-CH2C*FH-)n
287.9 CH3C*OCH3
288.0 Fe(CO)5
288.0 H2NCSNH2

288.2 CH3C*OONa
288.4 CH3C*ONH2
288.7 H2NCONH2
289.3 CH3C*OOH
289.4 Na2CO3
289.5 Cl3C*COONa
289.6 CaCO3
289.6 HCCl3
290.0 NaHCO3
290.9 (-CH2C*F2-)n
291.9 CO2
292.2 Teflon(-CF2CF2-)n
292.4 CCl4
292.9 C*F3COOEt
294.7 HCF3
296.7 CF4

Ca (L23M23M23).pos

298.2 Ca
292.5 CaO
291.9 CaCO3
291.9 CaCl2
288.9 CaF2

Ca 2p3.pos

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

Cd (M4N45N45).pos

384.0 Cd
382.4 CdO
382,4 CdTe
381.7 CdSe
381.3 CdS
381.2 CdI2
379.0 CdF2

Cd 3d5.pos

404.2 CdO

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

Ce 3d5.pos

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

Cl 2p3.pos

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

Co (L3M45M45).pos

773.0 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 Na₂SO₄
 1071.4 NaNO₃
 1071.5 Na₂CO₃
 1071.5 Na₂HPO₄
 1071.6 NaI
 1071.6 NaPO₃
 1071.6 NaCl
 1071.7 Na₂SiF₆
 1071.7 NaBr
 1071.8 Na
 1072.0 NaH₂PO₄
 1072.5 Na₂O
 1072.7 NaBF₄

Nb (M45N23V).pos

167.8 Nb
 165.6 NbH_x
 161.6 Nb₂O₅

Nb 3d5.pos

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

Nd 3d5.pos

980.8 Nd
 982.0 Nd₂O₃
 984.9 Nd₂(SO₄)₃

Nd 4d.pos

120.8 Nd₂O₃
 122.5 Nd₂(SO₄)₃

Ne (KL23L23).pos

818.0 Ne in Fe

Ne 1s.pos

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

Ni (L3M45M45).pos

846.2 Ni
 842.4 Ni(acac)₂
 842.4 NiF₂

Ni 2p3.pos

852.7 Ni
 852.8 NiS
 854.4 NiO
 855.7 Ni(acac)₂
 855.9 Ni(OH)₂

856.0 Ni₂O₃
 856.7 NiCl₂
 856.8 NiSO₄
 857.1 Ni(NO₃)₂
 857.5 NiF₂·4H₂O
 861.0 K₂NiF₆

O (KL23L23).pos

515.1 PbO₂
 513.1 PbO
 510.8 ZrO₂
 509.7 CaCO₃
 509.3 CaO
 508.8 CaSiO₃
 508.7 CaSO₄
 508.6 Al(OH)₃
 508.5 Al₂O₃
 507.9 NaPO₃
 507.7 H₂O
 507.7 NaAlSi₃O₈
 506.8 SiO₂

O 1s.pos

529.3 CrO₂
 529.5 NiO
 529.6 Fe₂O₃
 529.8 FeO
 529.9 Co₂O₃
 530.0 Fe₃O₄
 530.1 K₄P₂O₇
 530.2 Co₃O₄
 530.2 CrO₃
 530.2 CoO
 530.4 K₃PO₄
 530.6 Na₂SiO₃·3H₂O
 531.0 Al₂O₃/sapphire
 531.2 Ni(OH)₂
 531.4 Al(OH)₃
 531.4 CaCO₃
 531.5 Cr₂O₃
 531.6 Na₂CO₃
 531.7 BeO
 531.7 R-O-CO*-Ph
 531.8 Ni₂O₃
 532.1 NiSO₄
 532.2 KClO₄
 532.2 p-Benzoquinone
 532.2 PhCONH₂

532.2 R-O-CO*-(CH₂)_n-
 532.3 KClO₃
 532.5 Na₂SiO₃·H₂O*
 532.9 -(CH₂)_n-OH
 533.0 B₂O₃
 533.0 Ba(NO₃)₂
 533.0 SiO₂
 533.1 R-O*-CO-Ph
 533.1 H₂O
 533.5 Hydroquinone
 533.6 R-O*-CO-(CH₂)_n-

Os 4f7.pos

50.7 Os
 51.9 K₂O₈I₆
 52.0 OsO₂
 52.2 Os(HSO₃)₂
 52.9 K₂O₈Br₆
 53.1 OsCl₃
 53.2 K₂O₈Cl₆
 53.4 K₂O₈(NO)Cl₅
 55.2 K₂O₈O₂(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 PbSO₄

Pd (M4N45N45).pos

323.1 K₂PdCl₄
 327.8 Pd

Pd 3d5.pos

335.1 Pd
 336.3 PdO
 336.4 PdI₂

336.6 Pd₂(Ph₃P)₂
 337.1 PdBr₂
 337.7 K₂PdBr₄
 337.8 PdCl₂
 337.9 PdO₂
 337.9 K₂PdCl₄
 338.6 Pd(OAc)₂
 338.8 K₂Pd(NO₂)₄
 340.3 K₂PdCl₆

Pm 3d5.pos

1033..5 PmCl₃

Pr 3d5.pos

931.8 Pr
 933.6 Pr₂O₃
 935.3 PrO₂

Pr 4d.pos

116.1 Pr₂O₃
 116.2 PrO₂

Pt (M4N67N67).pos

2040.5 Pt
 2035.2 K₂PtCl₄

Pt (M5N67N67).pos

1960.7 Pt

Pt 4f7.pos

71.2 Pt
 71.4 Pt(Ph₃P)₃
 71.4 Pt(Ph₃P)₄
 72.5 Pt₂Si
 72.6 I₂Pt(Me₃P)₂/cis
 72.6 K₂PtBr₄
 72.6 Pt(OH)₂
 72.7 I₂Pt(Me₃P)₂/trans
 73.0 PtSi
 73.0 Cl₂Pt(Ph₃P)₂/cis
 73.4 K₂PtCl₄
 73.4 K₂PtI₆
 73.4 Pt(NH₃)₄Cl₂
 73.6 PtCl₂

74.2 PtO
 74.6 K₂PtBr₆
 75.0 PtO₂
 75.4 K₂PtCl₆
 75.5 PtCl₄
 75.9 Cl₄Pt(Et₃P)₂
 76.3 Pt(NH₃)₆Cl₄
 77.6 K₂PtF₆

Rb 3d5.pos

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

Re 4f7.pos

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

Rh 3d5.pos

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

Ru 3d5.pos

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

S (KL23L23).pos

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 Na₂SO₄
 169.7 CaSO₄
 174.4 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 SnCl₂
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 Hg_{0.8}Cd_{0.2}Te
572.7 CdTe
572.7 GeTe
572.9 Te
573.9 Ph₂Te₂
575.5 K₂TeO₃
575.8 TeI₄
576.1 TeO₂
576.2 Cl₂TePh₂
576.7 TeBr₄
576.8 Na₂TeO₄
576.9 TeCl₄

576.9 (NH₄)₂TeCl₆
 577.1 Te(OH)₆
 577.3 TeO₃

Th 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 YH_x

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 ZrH_x
141.9 ZrO₂

Zr 3d5.pos

179.0 Zr
179.6 ZrH_x
183.3 ZrO₂
184.2 K₂ZrF₆
185.3 ZrF₄

2 Auger Parameters

All photoelectron lines are in BE, all Auger lines are in KE [1, 2, 3]! The Auger parameters are the sum of the energy of the photoelectron line (BE) and Auger line (KE). The values are saved in the directory Unifit_2012_User_Files\auger parameters*.aup.

Ag 3d5 + Ag (M4N45N45).aup

2099.7=84.0+2015.7 Au

727.0=368.8+358.2 Mg97Ag3

726.0=368.2+357.8 Ag

725.3=368.1+357.2 Ag2S

725.2=367.8+357.4 Ag2Se

724.5=367.8+356.7 Ag2O

724.1=368.0+356.1 AgI

724.0=367.4+356.6 AgO

723.0=367.7+355.3 AgF

722.9=367.3+355.6 AgF2

722.0=367.8+354.2 Ag2SO4

Al 2p + Al (KL23L23).aup

1466.2=72.9+1393.3 Al

1464.8=73.6+1391.2 AlAs

1463.0=74.0+1389.0 AlN

1462.1=73.9+1388.2 Al2O3/alpha

1461.5=73.7+1387.8 Al2O3/gamma

1462.0=74.1+1387.9 Al2O3/sapphire

1461.8=74.2+1387.6 AlOOH/boehmite

1461.5=74.6+1386.9 Al2SiO5/sillimannite

1461.4=74.3+1387.1 Mica/muscovite

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

1460.3=74.8+1385.5 H Zeolon

1460.6=73.7+1386.9 Mol Sieve A

As 3d + As (L3M45M45).aup

1266.5=41.5+1225.0 As

1266.4=43.5+1222.9 AsI3

1266.2=41.2+1225.0 GaAs

1265.4=43.4+1222.0 As2S3

1263.9=42.8+1221.1 Ph3As

1263.8=44.3+1219.5 Ph3AsO

1263.6=44.9+1218.7 As2O3

1263.5=46.1+1217.4 As2O5

1263.4=45.3+1218.1 AsBr3

1261.6=47.8+1213.8 KAsF6

Au 4f7 + Au (M5N67N67).aup

Ba 3d5 + Ba (M4N45N45).aup

1381.6=780.6+601.0 Ba

1377.9=779.9+598.0 BaO

1376.9=780.8+596.1 BaSO4

1376.6=781.7+594.9 BaF2

Br 3d + Br (L3M45M45).aup

1458.0=68.9+1389.1 LiBr

1459.2=74.8+1384.4 KBrO3

1456.7=68.7+1388.0 KBr

Ca 2p3 + Ca (L23M23M23).aup

644.1=345.9+298.2 Ca

639.8=347.3+292.5 CaO

640.2=348.3+291.9 CaCl2

636.8=347.9+288.9 CaF2

638.8=347.0+291.8 CaCO3

Cd 3d5 + Cd (M4N45N45).aup

789.0=405.0+384.0 Cd

787.6=405.2+382.4 CdTe

786.7=405.0+381.7 CdSe

786.6=405.3+381.3 CdS

786.6=404.2+382.4 CdO

786.6=405.4+381.2 CdI2

784.9=405.9+379.0 CdF2

Co 2p3 + Cu (L3M45M45).aup

1551.8=783.6+768.3 CoSiF6

1551.2=778.2+773.0 Co

1550.3=781.7+768.6 Co(NH3)6Cl3

1548.7=781.9+766.8 K3Co(CN)6

Cr 2p3 + Cr (L3M23M45).aup

1101.5=574.3+527.2 Cr

Cs 3d5 + Cs (M4N45N45).aup

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

Cu 2p3 + Cu (L3M45M45).aup

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

F 1s + F (KL23L23).aup

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

Fe 2p3 + Fe (L3M45M45).aup

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

Ga 3d + Ga (L3M45M45).aup

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

Ge 3d + Ge (L3M45M45).aup

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

I 3d5 + I (M4N45N45).aup

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

In 3d5 + In (M4N45N45).aup

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

K 2p3 + K (L2M23M23).aup

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

Mg 2p + Mg (KL23L23).aup

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

Mn 2p3 + Mn (L2M23M45).aup

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

Mo 3d5 + Mo (L3M45M45).aup

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

N 1s + N (KVV).aup

803.9=407.3+396.6 Gd(NO₃)₃.5H₂O
 782.1=397.1+385.0 GaN
 777.3=398.1+379.2 BN
 775.4=398.8+376.6 NH₃

Na 1s + Na (KL23L23).aup

2066.1=1071.8+994.3 Na
 2062.8=1071.6+991.2 NaI
 2062.3=1072.5+989.8 Na₂O
 2062.3=1071.7+990.6 NaBr
 2061.9=1071.6+990.3 NaCl
 2061.3=1071.5+989.8 Na₂CO₃
 2061.3=1070.8+990.5 Na₂C₂O₄
 2061.3=1071.1+990.2 Na₃PO₄
 2061.2=1071.5+989.7 Na₂HPO₄
 2061.1=1071.6+989.4 NaPO₃
 2061.1=1072.0+989.1 NaH₂PO₄
 2061.0=1071.2+989.8 Na₂SO₄
 2061.0=1071.1+989.9 NaOAc
 2060.8=1071.4+989.4 NaNO₃
 2059.8=1072.7+987.1 NaBF₄
 2059.8=1071.2+988.6 NaF
 2059.4=1071.7+987.7 Na₂SiF₆

Nb 3d₅ + Nb (M45N23V).aup

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

Ne 1s + Ne (KL23L23).aup

1681.4=863.4+818.0 Ne in Fe

Ni 2p₃ + Ni (L3M45M45).aup

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

O 1s + O(KL23L23).aup

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

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

P 2p + P (KL23L23).aup

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

Pb 4f₇ + Pb (N6O45O45).aup

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

Pd 3d₅ + Pd (M4N45N45).aup

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

Pt 4f₇ + Pt (M4N67N67).aup

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

S 2p + S (KL23L23).aup

2278.9=162.8+2116.1 NiS
 2278.8=163.0+2115.8 FeS₂/Pyrite

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

Sb 3d5 + Sb (M4N45N45).aup

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

Se 3d5 + Se (L3M45M45).aup

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

Si 2p + Si (KL23L23).aup

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

Sn 3d5 + Sn (M4N45N45).aup

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

Ta 4f7 + Ta (M5N67N67).aup

1696.6=21.9+1674.7 Ta

Te 3d5 + Te (M4N45N45).aup

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

Ti 2p3 + Ti (L3M23M45).aup

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

V 2p3 + V (L3M23M45).aup

984.2=512.2+472.0 V

W 4f7 + W (M5N67N67).aup

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

Xe 3d5 + Xe (M4N45N45).aup

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

Y 3d5 + Y (M45N23V).aup

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

Zn 2p3 + Zn (L3M45M45).aup

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

2011.5=1022.0+989.5 ZnSe

2011.3=1021.6+989.7 ZnS

2011.3=1021.9+989.4 ZnCl₂

2011.2=1022.5+988.7 ZnI₂

2010.7=1023.4+987.3 ZnBr₂

2009.8=1022.1+987.7 ZnO

2009.2=1023.0+986.2 ZnSO₄

2009.1=1021.4+987.7 Zn(acac)₂

2008.0=1021.8+986.2 ZnF₂

Zr 3d₅ + Zr (M45N23V).aup

327.6=179.0+148.6 Zr

325.2=183.3+141.9 ZrO₂

324.9=179.6+145.3 ZrHx

3 Experimental Files

3.1 VG ESCALAB 220i-XL (*.TAP)

Eclipse Standard Data Transfer Format v2.0
File: 'C:\STS\DAT\AU041201' contains 5 spectra.

Spectrum: 1

Name (Spectrum): Au4f
Label: Gold auf Glimmer vom 03-12-96
Data Version: 1
Technique: XPS
Acquired at 11:30:41 on Wednesday 4-12-1996
ANALYSER:
Mode: CAE
Value: 10
Magnification: 1
Work function: 4.6
Width x: 0
Width y: 0
Source azimuth: 0
Polar angle: 0
Target bias: 0
Lens mode ID: 6
Lens name: Small Area 150
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: 10
Correction: 0
SAMPLE:
Charging: 0
Polar angle: 0
Azimuth: 0
Rotation: 0
PROFILE INFO:
None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 1393.6
Abscissa end: 1407.6
Abscissa increment: 0.05
Ordinate label:
Ordinate units: Counts
Ordinate data: 281 values
Ordinate minimum, maximum: 4718.24 52176.4

8281.36
8249.04
8191.44
8204.46
8163.56
8128.64
...
4918.28
4931.82

Spectrum: 2

Name (Spectrum): Cls
Label: Gold auf Glimmer vom 03-12-96
Data Version: 1
Technique: XPS
Acquired at 11:30:41 on Wednesday 4-12-1996
ANALYSER:
Mode: CAE
Value: 10
Magnification: 1
Work function: 4.6
Width x: 0
Width y: 0
Source azimuth: 0
Polar angle: 0
Target bias: 0
Lens mode ID: 6
Lens name: Small Area 150
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: 50
Correction: 0
SAMPLE:
Charging: 0
Polar angle: 0
Azimuth: 0
Rotation: 0
PROFILE INFO:
None
INSTRUMENT INFO:
Model: EscaLab 220-IXL
Transmission function coefficients:
Abscissa label: Kinetic Energy
Abscissa units: eV
Abscissa start: 1195.1
Abscissa end: 1206.1
Abscissa increment: 0.05
Ordinate label:
Ordinate units: Counts
Ordinate data: 221 values
Ordinate minimum, maximum: 49487.6 75395.6
51499.9

51187.6

...

3.2 ESCALB Avantage (*.AVG)

```

;=====
;Dump of DataSpace 'C:\temp\pet.DATA\C1s.VGD'
; on 9/11/2005 at 15:04:07
;=====

;[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 = 'C1s'
DS_EXT_SUPROPID_SUBJECT    : VT_BSTR = 'C1s'
DS_EXT_SUPROPID_AUTHOR     : VT_BSTR = 'Kevin Robinson'
DS_EXT_SUPROPID_COMMENTS   : VT_BSTR = ''
DS_EXT_SUPROPID_CREATED    : VT_DATE = 30/12/1899   00:00:00
DS_EXT_SUPROPID_SAVED     : VT_DATE = 9/11/2005   15:02:46

;Standard Properties present:
$PROPERTIES=STD
DS_GEPROPID_TECHNIQUE      : VT_I4   = 1
DS_GEPROPID_INSTRUMENT     : VT_BSTR = 'EscaLab 220-IXL'
DS_GEPROPID_SIGNAL2NOISE   : VT_R4   = 0.000000
DS_GEPROPID_SOURCE_TYPE    : VT_I4   = 3
DS_GEPROPID_GUID           : VT_BSTR = '{2258C2E6-6F66-48E8-
845F-380D4A3DF6B9}'
DS_GEPROPID_SOURCE_GUID    : VT_BSTR = '{56DF557E-B4F1-40AD-
8233-41D08B33D03C}'
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_SOPROPID_STYPE         : VT_I4   = 10
DS_SOPROPID_MONO          : VT_BOOL  = False
DS_SOPROPID_ENERGY        : VT_R4   = 1486.599976
DS_SOPROPID_VOLTAGE       : VT_R4   = 0.000000
DS_SOPROPID_CURRENT       : VT_R4   = 0.000000
DS_SOPROPID_WIDTH         : VT_R4   = 0.000000
DS_SOPROPID_LENGTH        : VT_R4   = 0.000000
DS_SOPROPID_AZIMUTH       : VT_R4   = 0.000000
DS_SOPROPID_POLAR        : VT_R4   = 0.000000
DS_SOPROPID_NUMBER        : VT_I2   = 0
DS_SOPROPID_ATOMS         : VT_I2   = 0
DS_SOPROPID_CHARGE        : VT_I2   = 0
DS_SOPROPID_ION           : VT_BSTR = 'Al K-alpha'
DS_ACPROPID_START_TIME    : VT_DATE = 14/7/1998   11:50:17
DS_ACPROPID_ACQ_TIME      : VT_R4   = 0.100000
DS_ACPROPID_PERIODS       : VT_I4   = 4
DS_ACPROPID_CORRECTION    : VT_R4   = 0.000000
DS_ACPROPID_MODE          : VT_I2   = 0
DS_ACPROPID_DIRECTION     : VT_I2   = 0
DS_ACPROPID_EV_SCALE      : VT_I2   = 1
DS_ANPROPID_MODE          : VT_I2   = 1
DS_ANPROPID_PASS          : VT_R4   = 20.000000
DS_ANPROPID_MAG           : VT_R4   = 1.000000
DS_ANPROPID_WORK_FTN      : VT_R4   = 4.400000
DS_ANPROPID_WIDTH         : VT_R4   = 0.000000
DS_ANPROPID_LENGTH        : VT_R4   = 0.000000

```

```

DS_ANPROPID_AZIMUTH           : VT_R4   = 0.000000
DS_ANPROPID_POLAR            : VT_R4   = 0.000000
DS_ANPROPID_LENS_MODE_NAME   : VT_BSTR = 'Large Area XL '
DS_ANPROPID_LENS_MODE_ID     : VT_I4   = 8
DS_ANPROPID_TXFN_COEFFS      : VT_I4   = 8
; Property list for DS_ANPROPID_TXFN_COEFF (expecting 8) follows:
DS_ANPROPID_TXFN_COEFF[0]    : VT_R4   = 3.867640
DS_ANPROPID_TXFN_COEFF[1]    : VT_R4   = -0.075012
DS_ANPROPID_TXFN_COEFF[2]    : VT_R4   = 0.003691
DS_ANPROPID_TXFN_COEFF[3]    : VT_R4   = -0.045752
DS_ANPROPID_TXFN_COEFF[4]    : VT_R4   = 0.000000
DS_ANPROPID_TXFN_COEFF[5]    : VT_R4   = 0.000000
DS_ANPROPID_TXFN_COEFF[6]    : VT_R4   = 0.000000
DS_ANPROPID_TXFN_COEFF[7]    : VT_R4   = 0.000000

;Extended Properties present:
$PROPERTIES=EXT
; NONE found

;=====

;DataSpace has 1 data axes as follows:
;   #=      start,      end,      numSpaceAxes
$DATAAXES=1,#empty#
   0=      0,      150,      1

;=====

;DataSpace has 1 space axes as follows:
;   #=      start,      width,      numPoints,      axisType,      linear,
symbol,      unit,      label
$SPACEAXES=1
   0=      1196.599976,      0.100000,      151,      ENERGY,      LINEAR,      'E',
'eV',      'Energy'

;=====

;Values on axis 0
$DATA=*
LIST@  0=      895.820068,      909.259827,      858.680054,      850.800049
LIST@  4=      814.080078,      857.560059,      862.439941,      808.340088
LIST@  8=      877.380005,      840.320007,      877.179993,      893.559998
LIST@ 12=      839.340027,      858.160034,      885.719971,      922.399902
LIST@ 16=      907.840027,      890.119934,      927.399963,      924.560059
LIST@ 20=      867.880127,      932.400024,      900.040100,      975.600098
LIST@ 24=      973.459961,      964.400024,      1028.039795,      1091.319946
LIST@ 28=      1074.219849,      1122.379883,      1088.239868,      1112.239990
LIST@ 32=      1141.780151,      1206.059937,      1181.860107,      1163.559937
LIST@ 36=      1146.939941,      1097.399902,      1108.960083,      1046.899902
LIST@ 40=      1013.499939,      1023.640076,      967.739990,      952.520020
LIST@ 44=      983.839966,      945.760010,      922.880005,      921.700012
LIST@ 48=      920.480042,      971.339966,      1097.359985,      1331.140259
LIST@ 52=      1662.020020,      2090.840332,      2679.299805,      3487.500244
LIST@ 56=      4361.740234,      4966.740723,      5592.619629,      5969.719727
LIST@ 60=      5925.180664,      5474.399902,      4749.800293,      4004.160645
LIST@ 64=      3037.959961,      2288.680176,      1705.000000,      1250.380005
LIST@ 68=      940.979980,      822.819946,      762.059937,      798.180054
LIST@ 72=      916.840027,      1141.500000,      1405.040161,      1697.299927
LIST@ 76=      2082.139893,      2637.520020,      3250.319824,      3792.460449
LIST@ 80=      4558.479980,      5024.319824,      5323.779297,      5587.600098
LIST@ 84=      5456.179688,      5257.540527,      4836.060059,      4408.620117
LIST@ 88=      4110.520020,      3861.579590,      4151.659668,      4772.479492
LIST@ 92=      5499.841309,      6874.199707,      8501.819336,      10431.880859
LIST@ 96=      12201.060547,      13960.781250,      15098.138672,      15826.120117
LIST@ 100=     15894.478516,      15339.280273,      13962.121094,      12477.199219
LIST@ 104=     10745.699219,      8755.339844,      7066.100098,      5598.081055
LIST@ 108=     4417.320313,      3485.000244,      2760.500000,      2172.459961

```

LIST@ 112=	1781.259888,	1387.240112,	1116.459961,	913.759949
LIST@ 116=	731.320068,	575.799988,	488.040039,	405.160004
LIST@ 120=	354.299957,	299.520020,	249.760025,	229.920029
LIST@ 124=	240.460022,	200.919983,	193.119995,	189.180008
LIST@ 128=	188.100006,	172.180023,	168.779999,	169.280029
LIST@ 132=	142.180008,	136.460007,	151.059998,	155.120010
LIST@ 136=	175.639999,	151.620010,	163.860016,	167.599991
LIST@ 140=	155.760010,	140.000000,	146.539993,	145.999985
LIST@ 144=	153.739990,	150.139984,	145.100006,	161.479980
LIST@ 148=	148.720001,	159.139999,	136.119995	

3.3 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

```

**P4C1S100
80*****1208*****.2*****20*****1486.6**2*****1*****
5047          4909          4997          4840          4996          4967
4947          5017          4980          5039
5026          5085          4998          5134          5114          4986
5129          5087          5225          5179
5264          5436          5609          5766          5973          6327
6938          7414          8192          9081
9703          10514         10916         11288         11083         10756
10224         9358          8562          7686
7170          6719          6293          6024          5953          5689
5634          5627          5575          5421
5539          5485          5342          5439          5445          5331
5438          5363          5483          5457
5437          5387          5389          5494          5410          5370
5269          5313          5223          5299
5238          5288          5303          5352          5271          5231
5387          5444          5286          5256

**4AG3D100
100*****1124*****.2*****20*****1486.6**2*****1*****
5852          5794          5862          5925          5903          6142
5933          5933          5886          5868
5960          5831          5950          6062          6022          6025
5949          5990          6015          5953
5928          6016          6022          6316          6713          7039
7541          8025          8639          9241
9765          9804          9862          9093          8486          7634
7193          7131          6751          6480
6373          6153          6203          6225          6198          6259
6310          6302          6244          6312
6197          6366          6502          6343          6659          7113
7257          7798          8160          8568
9000          8976          8908          8529          7788          7342
7161          6905          6798          6550
6523          6469          6398          6425          6390          6309
6283          6271          6327          6272
6295          6255          6297          6290          6388          6229
6369          6346          6273          6314
6370          6313          6268          6312          6394          6287
6379          6400          6306          6307

**4SN3D100
120*****1007*****.2*****20*****1486.6**2*****1*****
8161          7937          7869          7923          7996          8062
7941          8203          8309          8297

```

8398	8579	8573	8646	8686	9087
8983	9468	9776	9905		
10500	10809	10954	11347	12001	12533
13512	14514	16082	18116		
20786	24045	28404	34160	39768	46171
52343	57094	59766	61091		
57945	52871	46186	39199	31967	25695
21428	18224	15773	14506		

...

3.4 BESSY (*.*)

Comment:

- 1. – 14. row: acquisition parameters
- from row 15: column1: kinetic energy, column 2: intensity, column 3: flux
- Intensities are divided by flux (only flux > 0)

1. Version

```

komm_zeile : 10-4 MBT Borat Luft
prob_zeile : Galenit
date       : MON 19.02.1996
time       : 22:02:19
source     : HE_PGM3
MessMode   : EDC
max_energy : 55.0000
min_energy : 35.0000
pass energy : 10.0000
step_w     : 0.0500
anz_scans  : 4
count_time : 300
num_of_data : 401
E_kin;resCh ;secCh
35.0000;10126.0000;10.4164
35.0500;10112.0000;10.4168
35.1000;10205.0000;10.4171
...

```

2. Version

```

komm_zeile :
prob_zeile :
date       : TUE 27.01.1981
time       : 01:17:39
source     : noMono
MessMode   : EDC
max_energy : 23.5000
min_energy : 16.5000
phot_energy : 55.00
pass energy : 2.5000
step_w     : 0.0250
anz_scans  : 3
count_time : 500
num_of_data : 281
E_kin;setEn.;ch1 ;ch2 ;ch3 ;ch4 ;ch5 ;resCh ;secCh
16.5000;16.3750;676.0000;1152.0000;574.0000;188.0000;702.0000;3168.0000;0.0000
16.5250;16.4000;675.0000;1141.0000;525.0000;187.0000;719.0000;3233.0000;0.0000
...

```

3.5 VSI (*.GPH)

```

%%%%% 001 # General data
2.10 0.40 HSA FFFFFFFF # P-Version, C-Version, Type
05.12.1997 11:00 # Date, Time

```

```

14      #      Unit TYPE
%%%%% 010  #      Comment

%%%%% 002  #      Modul data
KINETIC      1000.0000000000  1  1      1.0000000000      0.0000000000  FFFFF529
CHANNELT     2000.0000000000  6  1      1.0000000000      0.0000000000  FFFFF651
%%%%% 003  #      Segment
0      #      Flag für Segmentauswahl
      865.0000000000  890.0000000000  0.0500000007  #      min max inc
2      #      Segmentanzahl
      0.00999999998  860.0000000000  885.0000000000  0.29999999821
0.2000000030  #      wait start stop inc
      0.00999999998  1100.0000000000  1130.0000000000  0.29999999821
0.2000000030  #      wait start stop inc
%%%%% 004  #      Channel data
0      #      main channel
COUNTER      0.0000000000      1.0000000000  0  1  1
FFFFD5D0
Channel 2      0.0000000000      1.0000000000  0  0  0
FFFFF3D0
Channel 3      0.0000000000      1.0000000000  0  0  0
FFFFE4D0
Channel 4      0.0000000000      1.0000000000  0  0  0
FFFFD5D0
Channel 5      0.0000000000      1.0000000000  0  0  0
FFFFC6D0
%%%%% 005  #      Averagedata
\SAVEMEAS    #      Filename Measure Values
0063 #      Flags
0003 #      Anzahl
000 #      Start extension
003 #      Save extension
\SAVEAV      #      Filename Average Values
\EXPMEAS     #      Filename Export Measure Values
\EXPAV       #      Filename Export Average Values
\expmcd      #      Filename MCD Values
%%%%% 006  #      Options
      1.0000000000 #      xFactor
      0.0000000000 #      xOffset
1000000.0000000000 #      warning level
%%%%% 007  #      Ramp Mode Parameter
1      #      mode
      5.000 #      parameter FRR
      5.000 #      parameter FAT
0      #      kinetic energy mode
2      #      MCD
0      #      adjustable magnification
0.000000 #      XPS-Gain

```

```

0      #      polarity
##### 008  #      Timedata
      0.1999999285 #      Meas time
      5.3999977112 #      startTime
      0.0099999998 #      sleepTime
##### 009  #      Graphicoptionen
880.000000 882.000000# X-Zoom
20000.000000 30000.000000# Y-Zoom
##### 011  #      Transformation
-1 #      Length of Differentiation
-1 #      Length of Smoothing
##### 012  #      Background Correction
0 #      Active
0.000000 #      LeftX
0.000000 #      LeftY
0.000000 #      RightX
0.000000 #      RightY
##### 020  #      Measure Global
12-05-1997 10:51:01 #      Startzeit
12-05-1997 10:59:53 #      Endzeit
  3 #      Averageanzahl
000 #      Scanindex
10000 #      Kanäle
##### 021  #      Measure Segment
1 #      Number of Segments
501      0.0099999998      865.0000000000      890.0000000000      0.0500000007
0.1999999285 #      Segmentsize wait start stop inc meastime
0.000000 #      MCD Correction
##### 022  #      Measure Data
COUNTER
S 0000 865.000000
M 0000 552.333313
S 0001 865.049988
M 0001 567.000000
S 0002 865.099976
M 0002 557.333374
S 0003 865.149963
M 0003 574.333313
...
S 0496 889.793945
M 0496 305.666687
S 0497 889.843933
M 0497 308.000000
S 0498 889.893921
M 0498 302.666656
S 0499 889.943909
M 0499 291.666656
S 0500 889.993896
M 0500 294.000000
##### ENDE #      end of file

```

3.6 HHUD (*.DAT)

Comment:

1. row: XPS2 for file identification
2. row: date and time
3. row: comment
4. row: comment
5. row: excitation source (Magnesium, Aluminium ...)
6. row: reserved for Xfit
7. row: region name (O 1s, ...)
8. row: analyser mode (e.g. CAE 10)
9. row: number of scans, dwell time in ms and acquisition time in min

10. row: cross section, area,... (no relevance for UNIFIT!)
11. row to 20. row no relevance for UNIFIT!
21. row: lowest binding energy in eV, highest binding energy in eV, smallest intensity, highest intensity, number of steps, total area of the spectrum
22. row: ,@' start of experimental data
from row 23: binding energy, intensity

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
80.55,72874.45
80.60,72654.45
80.65,72118.89
80.70,72658.89
80.75,71930.00
80.80,71623.34
80.85,72298.89
80.90,72380.00
80.95,72585.55
81.00,73012.23
81.05,73135.55
81.10,73691.11
81.15,73612.22
81.20,74097.77
81.25,74570.00
81.30,75167.78
81.35,75688.88
81.40,76543.33
81.45,77097.77
81.50,77885.55
81.55,78811.12
81.60,80141.12
81.65,81398.89
81.70,82586.67
81.75,83441.11

```
81.80,84680.00
81.85,86532.22
81.90,88875.55
81.95,89601.12
82.00,92637.78
...
```

3.7 LUND (*.*)

Comment:

- rows: 7 characters binding energy, 8 characters intensity

```
27.990      583
27.960      595
27.930      598
27.900      562
27.870      586
27.840      561
27.810      550
27.780      577
27.750      582
27.720      574
...
26.070     1125
26.040     1210
26.010     1329
25.980     1427
25.950     1529
...
21.300      245
21.270      253
21.240      250
21.210      242
21.180      262
21.150      239
21.120      248
21.090      238
21.060      240
21.030      252
21.000      217
```

3.8 CAF (*.CAF)

Comment:

- 1. row: start energy, 2. row: step width, 3. row: number of steps, from row 6: intensities

```
xstart 34
xstep 0.025
nop 321
mmean 3206.87961931464
BEGIN
936.83042
914.93686
930.38953
998.73214
905.29033
964.29078
908.19923
956.30381
...
283.63007
296.45818
282.19061
307.78396
```

```
252.03781  
END
```

```
END
```

3.9 SCIENTA

3.9.1 Standard Format (*,*)

Comment:

- 6 characters kinetic energy, space, intensity with three places after the decimal point
- recorded with increasing kinetic energy
- file structure changeable in SCIENTA acquisition program!

```
37.000 6299.000  
37.050 6404.000  
37.100 6410.000  
37.150 6438.000  
37.200 6266.000  
...  
54.900 5893.000  
54.950 5864.000  
55.000 5870.000
```

3.9.2 Parameter Dependent Measurement (Depth Profile) (*,*)

Comment:

- series (angle dependent), 1. row space, 2. row angle, 3. row space
- 6 characters kinetic energy, space, intensity
- recorded with increasing kinetic energy
- file structure changeable in SCIENTA acquisition program!

```
7.273
```

```
41.000 40.0  
41.020 0.0  
41.040 0.0  
...  
48.980 1861.0  
49.000 2393.0
```

```
8.364
```

```
41.000 152.0  
41.020 541.0  
...
```

3.10 KRATOS (*.CLI)

```
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 -3.024e+02 7.040e+02  
xywe -3.022e+02 1.024e+03  
xywe -3.020e+02 1.056e+03  
xywe -3.018e+02 9.920e+02  
...
```

3.11 PHI-5400 (*.INF), (*.ASC)

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_ratio
0.000000	yx_ratio
0	abs_bias

ION GUN: ion gun control information

04-300 ION GUN	Gun currently in system
----------------	-------------------------

3.000000	Ion gun voltage
0.000000	Ion gun current
25.000000	Emission current
10.000000	x raster range
0.000000	y raster range
1.000000	Ratio of y raster to x raster
Ar	Ion source gas type
75.000000	Focus voltage
0.000000	Condenser setting
190.000000	Grid voltage
15.000000	spc charge offset

X-RAY: x-ray control settings

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

ANGLES: angle information

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

SIMS ANALYZER: SIMS analyzer information

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

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

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

REGION INFORMATION: acquisition control block

5	Number of acb_region structures stored
Region acquisition control block structure	
S1	Element name
100	Old time per step
8	Number of sweeps
174.000000	Energy upper limit
18.000000	Energy range
174.000000	Analysis upper limit

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

Region acquisition control block structure

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

```
100.000000          Time per step

Region acquisition control block structure
01                Element name
100              Old time per step
4                Number of sweeps
538.000000      Energy upper limit
12.000000       Energy range
538.000000      Analysis upper limit
12.000000       Analysis range
0.100000        Volts per step
121             Steps per sweep
5               Number of diff points
0.000000        Window width for test acq
1               Flag, acquire data
0               Flag, triggered acquisition
2               Resolution
1               Calculation type
0               Gate trigger
0               Ion polarity
1               Transition
0.000000        Trigger relative rise %
0.000000        Trigger relative fall %
1832            Minimum counts
2281            Maximum counts
2147483647     Peak to peak minimum
0               Peak to peak maximum
0.000000        Actual sputter time
35.750000       Pass energy
35.750000       Retard ratio
2               Number of mcd channels
0.000000        Trigger fracture beam gating
0.000000        Trigger time beam gating
0.000000        Retard energy
0.000000        Ion energy
0.000000        Focus voltage
0.000000        Acceleration voltage
500             Signal to noise limit
100.000000     Time per step

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

35.750000	Retard ratio
2	Number of mcd channels
0.000000	Trigger fracture beam gating
0.000000	Trigger time beam gating
0.000000	Retard energy
0.000000	Ion energy
0.000000	Focus voltage
-7.625010	Acceleration voltage
50	Signal to noise limit
100.000000	Time per step

Region acquisition control block structure

S2	Element name
100	Old time per step
16	Number of sweeps
240.000000	Energy upper limit
20.000000	Energy range
240.000000	Analysis upper limit
20.000000	Analysis range
0.100000	Volts per step
201	Steps per sweep
5	Number of diff points
0.000000	Window width for test acq
1	Flag, acquire data
0	Flag, triggered acquisition
2	Resolution
1	Calculation type
0	Gate trigger
0	Ion polarity
1	Transition
0.000000	Trigger relative rise %
0.000000	Trigger relative fall %
6087	Minimum counts
8912	Maximum counts
2147483647	Peak to peak minimum
0	Peak to peak maximum
0.000000	Actual sputter time
35.750000	Pass energy
35.750000	Retard ratio
2	Number of mcd channels
0.000000	Trigger fracture beam gating
0.000000	Trigger time beam gating
0.000000	Retard energy
0.000000	Ion energy
0.000000	Focus voltage
0.000000	Acceleration voltage
50	Signal to noise limit
100.000000	Time per step

File (*.ASC)

Comment:

- 10 characters binding energy, 11 characters intensity

174.000000	3647.000000
173.899994	3789.000000
173.799988	3685.000000
173.699982	3817.000000
...	
156.198914	4158.000000
156.098907	4194.000000
155.998901	4324.000000
292.000000	1739.000000

```
291.899994 1708.000000
291.799988 1711.000000
...
282.099396 1711.000000
281.999390 1707.000000
538.000000 1902.000000
537.900024 1965.000000
...
527.002686 1977.000000
526.902710 1990.000000
526.802734 1921.000000
526.702759 1939.000000
526.0029301886.000000
...
149.000000 469.000000
148.899994 459.000000
133.199036 87.000000
133.099030 83.000000
132.999023 87.000000
240.000000 6346.000000
239.899994 6278.000000
...
220.198792 6255.000000
220.098785 6193.000000
219.998779 6303.000000
```

3.12 PHI-545/590 (*.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
339.85 2789
339.8 2736
339.75 2786
339.7 2800
...
275.3 1782
275.25 1704
275.2 2049
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
1036.7 14610
1036.6 14191
...
957.5 8118
957.4 8105
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
539.7	3290
539.6	3474
539.5	3380
...	
525.6	3249
525.5	3117
525.4	3134
525.3	3153
525.2	3271
525.1	3867
525	3282

3.13 PHI-1600/1600C

3.13.1 Standard Format, Typ 1 (*.csv)

```
[ID INFO]
App,PHI SCA XPS
Technique,XPS
Type,MULTIPLEX
Mode,FAT
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
```

3.13.2 Standard Format, Typ 2 (*.csv)

Comment:

- Example shows a measurement of 2 regions (Ag 3d, Au 4d3), Dwell Time, Scans, Pass Energy, Excitation Energy, Analyser Mode are not saved and has to be defined manually

Areal

```
Ag3d
1
378.0000,4067.9966
377.9000,4137.0375
377.8000,4127.4420
377.7000,4157.1693
377.6000,4107.0045
...
362.2000,2712.6659
362.1000,2768.1670
362.0000,2801.7648
```

Areal

```
Au4d3
1
364.0000,2823.8659
363.9000,2844.2625
363.8000,2902.7648
363.7000,2826.6830
363.6000,2713.9750
363.5000,2794.8943
363.4000,2785.0761
...
344.3000,2473.8477
344.2000,2479.6977
344.1000,2547.6761
344.0000,2434.0284
```

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

Comment:

- Example shows a measurement of 5 regions (C 1s, O 1s, Pt 4f, Cu 2p₃, Si 2p) and 35 parameter steps (Cycles)

```
[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,

```

3.14 VGX-900 (*.1)

Comment:

- VGX-900 files can be recorded with decreasing or increasing kinetic 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
- 3. row: region name (here: WIDE SCAN, AG 3D, C 1S, O 1S)

```

XPS
    0.00000 1000.00000    1.00000    3.00000    0.10000 1001    50.0
    WIDE SCAN
474
526
...
12511
12483
12488
12756
    365.00000 380.00000    0.10000    5.00000    0.50000 151    20.0
    AG 3D
7442
7283
...
10344
10464
10400
    280.00000 290.00000    0.10000    5.00000    0.50000 101    20.0
    C 1S
2769
2846
...

```

```

2961
2874
3014
2877
  526.00000  536.00000  0.10000  5.00000  0.50000  101  20.0
  O 1S
12623
12991
12625
...
12891
13195
13052
13016
12906
13046

```

3.15 VAMAS

3.15.1 Standard Format (*.VMS)

Comment:

,NORM' in 7. row means ,Ordinary Spectrum File

VAMAS Surface Chemical Analysis Standard Data Transfer Format 1988 May 4

Univ. Leipzig, Fachbereich Chemie

EscaLab 220-IXL

Ronald Hesse

C:\RH\DAT\FREIBERG\PVPI900

0

NORM

REGULAR

4

0

0

0

0

0

4

Region 1

1998

10

6

12

50

23

255

0

XPS

Mg K-alpha

1253.6

0

0

0

0

0

FAT

10

1E+37

4.61

0

```
0
0
0
0
C1s
C1s
-1
Kinetic Energy
eV
960.6
0.1
1

Counts
pulse counting
0.3
2
0
0
0
0
0
121
547.27
10446.7
1042.69
1098.76
1123.82
...
595.89
573.78
Region 2

1998
10
6
12
50
23
255
0
XPS
Mg K-alpha
1253.6
0
0
0
0
0
FAT
10
1E+37
4.61
0
0
0
0
0
N1s
N1s
-1
Kinetic Energy
eV
844.6
0.1
1
```

Counts
pulse counting
0.3
50
0
0
0
0
0
141
50984.5
55340.7
...
51039.6
Region 3

1998
10
6
12
50
24
255
0
XPS
Mg K-alpha
1253.6
0
0
0
0
0
FAT
10
1E+37
4.61
0
0
0
0
0
O1s
O1s
-1
Kinetic Energy
eV
713.6
0.1
1

Counts
pulse counting
0.3
20
0
0
0
0
0
121
23322.8
33140.8
24362
24182.1
24011.2
...
23644.9

```
23238
Region 4

1998
10
6
12
46
29
255
0
XPS
Mg K-alpha
1253.6
0
0
0
0
0
FAT
50
1E+37
4.61
0
0
0
0
0
US
US
-1
Kinetic Energy
eV
253.6
0.5
1

Counts
pulse counting
0.1
1
0
0
0
0
0
2001
124.2
25532.9
12217.9
...
119.7
118.44
end of experiment
```

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

Comment:

- Example consists of 21 spectra, i.e. 3 regions (O 1s, C 1s, Si 2p) with 7 steps (sputter time, angle etc.)
- ‚SDP‘ in 7. row means series of spectra (e.g. sputter depth profile)

EscaLab 220-IXL
Ronald Hesse
C:\RH\DAT\SIDP
0
SDP
REGULAR
3
1
Etch Time
Seconds
0
0
0
0
21
Region 0

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

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

```
0
0
0
0
81
7149.84
14129.2
7388.86
7285.92
7355.6
...
7163.96
7177.98
7190.72
...
Region 0

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

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

```
0
0
0
0
81
7400.7
7973.76
7469.58
7452.52
...
7727.98
7659.92
Region 1

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

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

```
0
111
7487.76
33338.5
7731.46
...
7688.62
7509.76
7502.9
...
Region 1

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

Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
0
Cyclic
0
0
0
0
111
```

7187.1
8566.98
7359.68
...
7362.26
7240
7220.72
7265.28
Region 2

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

Counts
pulse counting
0.3
3
0
0
1
1
1
0
0
Cyclic
0
0
0
0
131
1785.06
18039.9

```
...
1837.52
1842.62
...
Region 2

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

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

3.16 NPL (*.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

3.17 SPECSLAB (*.exp)

Comment:

- Example shows ten spectra in parameter depends acquisition mode (sputter profile):
Ag 3d_1 with 30 eV Pass and Ag 3d_2 with 120 eV Pass
- “tag” Ag 3d_1 is the name of the first region
- “tag” Ag 3d_” is the name of the second region
- Sputter steps: 0 s, 60 s, 120 s, 240 s, 360 s
- Only the data set “original” is read

```
#SPX
region: 1
method: XPS
active: 1
range: 876 889 0.05
scans: 1
dwell: 0.1
x_shift: 0
x_gain: 1
work_function: 0
Source: XRayGun
{
    xrs_anode = Mg;
    xrs_voltage = 10000;
    xrs_emission_current = 0.01;
}
EnergyAnalyser: ea200
{
    ea_mode = esca_c_ep;
    ea_serial = 0;
    ea_vers = 0;
    ea_const = 120;
    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: Sage
{
    ma_type = Sage;
    ma_x = 0.0505;
    ma_y = 0.045;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = -1;
    mi_acp_pascal = -1;
    mi_tcp_pascal = -1;
}
flood_gun_U: 0
tag: "Ag 3d_1"
ManipulationProtocol:
{
```

```
    mp_nstrings = 0;
    mp_strings = {
  }
}
measure_date: 14 06 2002 11 41
filename: "1406x02"
visible: 1
depth: 5
sputter_def: 1: 0, 2: 60, 4: 120
data: 261 long 1547
12496
12723
...
7451
7475
enddata
background: 261 double 2535
12603.053
12602.994
...
7465.688
7465.667
endbackground
original: 261 long 1547
12496
12723
...
7451
7475
endoriginal
data: 261 long 1546
12502
12512
...
56
26311
24734
7464
enddata
background: 261 double 2535
12532.011
12532.018
...
7480.628
7480.667
endbackground
original: 261 long 1546
12502
12512
...
endoriginal
data: 261 long 1548
12596
12684
...
7543
7481
enddata
background: 261 double 2536
12625.333
12617.633
...
7551.837
7552.000
endbackground
original: 261 long 1548
12596
```

```
12684
...
7543
7481
endoriginal
data: 261 long 1547
12711
12639
...
7702
7651
enddata
background: 261 double 2536
12693.768
12693.768
...
7643.113
7658.333
endbackground
original: 261 long 1547
12711
12639
...
7702
7651
endoriginal
data: 261 long 1402
6450
6452
...
3793
3768
enddata
background: 261 double 2349
6416.333
6418.647
...
3782.965
3783.000
endbackground
original: 261 long 1402
6450
6452
...
3793
3768
endoriginal
endregion
region: 2
method: XPS
active: 1
range: 976 989 0.1
scans: 1
dwell: 0.1
x_shift: 0
x_gain: 1
work_function: 0
Source: XRayGun
{
    xrs_anode = Mg;
    xrs_voltage = 10000;
    xrs_emission_current = 0.01;
}
EnergyAnalyser: ea200
{
    ea_mode = esca_c_ep;
    ea_serial = 0;
```

```
    ea_vers = 0;
    ea_const = 30;
    ea_ampl_fact = 0;
    ea_particle_polarity = -1;
    ea_detector_U = 2249.9;
    ea_conversion_U = 0;
    ea_aperture = 10;
    ea_is_small_spot = 0;
}
Manipulator: Sage
{
    ma_type = Sage;
    ma_x = 0.0505;
    ma_y = 0.045;
}
MiscAcqInfo:
{
    mi_sample_ampere = 0;
    mi_sample_kelvin = -1;
    mi_acp_pascal = -1;
    mi_tcp_pascal = -1;
}
flood_gun_U: 0
tag: "Ag 3d_2"
ManipulationProtocol:
{
    mp_nstrings = 0;
    mp_strings = {
    }
}
measure_date: 14 06 2002 11 44
filename: "1406x02"
visible: 1
depth: 5
sputter_def: 1: 0, 2: 60, 4: 120
data: 131 long 563
368
349
...
312
308
enddata
background: 131 double 1048
387.287
387.287
...
300.065
304.000
endbackground
original: 131 long 563
368
349
...
312
308
endoriginal
data: 131 long 563
365
389
...
299
315
enddata
background: 131 double 1048
378.010
378.002
...
```

```
300.012
300.000
endbackground
original: 131 long 563
365
389
...
315
endoriginal
data: 131 long 563
355
384
...
294
299
enddata
background: 131 double 1048
389.697
389.702
...
299.999
300.000
endbackground
original: 131 long 563
355
384
...
429
453
517
294
299
endoriginal
data: 131 long 564
390
430
...
309
305
enddata
background: 131 double 1048
422.035
422.026
...
312.325
312.333
endbackground
original: 131 long 564
390
430
...
309
305
endoriginal
data: 131 long 545
204
210
...
143
147
enddata
background: 131 double 1048
217.017
217.027
...
149.330
149.333
```

```

endbackground
original: 131 long 545
204
210
...
143
147
endoriginal
endregion

```

3.18 VSW-Tübingen (*.dat)

Comment:

- Example of a Cu 2p spectrum
- Excitation energy: 1253.6 eV, Start energy: 320.086, End energy: 288.001, Step width: 0.0515, Number of points: 624, Accumulations: 5, Analyser mode: FAT, Pass energy: 50 eV, Dwell time: 0.2 s

```

PCF
EISCA
4. 6.2003

```

```

Goertz,1,Cu2p
frei
Au/Ag/Cu 473 mm 105ø
Gesamtsignal
50.69 Prozent Totzeit
*
1
XPS
FAT
5
X-Ray
1
1.0000000000E+01
1.0000000000E+04
*
624
288.002
320.086
50.0
0.051
0.200
*
185696.000000
186616.000000
...
159068.000000
159438.000000
*
*

```

3.19 VGS2000 (*.xps)

Comment::

- Example of a survey
- Excitation energy not available
- Dwell time has to be calculated in a special manner

```

30308IA      1 Bereich
tv30308 interkaliert ungesputtert
24 19,35 158 33,5 Mg

```



```
...
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
122.20000 122.30000 122.40000 122.50000 122.60000 122.70000 122.80000 122.90000
```

```

123.00000 123.10000 123.20000 123.30000 123.40000 123.50000 123.60000 123.70000
123.80000 123.90000 124.00000 124.10000 124.20000 124.30000 124.40000 124.50000
124.60000 124.70000 124.80000 124.90000 125.00000 125.10000 125.20000 125.30000
...
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

```

3.21 SCIENTA3000 (*.txt)

Comment:

- Example with 1 region: Ag3d
- ‚Number of Slices’ is the number of separate intensities per channel
- The sum of all intensities per slice gives the intensity shown in the spectrum.

[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

```

3.22 PHI Spectrometer/Single Spectra (*.spe)

Comment:

- Example of 6 regions: Cu 2p, Ag3p1, Ag3d, Au 4f, Au 4d3, Au 4d5, O 1s
- Header in ASCII from SOFH to EOFH
- Intensities saved on the end of the file as single float or double float number (number of bytes: 4 x or 8 x number of channels of all regions)

```

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 Cl1s 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 Areal 1 (1024.0 1024.0 0.0 90.0 45.0)
SpatialAreaDesc: 1
EOFH
_ß"@,ëxJ°V@@@8\33...33ó@°-í+6L@2<,<|>@ö°èç
g"@-!-}Ãm"@øæJ •b@@‡|°èÃÃ"@ĐBä)Á7@@"ö-c"@¶ÃÚ·Y"@

```

3.23 PHI Spectrometer/Profile (*.pro; ang)

Comment:

- Example of sputter depth profile with 2 regions (Ta 4f, O 1s) and 60 sputter cycles (2 s per cycle)
- Header in ASCII from SOFH to EOFH

- Intensities saved on the end of the file as single float or double float number (number of bytes: 4 x or 8 x number of channels of all regions)

```

SOFH
Platform: PC
Technique: XPS
FileType: DEPTHPRO
FileDesc: Ta2O5 PHI 100nm
FileDate: 96 6 28
AcqFileDate: 96 6 28
AcqFilename: /usr/userdata/DATA/INE/Schild/sputterref/TaO_1.pro
ScanMode: scan
XraySource: Mg 1253.6 std
XrayPower: 400.00 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: 3He
SputterEnergy: 3.000 keV
SputterCurrent: 0.0 nA
SputterRaster: 10.0 0.0 um
PreAcqSputterTime: 4 s
PreAcqSputterRate: 1.0 A/s
NoSpectralReg: 2
SpectralRegDef: 1 1 O1 8 105 -0.1250 538.0 525.0 537.0 526.0 0.150000 58.70 none
SpectralRegDef: 2 2 Ta1 73 121 -0.1250 33.0 18.0 33.0 20.0 0.100000 58.70 none
NoDPDataCyc: 60
NoPreSputterCyc: 2
SputterInterval: 2.000 s
SputterMode: alt
SampleRotation: on
DepthRecal: no
NoSpatialArea: 1
SpatialAreaDef: 1 Full 1 (0.0 0.0 0.0 0.0 0.0)
EOFH
G«æ!G«@'G«G«ª...

```

3.24 Focus CSA (*.dat)

Comment:

- example of one region (VB), 20 Scans
- 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

```

[REGION_CONFIG]
TIMESTAMP="9/11/2009 / 10:17:40 AM"
USE=TRUE
E_START=10000.000000000000
E_STOP=10070.000000000000
E_STEP=0.318437500000
E_SCAN=1
EPASS=100.000000000000
N_SCAN=20
N_IMAGE=1000
PE=10050.000000

```

```

T_DWELL=5000.000000
SLIT=9
COMMENT=" "
PATH_LENS_TAB=/C/Program Files/FOCUS ProCSA/lens tables/Mode2/M06_Mo2.lens
PATH_DATA_FILE=/C/Data/090910/ST010KeV/VBdef.dat
[DETECTOR]
CAMRES_X=1280
CAMRES_Y=1024
CAMRANGE_XMIN=100
CAMRANGE_XMAX=599
CAMRANGE_YMIN=115
CAMRANGE_YMAX=350
T_EXPOSURE=5.000000
K_DET=0.101900
WA=4.500000
NX0=337
BINNING=1
K_SPEC=0.859900
CHANNELS=25
U_MCP=2400.000000
U_SCR=4500.000000
IP=127.0.0.1
PORT=5555
[DATA_CONFIG]
TIMESTAMP="9/11/2009 / 3:20:44 AM"
T_EXPOSURE=5.000000
N_SCAN=20
N_Image=1000
PE=10050.000000
WA=4.500000
[DATA]
10000.00000 1537 41 0 0
10000.31844 1553 41 0 0
10000.63688 1538 41 0 0
...
10069.73781 702 43 0 0
10070.05625 688 42 0 0
[DATA_1]
10000.00000 77 2 0 0
10000.31844 96 2 0 0
...
10069.73781 26 3 0 0
10070.05625 45 2 0 0
[DATA_2]
10000.00000 90 2 0 0
10000.31844 85 2 0 0
...
10069.73781 46 2 0 0
10070.05625 31 2 0 0
[DATA_3]
10000.00000 79 2 0 0
10000.31844 65 2 0 0
...
10069.73781 33 2 0 0
10070.05625 38 2 0 0
[DATA_4]
10000.00000 81 2 0 0
10000.31844 84 2 0 0
...
10069.73781 38 2 0 0
10070.05625 39 2 0 0
[DATA_5]
10000.00000 78 2 0 0
10000.31844 83 2 0 0
...
10069.73781 39 2 0 0
10070.05625 26 2 0 0

```

```
[DATA_6]
10000.00000 84    2    0    0
10000.31844 90    2    0    0
...
10069.73781 40    2    0    0
10070.05625 37    2    0    0
[DATA_7]
10000.00000 55    2    0    0
10000.31844 67    2    0    0
...
10069.73781 41    2    0    0
10070.05625 37    2    0    0
[DATA_8]
10000.00000 66    2    0    0
10000.31844 74    2    0    0
...
10069.73781 47    2    0    0
10070.05625 32    2    0    0
[DATA_9]
10000.00000 58    2    0    0
10000.31844 71    2    0    0
...
10069.73781 33    2    0    0
10070.05625 41    2    0    0
[DATA_10]
10000.00000 68    2    0    0
10000.31844 66    2    0    0
...
10069.73781 28    2    0    0
10070.05625 32    2    0    0
[DATA_11]
10000.00000 71    2    0    0
10000.31844 70    2    0    0
...
10069.73781 51    3    0    0
10070.05625 28    3    0    0
[DATA_12]
10000.00000 92    2    0    0
10000.31844 96    2    0    0
...
10069.73781 31    3    0    0
10070.05625 40    3    0    0
[DATA_13]
10000.00000 72    2    0    0
10000.31844 76    2    0    0
...
10069.73781 24    2    0    0
10070.05625 29    2    0    0
[DATA_14]
10000.00000 90    2    0    0
10000.31844 89    2    0    0
...
10069.73781 35    2    0    0
10070.05625 27    2    0    0
[DATA_15]
10000.00000 88    2    0    0
10000.31844 79    3    0    0
...
10069.73781 31    2    0    0
10070.05625 35    2    0    0
[DATA_16]
10000.00000 84    2    0    0
10000.31844 77    2    0    0
...
10069.73781 33    2    0    0
10070.05625 35    2    0    0
[DATA_17]
```

```

10000.00000 73    2    0    0
10000.31844 67    2    0    0
...
10069.73781 30    2    0    0
10070.05625 38    2    0    0
[DATA_18]
10000.00000 87    3    0    0
10000.31844 80    2    0    0
...
10069.73781 45    2    0    0
10070.05625 37    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

```

3.25 Croissant (*.pesp)

Comment:

- Measurement data format of the University Basel
- Example of 1one region (O 1s), 20 Scans
- 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

```

[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_S1s.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
GroupName=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
525.100 961.500 3907 854 736 759 823 735
525.150 961.450 3879 864 705 768 799 743
525.200 961.400 4042 898 740 831 837 736
...
539.750 946.850 4101 853 783 853 887 725
539.800 946.800 4002 899 754 804 832 713
539.850 946.750 4066 872 734 851 862 747
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

```

3.26 NEXAFS (*.dat)

Comment:

- Data format of a NEXAFS measurement with non-ecquidistant steps
- Example of a region (C 1s)
- no header
- Data: 1. column: Photon enenergy, 2. column: Intensity

```

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
...
3.2100000e+002 1.1158779e+000
3.2150000e+002 1.1052257e+000
3.2200000e+002 1.1062839e+000
3.2250000e+002 1.0904328e+000

```

3.2300000e+002	1.0875981e+000
3.2350000e+002	1.0741955e+000
3.2400000e+002	1.0674672e+000
3.2450000e+002	1.0636128e+000
3.2500000e+002	1.0502793e+000
3.2550000e+002	1.0514595e+000
3.2600000e+002	1.0403178e+000
3.2650000e+002	1.0262274e+000
3.2700000e+002	1.0092817e+000
3.2750000e+002	1.0000000e+000
3.2800000e+002	9.8856950e-001
3.2850000e+002	9.8077209e-001
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 with of exported data: 0.01 eV,
- Not available intensities are interpolated,
- 1. row: energy, series name of spectrum 1, series name spectrum 2, ...,
- 1. column: energy, 2-13 columns: intensities

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

4.1.1.5 Parameter Plot

Comment:

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

Energy	0	1	2	3	...	9	10
Parameter	C1s Peak1	O1s Peak1	O1s Peak2	Si2p Peak1	Si2p Peak2	Si2p Peak3	
0	199.999999999994	1.00000000000031	999.999999999999	998.985316335666	...		
1	799.999999999998	99.999999999998	899.999999999997	367.799999999992	...		
2	799.999999999998	199.999999999995	799.999999999996	135.299999999989	...		
3	199.999999999994	299.999999999996	699.999999999995	49.7799999999993	...		
4	199.999999999994	399.999999999998	599.999999999997	18.37000000000051	...		
5	799.999999999998	499.999999999999	499.999999999999	0	...		

```

6      799.999999999998  599.999999999995  399.999999999995  2.47800000000605  ...
7      199.999999999994  699.999999999995  299.999999999994  0                  ...
8      199.999999999994  799.999999999996  199.999999999998  0                  ...
9      799.999999999998  899.999999999996  99.9999999999967  0                  ...
10     799.999999999998  999.999999999999  0.999999999999153  0                  ...

```

4.1.1.6 Wagner Plot

Comment:

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

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

4.1.2 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
...
88.3;4.30237286;1.87729082;1.18719752;1.26836160;2.10025394;3.53868276;2.3907214
4;1.77791470;1.69478584;1.76560963;1.89092669
88.2;4.24587888;1.85379198;1.17395666;1.25563898;2.07963854;3.50366688;2.3679526
2;1.76182747;1.67988702;1.75030776;1.87465846
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
 48.69;702.37;351.18;0.865;0.865;99.31;99.91;0.853;0.853;0;0;152.97;76.48;0.986;0
 .986;103.13;103.73;1.669;1.669;0;0
 44.54;751.03;375.51;0.869;0.869;99.32;99.92;0.883;0.883;0;0;149.31;74.65;0.913;0
 .913;103.16;103.76;1.747;1.747;0;0
 40.39;915.1;457.55;0.812;0.812;99.31;99.91;0.896;0.896;0;0;143.15;71.57;0.962;0.
 962;103.15;103.75;1.847;1.847;0;0
 36.24;1071;535.84;0.851;0.851;99.32;99.92;0.843;0.843;0;0;138.81;69.4;0.961;0.96
 1;103.13;103.73;1.907;1.907;0;0
 32.09;941.64;470.82;0.834;0.834;99.31;99.91;0.871;0.871;0;0;140.83;70.41;1;1;103
 .2;103.8;1.798;1.798;0;0
 27.94;843.65;421.82;0.791;0.791;99.34;99.94;0.922;0.922;0;0;127.75;63.87;0.999;0
 .999;103.21;103.81;1.942;1.942;0;0
 23.79;799.36;399.68;0.792;0.792;99.34;99.94;0.867;0.867;0;0;124.17;62.08;1;1;103
 .22;103.82;1.728;1.728;0;0
 19.64;825.95;412.97;0.777;0.777;99.34;99.94;0.891;0.891;0;0;124.24;62.12;0.965;0
 .965;103.2;103.8;1.819;1.819;0;0
 15.49;1116;558.47;0.756;0.756;99.34;99.94;0.9;0.9;0;0;127.7;63.84;1;1;103.12;103
 .72;1.751;1.751;0;0
 11.34;966.93;483.46;0.776;0.776;99.35;99.95;0.884;0.884;0;0;121.47;60.73;0.988;0
 .988;103.19;103.79;1.995;1.995;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
-56.99;2318.28221;935.216392
-52.84;2630.11575;902.130651
-48.69;3002.31938;723.771260
-44.54;3188.35669;628.572714
-40.39;3931.40240;651.207306
-36.24;4442.72429;698.772095
-32.09;3937.65000;633.781393
-27.94;3673.67811;542.044884
-23.79;3290.39233;534.863938
-19.64;3442.94725;514.461365
-15.49;4652.76778;459.804089
-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_2012_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 2008
1
Calibration of intensity scale
Acquisition conditions:
Twin, LAX, 50eV pass
0
0
```

```
1
0
4
1
1
0
0
0
0
0
1
0
1
1
1
1
Peak
0
119857.939026664
206
411
C:\Programme\Unifit 2008\examples\projects
(ufp)\Calibration_Intensity_Cu\CUATLX19.VMS
1
12
Cu2p3_0
0
411
523.6
564.6
0.1
10
1486.6
3
0.3
FAT
3-5-2004

23295.2
23118.5
23312.2
...
32442.9
33900.1
35115.9
36240.8069376146
37541.5569991501
39214.8001599847
...
13853.8771398518
13892.2199001605
13808.5401490263
0
0
0
...
0
0
0
19529.1596516772
19506.9264511183
19484.7781521874
...
13731.561604792
13728.8334511621
13726.2060140308
Peak
```

401
0
5000000
67049.4005509924
0
0
5000000
0
1
0.1
5
0.668837328491432
0
0.1
5
0
1
922
963
932.691983684025
0
922
963
932.691983684025
1
0.1
5
0.919872177669453
0
0.1
5
0
1
0
0
0
1
0
0
0
1
15250.8303328187
Falsch
2.35204675390576
Falsch
0.0532203056627311
Falsch
0
Wahr
0.00314371152907954
Falsch
0
Wahr
0
0
0
0
Kurve 1
Kurve 2
Kurve 3
Kurve 4
Kurve 5
Kurve 6
Kurve 7
Kurve 8
Kurve 9
Kurve 10

```
Kurve 11
Kurve 12
Kurve 13
Kurve 14
Kurve 15
0
0
1
1
1
0 2008
2
Calibration of intensity scale
Acquisition conditions:
Twin, LAX, 50eV pass
0
0
2
0
4
1
0
0
0
0
0
0
1
0
1
1
1
Dublett
0
12377.7387706924
1
401
C:\Programme\Unifit 2008\examples\projects
(ufp)\Calibration_Intensity_Cu\CUATLX19.VMS
1
12
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
...
1045.03
1112.55
1138.01
1104.13013692159
1071.3734276708
1091.82614278607
...
470.373049542057
```

470.150733992558
469.931656114573
Dublett
401
0
500000
2124.00000650975
0
0
500000
1090.70954552183
0
0.1
5
0.106849857450146
0
0.1
5
0.106849857450146
1
55
95
75.0783280298056
0
55
95
77.4946067800895
0
0.1
5
2.55230556411849
0
0.1
5
2.55230556411849
1
0
0
0
1
0
0
0
1
522.103137121386
Falsch
0.198301370092426
Falsch
0.00158693097340261
Falsch
0
Wahr
0.00357535492084456
Falsch
0
Wahr
0
0
0
0
Kurve 1
Kurve 2
Kurve 3
Kurve 4
Kurve 5
Kurve 6
Kurve 7

```
Kurve 8
Kurve 9
Kurve 10
Kurve 11
Kurve 12
Kurve 13
Kurve 14
Kurve 15
0
0
1
1
1
0 2008
3
Calibration of intensity scale
Acquisition conditions:
Twin, LAX, 50eV pass
0
0
4
0
0
0
0
0
0
0
0
0
0
1
0
0
0
1
Dublett
0
0
1
1361
C:\Programme\Unifit 2008\examples\projects
(ufp)\Calibration_Intensity_Cu\CUATLX58.VMS
1
12
US_0
0
1361
200
1560
1
50
1486.6
2
0.3
FAT
29-4-2004
264993
263826
262686
...
858.27
850.06
817.265
0
0
```

```

0
...
0
0
0
Kurve 1
Kurve 2
Kurve 3
Kurve 4
Kurve 5
Kurve 6
Kurve 7
Kurve 8
Kurve 9
Kurve 10
Kurve 11
Kurve 12
Kurve 13
Kurve 14
Kurve 15
0
0
1
1
1
2
AlScofld.sen
ESCALAB220_TWIN_LAXL_10EP.trm
1
Cu2p3
16.73
11.39
1.931
367.961
2
Cu3p
2.478
22.87
0.681
38.594

```

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
- For fitted background: last six rows = background parameters: constante parameter, linear parameter, square parameter, cubic parameter, Shirley parameter, Tougaard parameter

```

Dublett
402
1
1000000
3060
0
1
1000000
1530
-1
0

```

1
0.51
0
0
1
0.51
-1
1
1400
163.88
0
1
1400
165.08
-1
0.1
5
1.92
0
0.1
5
1.92
-1
0
0
0
-1
0
0
0
-1
1
1000000
414
0
1
1000000
207
-1
0
1
0
0
0
1
0
-1
1
1400
168.05
0
1
1400
169.25
-1
0.1
5
2.65
0
0.1
5
2.65
-1
0
0
0
-1

```
0
0
0
-1
579.382483765469
0
1.37578659957308
0
0
-1
0
-1
0
-1
1.39756699257826
0
```

4.4 Annotation/Design File (*.DSG)

Remark:

- saved in Unifit _2012_User_Files\design*.dsg

Annotation/Design

```
2011
0
1.5
16777215
0
1
0
0
1.5
16711680
0
1
0
3
1
65280
0
1
0
0
1.5
32768
0
1
0
0
2.5
255
0
1
0
0
1.5
8421504
0
1
0
6
3
255
0
1
```

0
2
1
16711680
0
1
0
1
1
0
0
1
0
2
1
0
0
1
0
1
1.5
255
1
1.5
255
1
1.5
8454143
2
1.5
8454143
1
1.5
65535
3
1.5
65535
1
1.5
16777088
4
1.5
16777088
1
1.5
16776960
5
1.5
16776960
1
1.5
16776960
6
1.5
16776960
1
1.5
8388863
7
1.5
8388863
1
1.5
4227327
8
1.5
33023

1
1.5
16711935
9
1.5
16711935
1
1.5
33023
10
1.5
33023
1
1.5
12632256
11
1.5
12632256
1
1.5
65408
11
1.5
65408
1
1.5
16776960
11
1.5
16776960
1
1.5
33023
12
1.5
4227327
1
1.5
12615808
1
2
12615808
15461355
14803425
13619151
12303291
10790052
9671571
8289918
6974058
8453888
16776960
16744703
16711680
33023
4227327
4227200
0
1.5
16777215
Arial
Falsch
16
Falsch
Falsch
Falsch
0

16777215
12
28
2
1.5
8421440
Arial
Falsch
12
Falsch
Falsch
Falsch
0
16777215
9
21
0
1
8421504
Arial
Falsch
14
Falsch
Falsch
Falsch
0
16777215
11
25
0
2
255
Arial
Falsch
12
Falsch
Falsch
Falsch
0
16777215
9
21
2
1
8421504

Falsch
0
Falsch
Falsch
Falsch
0
0
0
0
0
2
16711680

Falsch
0
Falsch
Falsch
Falsch
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0
0
0
0
0
5066061
0
1
1
1
1
1
1
0
1
1
1
1
1
0

```

1
1
8454143
65535
4227327
5
S 2p
0.787724329896907
0.654007591795021
S 2s
0.720920206185567
0.694229505803343
C 1s
0.705250103092784
0.0645485071903058
N 1s
0.534528453608248
0.60812381632815
O 1s
0.405868659793814
0.294398326132072
1
Survey
0.0314356701030929
0.0591042084850141
0
0
0
0
Kurve 1
Kurve 2
Kurve 3
Kurve 4
Kurve 5
Kurve 6
Kurve 7
Kurve 8
Kurve 9
Kurve 10
Kurve 11
Kurve 12
Kurve 13
Kurve 14
Kurve 15
1
1
1
Binding Energy / eV
Intensity / kcps

```

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

Remark:

- saved in Unifit _2012_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_2012_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\sensifivity 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,Bel1s,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,Na1s,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 linie ($1 = \alpha_3, 2 = \alpha_4, 3 = \alpha_5, 4 = \alpha_6, 5 = \beta$)
- 2nd row: energy position of satellite 1. set
- 3rd row: rel. height of the satellite 1. set
- 4th row: energy position of the satellite 2. set
- 5th row: rel. height of the satellite 2. set etc.

Aluminiumsatelliten 1

9.8
 0.064
 0
 0
 0
 0
 0
 0
 0
 0

Magnesiumsatelliten 1

8.4
0.08
0
0
0
0
0
0

...

0
0
0

Aluminiumsatelliten 5

69.7
0.0055
0
0
0
0
0
0
0
0
0

Magnesiumsatelliten 5

48.5
0.005
0
0
0
0
0
0
0
0

5.5 Doublet File (doublet.dda)

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

Comment:

- 1. value: name of the peaks
- 2. value: relative intensity
- 3. Wert: 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,0.66,1.0
Ca2p,0.5,3.5,Cd3p,0.5,34.1,Cd3d,0.666,6.76,Cd4d,0.666,0.6,Ce3d,0.666,18.3,Ce4d,0.666,4.0,Cl2p,0.5,1.6,Co2p,0.5,15.05
Co3p,0.5,2.0,Cr2p,0.5,9.3,Cr3p,0.5,1.0,Cs3d,0.666,13.9,Cs4d,0.666,2.3
Cu2p,0.5,19.8,Cu3p,0.5,2.4,Dy4d,0.666,0.0,Dy4p,0.5,40.3,Er4p,0.5,45.8,Er4d,0.666,0.0,Eu3d,0.666,31.1
Eu4d,0.666,0.0,Fe2p,0.5,13.2,Fe3p,0.5,1.0,Ga2p,0.5,26.8,Ga3p,0.5,3.0,Ga3d,0.666,0.4,Gd4d,0.666,0.0
Ge2p,0.5,31.1,Ge3p,0.5,4.1,Hf4d,0.666,8.5,Hf4f,0.75,1.55,Hg4d,0.666,19.4,Hg4f,0.75,4.1,Ho4d,0.666,0.0
Ho4p,0.5,36.8,I3d,0.666,11.52,I4d,0.666,2.0,In3p,0.5,37.9,In3d,0.666,7.6,In4d,0.666,0.9,Ir4d,0.666,15.6,Ir4f,0.75,2.95
K2p,0.5,2.8,Kr3p,0.5,7.8,La3d,0.666,16.8,La4d,0.666,2.8,Lu4p,0.5,53.2,Lu4d,0.666,9.8,Mg2p,0.5,0.4
Mn2p,0.5,11.25,Mn3p,0.5,1.0,Mo3p,0.5,16.6,Mo3d,0.666,3.15,Nb3p,0.5,15.5,Nb3d,0.666,2.8,Nd4d,0.666,0.0

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

6 References

- [1] G. Beamson, D. Briggs, High Resolution XPS of Organic Polymers, John Wiley & Sons, Chichester, 1992
- [2] J.F. Moulder, W.F. Stickle, P.E. Sobol, K.D. Bomben, Handbook of X-ray Photoelectron Spectroscopy, Physical Electronics, Inc., Eden Prairie , 1995
- [3] C.D. Wagner, A.V. Naumkin, A. Kraut-Vass, J.W. Allison, C.J. Powell, J.R. Rumble Jr. NIST X-ray Photoelectron Spectroscopy Database, NIST Standard Reference Database 20, Version 3.1, Gaithersburg 2000, <http://srdata.nist.gov/xps>