Fundamental XPS Data* to Assist Peak-fitting Elements, Binary Oxides and Chemical Compounds

*The "*XI Library of Monochromatic XPS Spectra*" is the source of BEs and FWHMs shown here. (US registered copyright, © TX 4-560-881)

Key (example box: 13 Al 2p3)

Atomic Number of Aluminum	13 Al 2p3	Principal XPS Signal for Aluminum
Abbreviation for Elemental Aluminum	Al° / Al_2O_3•	Pure Oxide - most common form - thermodynamically stable
Al 2p3 BE of Al° under Native Oxide	72.8 / 74.4	Al 2p3 BE of Oxide Species in Pure Oxide
Al 2p3 FWHM of Al° under Native Oxide	(0.62) / (1.39)	Al 2p3 FWHM of Oxide Species in Pure Oxide
C 1s BE of Principal Peak 10 hours after Ion Etch, Pure Al°	285.1 / 285.0	C 1s BE of Hydrocarbon Peak - if non-conductive, then defined = 285.0 eV
Al 2p3 BE (2nd decimal value included) of Ion Etched, Pure Al°	72.82 / 530.8	O 1s BE of Oxygen Species in Pure Oxide
Al 2p3 FWHM of Ion Etched, Pure Al°	(0.41) / (1.60)	O 1s FWHM of Oxygen Species in Pure Oxide

Non-conductive materials were referenced to adventitious hydrocarbon with C 1s BE at 285.0 eV.
Energy resolution settings for pure oxide data gave FWHM <0.75 eV for Ag 3d5 of ion etched Ag°.
All non-conductors were analyzed with the Flood-Gun Mesh-Screen 0.5-1.0 mm above the specimen.
C 1s BEs for "hydrocarbons" were collected from hydrocarbon peak that formed on ion etched elements.
Carbon from the cryo-pumped vacuum ($3x10^{-9}$ torr) was analyzed >10 hours after ion cleaning.
Energy resolution settings for ion etched elements gave FWHM <0.50 eV for Ag 3d5 of ion etched Ag°.
Calibration was: Cu 2p3 at 932.67 ±0.05 eV, Cu 3s at 122.45 ±0.05 eV and Au 4f7 at 83.98 eV.

The FWHM and BE values in this table were all obtained by one scientist using two SSI XPS systems with a theoretical resolution of 0.1 eV. Each system was equipped with a monochromatic Aluminum X-ray source which have a theoretical energy resolution limit of about 0.16 eV. The BEs for the ion etched elements are reliable secondary energy reference values with a standard deviation of 0.055 as measured by NIST. BEs for the chemical compounds should be accurate to ±0.15 eV.

The BEs of non-conductive materials are referenced to the hydrocarbon C 1s BE at 285.0 eV to match current day methods of charge referencing, but this method of charge referencing is not absolute. The C 1s BEs of the adventitious hydrocarbon components on various naturally formed, thin native oxides (metal signal visible) were measured to occur between 285.5 and 286.5 eV. The native oxides of Ag, Al, Be, Bi, Cd, Co, Ga, Ge, Hf, In, Lu, Mg, Ni, Pb, Pd, Sc, Si, Ta, Y, Zn and Zr give C 1s BEs that are 0.5-1.5 eV above 285.0 eV. Surface dipole moments are suspected to be the cause of this shift. BEs from native oxides for these metals are more correct. BEs from oxides marked with a small red dot "•" require further study.

Groups 1 and 2, 13–18

1 H 1s (group 1)	H_2° / LiH	
2 He 1s (group 18)	He^+/Be / He^+/C	
3 Li 1s	LiOH / Li_2O	54.9 / 55.6; (1.65) / (1.6); 285.0 / 285.0; 531.8 / 530.8; (1.6) / (1.5)
4 Be 1s (group 2)	Be° / BeO•	111.8 / 113.6; (0.79) / (1.73); 286.2 / 285.0; 111.88 / 531.2; (0.69) / (1.71)
5 B 1s (group 13)	B° / B_2O_3	187.5 / 193.7; (0.92) / (1.30); 285.2 / 285.0; 187.8 / 533.7; (1.03) / (1.6)
6 C 1s (group 14)	HOPG / Black	284.5 / 284.4; (0.42) / (1.04)
7 N 1s (group 15)	Kapton / BN	400.9 / 398.9; (1.31) / (1.10); 285.0 / 285.0; 191.3; (1.03)
8 O 1s (group 16)	CuO / SiO_2	529.6 / 532.4; (0.98) / (1.2.7); 284.7 / 285.0; 934.0 / 103.1; (1.42) / (1.19)
9 F 1s (group 17)	Teflon / CaF_2	689.2 / 685.1; (1.8) / (1.53); 285.0 / 285.0; 292.0 / 348.1; (1.6) / (1.6)
10 Ne 1s	Ne^+/Be / Ne^+/C	863.1; (1.3)
11 Na 1s	Na° / Na_2O	1071.8 / 1072.6; (1.1) / (1.78); 285.0; 530.6; (1.44)
12 Mg 2p	Mg° / MgO•	49.7 / 49.5; (0.58) / (1.25); 286.5 / 285.0; 49.77 / 529.9; (0.60) / (1.38)
13 Al 2p3	Al° / Al_2O_3•	72.9 / 74.4; (0.62) / (1.39); 284.9 / 285.0; 72.82 / 530.8; (0.41) / (1.60)
14 Si 2p3	Si° / SiO_2•	99.8 / 103.1; (0.57) / (1.19); 285.8 / 285.0; 99.35 / 532.4; (0.45) / (1.27)
15 P 2p3	P° / InP	130.1 / 128.8; (0.67) / (0.62); 285.0 / 285.5; 444.7; (0.78)
16 S 2p3	S° / MoS_2	164.0 / 162.7; (0.72) / (0.39); 285.0; 229.7; (0.80)
17 Cl 2p3	PVC / NaCl	199.8 / 199.3; (1.7) / (1.19); 285.0 / 285.0; 1072.0; (1.40)
18 Ar 2p3	Ar^+/B / Ar^+/HOPG	241.8 / 241.8; (1.4) / (0.89); 285.2 / 284.5; 188.1
19 K 2p3	K° / K_2O	294.4 / 292.7; (0.9) / (1.37); 285.0; 531.0; (1.6)
20 Ca 2p3	Ca° / $CaCO_3$	
21 Sc 2p3 (3)	Sc° / Sc_2O_3•	
22 Ti 2p3 (4)	Ti° / TiO_2	
23 V 2p3 (5)	V° / V_2O_5	
24 Cr 2p3 (6)	Cr° / Cr_2O_3	
25 Mn 2p3 (7)	Mn° / MnO_2	
26 Fe 2p3 (8)	Fe° / α-Fe_2O_3	
27 Co 2p3 (9)	Co° / Co_3O_4•	
28 Ni 2p3 (10)	Ni° / NiO•	
29 Cu 2p3 (11)	Cu° / Cu_2O	
30 Zn 2p3 (12)	Zn° / ZnO•	
31 Ga 3d5	Ga° / Ga_2O_3•	
32 Ge 3d5	Ge° / GeO_2•	
33 As 3d5	As° / As_2O_3	
34 Se 3d5	Se° / SeO_x	
35 Br 3d5	KBr	
36 Kr 3d5	Kr^+/Be / Kr^+/C	86.9; (0.88); 285.0
37 Rb 3d5	Rb° / RbOAc	111.5 / 109.7; (0.8) / (1.40); 285.0; 530.6; (1.9)
54 Xe 3d5	Xe^+/Be / Xe^+/C	669.6; (1.13); 285.0
55 Cs 3d5	Cs° / Cs_2O	726.4 / 724.7; (1.3) / (2.00); 285.0; 198.9
86 Rn 4f7	Radioactive	
87 Fr 4f7	Radioactive	
88 Ra 4f7	Radioactive	
89 Ac 4f7	Radioactive	

Size and pricing for these tables:

Laminated 8.5x10" letter or A4 size:	$55 (includes shipping)
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Changes and improvements include:

A. Correction of several metal oxide metal signal BEs
B. Correction of BEs of several O 1s peak BEs
C. Coloration of chart to enhance readability and reveal related elements.
D. Highlighting of FWHM in blue lettering because these are the key to improved peak-fits.
E. Addition of alkali oxides replacing alkali halides to match presence of other oxides.
F. Marking of ionic oxides (red dot) that are expected to have C 1s BEs higher than 285.5 eV.
G. Addition of various BEs and FWHMs for Sr, La, Ce, Ne Os, U, Na, K, Rb, Cs and Th.
H. Introduction of C 1s BEs from Carbon recovered after ion etching and 10+ hr exposure to UHV.
I. Addition of radioactivity labels (bottom right corner of each box if radioactive)
J. Calibration and Std Dev info shown in bottom image below signature

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Updated: March 1, 2007

Lanthanides and Actinides

58 Ce 3d5	Ce° / CeO_2	883.8 / 882.1; (3.2) / (2.0); 285.0; 529.6; (2.00)
59 Pr 3d5	Pr° / Pr_2O_5	929.4 / 928.8; (2.96) / (3.2); 285.0; 528.5; (1.2)
60 Nd 3d5	Nd° / Nd_2O_3	980.8 / 983.2; (2.9) / (2.7); 285.6 / 285.0; 530.8; (1.3)
61 Pm 4d5	Pm° / Pm_2O_3	Radioactive
62 Sm 4d5	Sm° / Sm_2O_3	1081.1 / 1083.8; --- / (4.3); --- / 285.0; 128.7 / 529.9; (2.5) / (1.6)
63 Eu 4d5	Eu° / Eu_2O_3	128.2 / 136.2; --- / (3.6); 284.3 / 285.0; 128.18 / 530.5; (1.08) / (1.4)
64 Gd 4d5	Gd° / Gd_2O_3	140.2 / (1187.5); --- / (5.4); 281.4 / 285.0; 140.31 / 529.3; (1.05) / (1.5)
65 Tb 4d5	Tb° / Tb_4O_7	145.9 / (149.5); --- / (?); --- / 285.0; 145.95 / 529.7; (1.16) / (1.5)
66 Dy 4d5	Dy° / Dy_2O_3	152.4 / (153.5); --- / (1.9); --- / 285.0; 152.34 / 529.4; (0.90) / (1.7)
67 Ho 4d5	Ho° / Ho_2O_3	159.8 / 160.9; --- / (2.0); --- / 285.0; 159.58 / 529.3; (0.98) / (1.6)
68 Er 4d5	Er° / Er_2O_3	167.7 / 168.5; --- / (1.9); --- / 285.0; 167.25 / 529.7; (1.00) / (1.5)
69 Tm 4d5	Tm° / Tm_2O_3	175.3 / 176.3; --- / (1.1); 285.3 / 285.0; 175.37 / 529.6; (1.06) / (1.6)
70 Yb 4d5	Yb° / Yb_2O_3	182.4 / 185.0; --- / (2.7); 285.6 / 285.0; 182.39 / 529.2; (0.61) / (1.5)
71 Lu 4f7	Lu° / Lu_2O_3	7.1 / 8.0; (0.46) / (2.5); 284.6 / 285.0; 7.10 / 529.5; (0.69) / (1.4)
90 Th 4d5	Th° / ThO_2	333.2 / 334.5; (1.7) / (1.6)
91 Pa 4d5		Radioactive
92 U 4f7	U° / UO_3	377.3 / 381.7; (1.4)
93 Np		Radioactive
94 Pu		Radioactive
95 Am		Radioactive
96 Cm		Radioactive
97 Bk		Radioactive
98 Cf		Radioactive
99 Es		Radioactive
100 Fm		Radioactive
101 Md		Radioactive
102 No		Radioactive
103 Lr		Radioactive

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