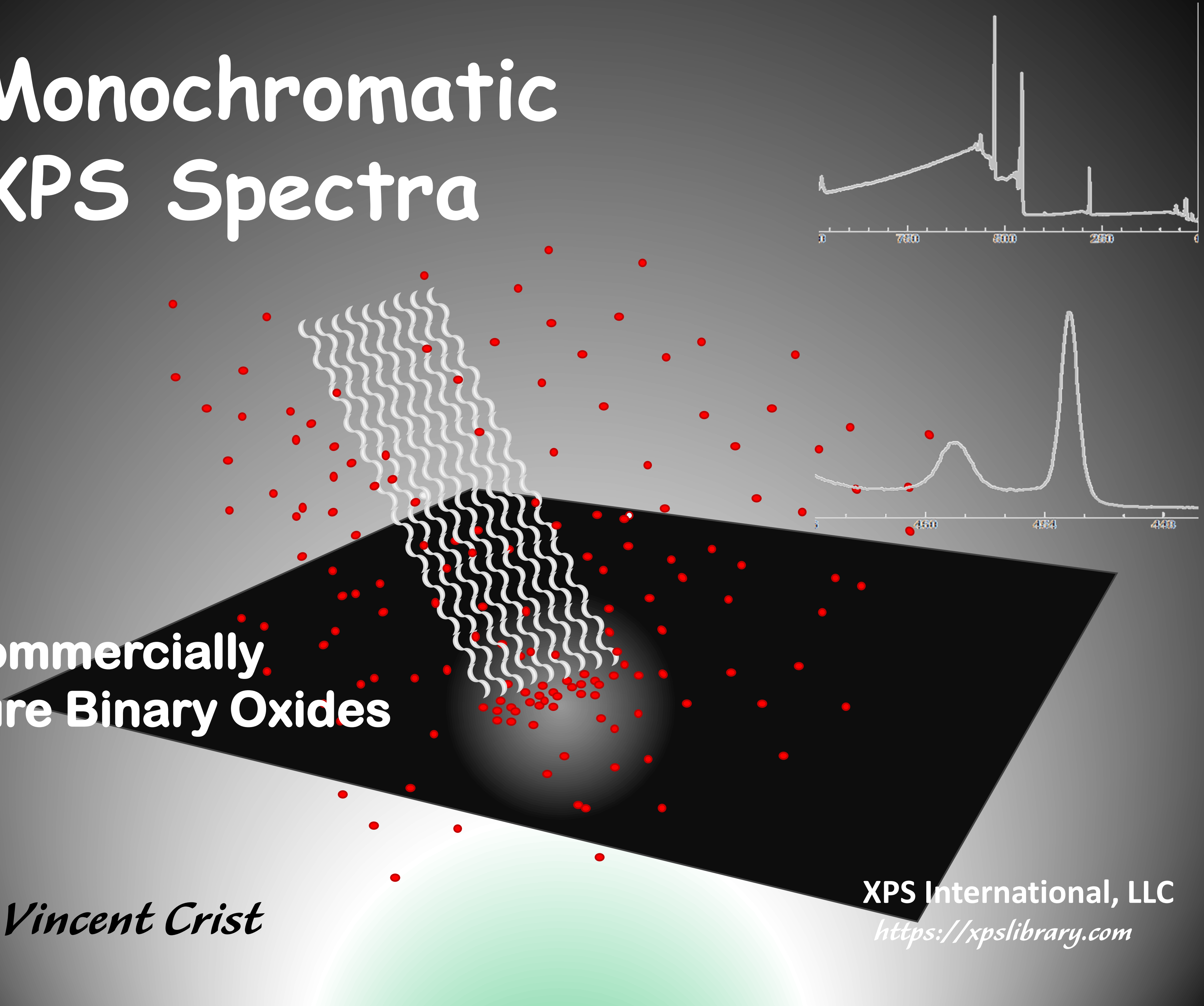
Monochromatic XPS Spectra



Commercially Pure Binary Oxides

B. Vincent Crist

XPS International, LLC
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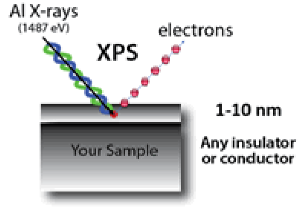
Monochromatic XPS Spectra

Commercially Pure Binary Oxides



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H 1s H_2° LiH																	**2 He 1s** 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** 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** 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** HOPG Black 284.5 284.4 (0.42) (1.04)	**7 N 1s** Kapton BN 400.9 398.9 (1.31) (1.10) 285.0 285.0 191.3 (1.03)	**8 O 1s** 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** 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 2p** 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 2p** 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° $CaCO_3$ 346.5 346.4 (1.0) (1.67) 284.6 285.0 346.5 530.8 (1.07) (1.64)	**21 Sc 2p3** Sc° Sc_2O_3* 398.5 401.9 (0.9) (1.27) 285.9 285.0 398.46 530.0 (0.69) (1.30)	**22 Ti 2p3** Ti° TiO_2 453.8 458.8 (0.90) (1.02) 285.1 285.0 453.95 530.0 (0.62) (1.20)	**23 V 2p3** V° V_2O_5 512.2 517.0 (0.79) (0.99) 285.0 284.8 512.22 530.0 (0.75) (1.33)	**24 Cr 2p3** Cr° Cr_2O_3 574.2 575.6 (1.05) (1.10) 284.8 285.0 574.37 530.1 (0.89) (1.27)	**25 Mn 2p3** Mn° MnO_2 638.7 641.4 (1.00) (1.12) 286.3 284.6 638.74 529.0 (0.89) (1.02)	**26 Fe 2p3** Fe° a-Fe_2O_3 706.6 709.8 (0.90) (1.31) 285.0 285.0 706.78 529.9 (0.99) (1.04)	**27 Co 2p3** Co° Co_3O_4* 778.1 779.5 (0.99) (1.51) 285.0 285.0 778.26 530.0 (0.85) (1.00)	**28 Ni 2p3** Ni° NiO* 852.6 853.7 (1.14) (1.19) 284.7 284.8 852.65 529.3 (1.02) (1.06)	**29 Cu 2p3** Cu° Cu_2O 932.7 932.7 (1.22) (1.16) 284.7 285.0 932.67 530.5 (0.92) (1.00)	**30 Zn 2p3** Zn° ZnO* 1021.8 1021.7 (1.10) (1.43) 284.8 285.0 1021.76 530.5 (0.97) (1.15)	**31 Ga 3d5** Ga° Ga_2O_3* 18.5 20.7 (0.70) (1.28) 285.6 285.0 18.5 531.4 (0.60) (1.51)	**32 Ge 3d5** Ge° GeO_2* 29.3 32.9 (0.68) (1.28) 285.1 285.0 29.28 532.1 (0.64) (1.40)	**33 As 3d5** As° As_2O_3 41.8 45.3 (0.65) (1.26) 284.8 285.0 41.69 532.0 (0.67) (1.71)	**34 Se 3d5** Se° SeO_2 54.8 59.3 (0.76) (1.09) 284.2 284.6 54.90 532.6 (0.78)	**35 Br 3d5** KBr 68.8 (0.92) 285.0 293.0 (1.31)	**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)	**38 Sr 3d5** Sr° $SrCO_3$ 134.3 133.4 (0.9) (1.56) 285.0 531.5 (1.9)	**39 Y 3d5** Y° Y_2O_3* 155.9 158.0 (0.60) (1.18) 286.0 285.0 155.92 530.7 (0.62) (1.30)	**40 Zr 3d5** Zr° ZrO_2* 178.9 182.5 (0.63) (1.20) 285.5 285.0 178.80 530.4 (0.63) (1.44)	**41 Nb 3d5** Nb° Nb_2O_5 202.1 207.2 (0.78) (1.12) 285.0 285.0 202.35 530.3 (0.57) (1.34)	**42 Mo 3d5** Mo° MoO_3 227.8 233.0 (0.66) (1.03) 285.1 284.9 227.94 530.9 (0.57) (1.23)	**43 Tc 3d5** Tc° TcO_2 256.8	**44 Ru 3d5** Ru° RuO_2 280.0 280.7 --- (0.77) 284.7 284.6 280.11 529.3 (0.59) (0.95)	**45 Rh 3d5** Rh° Rh_2O_3 307.2 308.6 (0.73) (0.90) 284.6 284.7 307.21 530.2 (0.69) (1.09)	**46 Pd 3d5** Pd° PdO* 335.1 336.9 (0.80) (0.98) 284.6 284.9 335.10 530.6 (0.77) (1.09)	**47 Ag 3d5** Ag° Ag_2O* 368.2 367.6 (0.64) (1.00) 284.8 284.3 368.28 530.1 (0.62) (1.20)	**48 Cd 3d5** Cd° CdO* 405.0 404.1 (0.80) (1.42) 285.0 285.0 405.04 528.6 (0.61) (1.28)	**49 In 3d5** In° In_2O_3* 443.8 444.3 (1.08) (1.33) 285.0 285.0 443.87 529.8 (0.71) (1.19)	**50 Sn 3d5** Sn° SnO_2 484.9 487.3 (0.81) (1.32) 284.9 285.5 485.01 531.1 (0.68) (1.14)	**51 Sb 3d5** Sb° Sb_2O_3 528.1 532.4 (0.88) (1.6) 284.8 285.0 528.26 531.0 (0.80) (1.6)	**52 Te 3d5** Te° TeO_2 572.7 576.6 (0.97) (1.48) 284.3 284.9 572.97 530.8 (0.83) (1.42)	**53 I 3d5** KI 619.2 (1.30) 285.0 293.2 (1.11)	**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	**56 Ba 3d5** Ba° $BaCO_3$ 780.6 779.9 (1.4) (2.07) 285.0 531.4 (1.77)	**57 La 3d5** La° La_2O_3 835.8 834.4 (1.3) (2.5) 285.0 529.0 (1.66)	**72 Hf 4f7** Hf° HfO_2* 14.4 17.2 (0.63) (1.31) 285.7 285.0 14.32 529.9 (0.62) (1.71)	**73 Ta 4f7** Ta° Ta_2O_5* 21.8 26.3 (0.72) (1.11) 285.1 285.0 21.78 530.4 (0.56) (1.47)	**74 W 4f7** W° WO_3 31.4 35.8 (0.58) (1.02) 285.1 285.1 31.38 530.6 (0.53) (1.28)	**75 Re 4f7** Re° Re_2O_7 40.3 46.9 (0.67) (1.47) 285.0 285.0 40.30 532.2 (0.54) (1.49)	**76 Os 4f7** Os° OsO_2 50.7 53.8 (1.2)	**77 Ir 4f7** Ir° IrO_2 60.8 61.7 (0.80) (0.84) 284.5 284.8 60.88 530.0 (0.82) (0.99)	**78 Pt 4f7** Pt° PtO_2 71.1 75.1 (0.96) (1.09) 284.4 284.9 71.15 531.3 (0.88) (1.52)	**79 Au 4f7** Au° Au_2O_3 84.0 85.1 (0.66) (1.37) 284.1 285.1 83.98 530.2 (0.68) (1.13)	**80 Hg 4f** Hg° HgO 99.8 100.9 --- (1.07) 285.0 285.0 99.81 530.0 (0.65) (1.00)	**81 Tl 4f7** Tl° Tl_2O_3* 117.8 118.1 (0.97) (1.1) 285.2 284.8 117.77 528.6 (0.66) (1.07)	**82 Pb 4f7** Pb° PbO* 136.9 137.5 (0.67) (1.17) 285.0 285.0 136.95 528.9 (0.63) (1.09)	**83 Bi 4f7** Bi° Bi_2O_3* 157.0 158.9 (0.73) (1.37) 284.9 285.0 157.05 529.6 (0.62) (1.52)	**84 Po 4f7** Radioactive	**85 At 4f7** Radioactive	**86 Rn 4f7** Radioactive
87 Fr 4f7 Radioactive	**88 Ra 4f7** Radioactive	**89 Ac 4f7** Radioactive															

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_3 929.4 928.8 (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_2O_3 145.9 (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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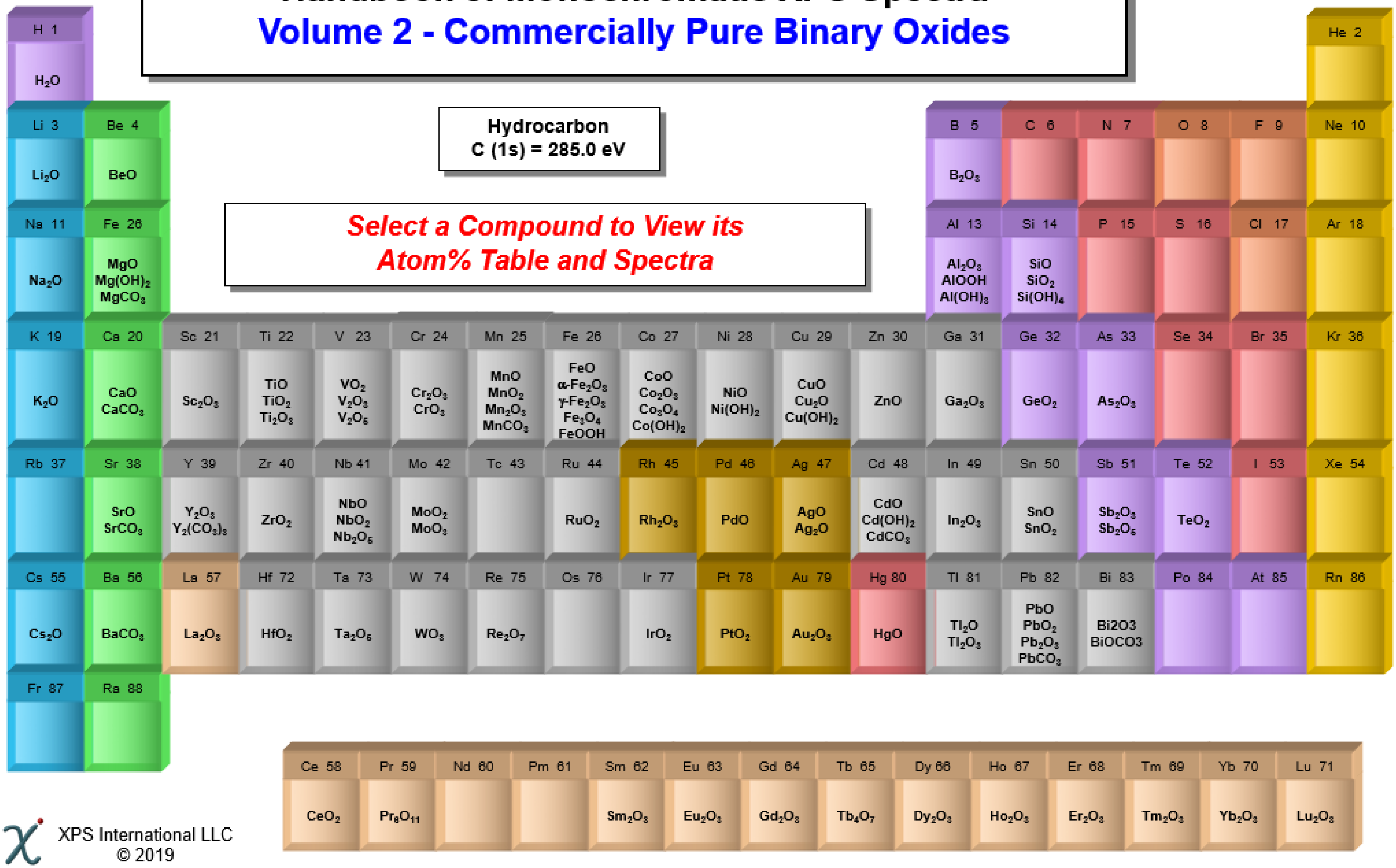
Handbooks of Monochromatic
XPS Spectra

Volume 2 – *Commercially Pure Binary Oxides*
and a few Common Carbonates and Hydroxides

by

B. Vincent Crist, Ph.D.

Handbook of Monochromatic XPS Spectra
Volume 2 - Commercially Pure Binary Oxides



Hydrocarbon
C (1s) = 285.0 eV

Select a Compound to View its Atom% Table and Spectra

H 1 H_2O																	He 2
Li 3 Li_2O	Be 4 BeO											B 5 B_2O_3	C 6	N 7	O 8	F 9	Ne 10
Na 11 Na_2O	Fe 26 MgO $Mg(OH)_2$ $MgCO_3$											Al 13 Al_2O_3 AlOOH $Al(OH)_3$	Si 14 SiO SiO_2 $Si(OH)_4$	P 15	S 16	Cl 17	Ar 18
K 19 K_2O	Ca 20 CaO $CaCO_3$	Sc 21 Sc_2O_3	Ti 22 TiO TiO_2 Ti_2O_3	V 23 VO_2 V_2O_3 V_2O_5	Cr 24 Cr_2O_3 CrO_3	Mn 25 MnO MnO_2 Mn_2O_3 $MnCO_3$	Fe 26 FeO α-Fe_2O_3 γ-Fe_2O_3 Fe_3O_4 FeOOH	Co 27 CoO Co_2O_3 Co_3O_4 $Co(OH)_2$	Ni 28 NiO $Ni(OH)_2$	Cu 29 CuO Cu_2O $Cu(OH)_2$	Zn 30 ZnO	Ga 31 Ga_2O_3	Ge 32 GeO_2	As 33 As_2O_3	Se 34	Br 35	Kr 36
Rb 37	Sr 38 SrO $SrCO_3$	Y 39 Y_2O_3 $Y_2(CO_3)_3$	Zr 40 ZrO_2	Nb 41 NbO NbO_2 Nb_2O_5	Mo 42 MoO_2 MoO_3	Tc 43	Ru 44 RuO_2	Rh 45 Rh_2O_3	Pd 46 PdO	Ag 47 AgO Ag_2O	Cd 48 CdO $Cd(OH)_2$ $CdCO_3$	In 49 In_2O_3	Sn 50 SnO SnO_2	Sb 51 Sb_2O_3 Sb_2O_5	Te 52 TeO_2	I 53	Xe 54
Cs 55 Cs_2O	Ba 56 $BaCO_3$	La 57 La_2O_3	Hf 72 HfO_2	Ta 73 Ta_2O_5	W 74 WO_3	Re 75 Re_2O_7	Os 76	Ir 77 IrO_2	Pt 78 PtO_2	Au 79 Au_2O_3	Hg 80 HgO	Tl 81 Tl_2O Tl_2O_3	Pb 82 PbO PbO_2 Pb_2O_3 $PbCO_3$	Bi 83 Bi2O3 BiOCO3	Po 84	At 85	Rn 86
Fr 87	Ra 88																

Ce 58 CeO_2	Pr 59 Pr_6O_{11}	Nd 60	Pm 61	Sm 62 Sm_2O_3	Eu 63 Eu_2O_3	Gd 64 Gd_2O_3	Tb 65 Tb_4O_7	Dy 66 Dy_2O_3	Ho 67 Ho_2O_3	Er 68 Er_2O_3	Tm 69 Tm_2O_3	Yb 70 Yb_2O_3	Lu 71 Lu_2O_3

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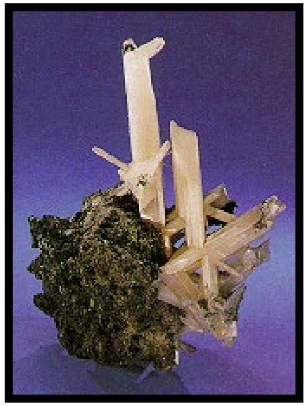
Cassiterite, SnO_2, black


Cuprite, Cu_2O, red


Cerrusite, $PbCO_3$, white


Anatase, TiO_2, black


Rhodochrosite, $MnCO_3$, red


Tenorite, CuO, black


Tellurite, TeO_2, yellow


Calcite, $CaCO_3$, yellow


Hematite, Fe_2O_3, brown


Diaspore, AlOOH, white

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TABLE OF CONTENTS

Alphabetical List of Materials in Volume Two – Handbook of Commercially Pure Binary Oxides

Binary Oxides, Carbonates and Hydroxides – Alphabetical by Chemical Formula

INTRODUCTION

This handbook contains wide scan survey spectra and high energy resolution narrows scan spectra from commercially pure samples of binary oxides, a few natural minerals, several hydroxides and carbonates. The spectra were collected under conditions that maximized the accuracy and reliability of the binding energies. The reference energies used to calibrate the energy scale were those reference energies recommended by the National Physical Laboratory in the UK, and now ISO TC/201. Section "F" provides the details of energy scale calibration. For those compounds that were non-conductive or semi-conductive in behavior, the reference energy for the hydrocarbon carbon (1s) signal from those samples was defined as 285.0 eV. The binding energies of all truly conductive samples were reported exactly as measured and without correction.

ORGANIZATION AND DETAILS OF SPECTRAL SETS

Organization

The spectra are organized alphabetically by using the chemical formula (e.g. AgO to ZrO_2). Data and spectra from the binary oxide known as “aluminum (III) oxide” has chemical formula “Al_2O_3” in the upper right and left corners of the pages that belong to that set of spectra. This means that spectra and data for “Antimony Oxide” will be found by looking for the chemical formula: “Sb_2O_3”. Just underneath of this chemical formula the mineral name is reported if the sample was a natural mineral.

Contents of Each Set of Spectra

The compounds in this volume include: AgO, Ag_2O, Al_2O_3, $Al(OH)_3$, AlOOH (Diaspore), As_2O_3, Au_2O_3, B_2O_3, $BaCO_3$, BeO, Bi_2O_3, $(BiO)_2CO_3$, CaO, $CaCO_3$ (Calcite), CdO, $Cd(OH)_2$, $CdCO_3$, CeO_2, CoO, Co_2O_3, Co_3O_4, $Co(OH)_2$, CrO_3, Cr_2O_3, Cs_2O, CuO, Cu_2O (Cuprite), $Cu(OH)_2$, $CuCO_3$ (Azurite), Dy_2O_3, Er_2O_3, Eu_2O_3, FeO, α-Fe_2O_3 (Hematite), γ-Fe_2O_3, Fe_3O_4, FeOOH (Goethite), Ga_2O_3, Gd_2O_3, GeO_2, HfO_2, HgO, Ho_2O_3, In_2O_3, IrO_2, K_2O, La_2O_3, Li_2O, Li_2CO_3, Lu_2O_3, MgO, $Mg(OH)_2$, $MgCO_3$, MnO, MnO_2, Mn_2O_3, $MnCO_3$ (Rhodochrosite), MoO_2, MoO_3, Na_2O, NbO, NbO_2, Nb_2O_5, NiO, $Ni(OH)_2$, PbO, PbO_2, Pb_2O_3, $PbCO_3$ (Cerrusite), PdO, Pr_6O_{11}, PtO_2, Re_2O_7, Rh_2O_3, RuO_2, Sb_2O_3, Sb_2O_5, Sc_2O_3, SiO, SiO_2 (Quartz), $Si(OH)_4$ (Opal), Sm_2O_3, SnO, SnO_2 (Cassiterite), $SrCO_3$, SrO, Ta_2O_5, Tb_4O_7, TeO_2, ThO_2, TiO, TiO_2, Ti_2O_3, Tl_2O_3, Tm_2O_3, VO_2, V_2O_3, V_2O_5, WO_3, Y_2O_3, $Y_2(CO_3)_3$, Yb_2O_3, ZnO, and ZrO_2.

The first page of each data set includes a title line that reports the chemical name, the oxidation state of the element, and its’ formula weight (FW). Just below the title line the “Surface Composition Table” lists the peak assignments from each wide scan survey spectrum, corrected and measured binding energies of all major and minor peaks, relative sensitivity factors, relative peak areas and the atom % abundance of each major signal. Each data set includes a wide scan survey spectrum, a valence band spectrum, a 1,000-1,400 eV range spectrum and high energy resolution spectra of the primary metal signal, secondary metal signals, the carbon (1s) signal, the oxygen (1s) signal and several Auger signals. The spectra and their annotations are presented exactly as produced and exported by the Spectral Data Processor v4.1 software from XPS International LLC.

Descriptions above each subsequent spectrum include the original key information about the sample, the source of the sample if known, and peak labels. Detailed information about the operating capabilities of the SSI XPS system and analysis conditions used to collect these data are presented in the next section of this book.

The remaining pages of each set include the high energy resolution narrow scan spectra which were obtained by measuring the main XPS signals found in the wide scan survey spectrum. These spectra contain detailed peak-fit results in a table at the top left corner of the spectrum and the actual peak-fit results. The binding energies of the non-conductive samples were corrected to the binding energy of the hydrocarbon carbon (1s) signal at 285.0 eV which is a common practice. This method of energy referencing non-conductive materials is widely used and accepted because there is currently no standard method for charge referencing spectra from insulating materials. Each peak-fit table includes the binding energies of each peak, their FWHM, peak height, percentage of Gaussian peak-shape used, percentage of asymmetry used, normalized peak area and relative peak area. The relative peak area percentages are based on the total peak area intensity of that signal only. Relative peak area percentages are not atom % values.

Philosophy of Data Collection

The spectra in this book were collected under analysis conditions that are practical, readily reproduced, and typically used in laboratories that use monochromatic X-ray sources and are working under real world practical analysis conditions. We have produced this volume of reference spectra because many XPS laboratories need practical reference spectra and do not have the time or money to produce XPS spectra from common reference materials. The signal to noise (S/N) ratios in the wide scan survey spectra is large enough to reveal the presence of minor components that are often not detected. The high energy resolution spectra were obtained under analysis conditions that would give a FWHM = 0.75 eV from the Ag ($3d_{5/2}$) signal of freshly ion etched silver (Ag).

A few high energy resolution spectra, labeled with the superscript “UR” were obtained under the “ultimate energy resolution” conditions available on the SSI S-Probe XPS system. This “ultimate” level of energy resolution produced a FWHM = 0.44 eV from the ($3d_{5/2}$) signal of freshly ion etched silver (Ag). In the production of these spectra we did not attempt to clean the surfaces of any sample because that would make charge referencing of the non-conductive samples a difficult task. For practical reasons we used the hydrocarbon carbon (1s) spectra from the naturally formed layer of adventitious hydrocarbons for charge referencing because that signal is the “de facto” standard for charge referencing non-conductive materials. This method of correcting for charge-up increases the uncertainty in the accuracy of the related binding energies.

The spectral data contained within this 5 volume series of handbooks are designed to assist engineers, scientists, analysts, theoreticians, and teachers who use XPS on an everyday basis under practical working conditions. We hope that these spectra will help XPS users to analyze industrial problems, gather high grade reference data, perform basic research, test theories and teach others. These spectra are designed to be practical tools for everyday use and were obtained under practical working conditions. We have not attempted to produce research grade spectra, but we have, in fact, produced research grade spectra because of our self-consistent methods. In the production of these spectra no attempt was made to produce a pure, clean surface, but an effort was made to produce surfaces with a minimum amount of natural surface contamination.

Peak-Fitting (Curve-Fitting) of High Energy Resolution Spectra

Peak-fitting was performed by using Spectral Data Processor (SDP v7.0) from XPS International LLC (www.xpsdata.com). This software allows the user to control the full width at half maxima (FWHM) value of any peak, the binding energy (BE) of any peak, peak areas, peak heights, the ratio of pairs of peak areas, the ratio of pairs of FWHM, the energy difference between two peak maxima, the shape of a peak as a sum-function of Gaussian and Lorentzian peak shapes, and the percentage of asymmetry in any peak.

By empirically peak-fitting the spectra from large sets of closely related materials in a trial and error method and analyzing the trends, it was possible to recognize several fundamental peak-shape and peak-fitting parameters for pure elements, binary oxides, polymers, and semiconductors. We have used those empirical findings to guide our efforts to peak-fit the many spectra which had complicated peak shapes. In some cases we used the theoretical peak area ratio of a spin-orbit coupled pair to assist the peak-fitting of a spectrum, and also the energy interval between spin-orbit coupled signals derived from pure element spectra.

The reduced “chi-squared” value, which indicates the goodness of a peak-fit, was used to determine if a peak-fit was reasonable or not. Based on practical experience a “chi-squared” value between 1 and 2 implies a relatively good peak-fit. A “chi-squared” value between 2 and 4 implies that the fit has not yet been optimized. A “chi-squared” value larger than four (4) implies that one or more signals are missing from the peak-fit.

A Shirley-type (sigmoid) baseline was used for most peak-fits. Peak-fits for the main XPS signals were optimized by using a Gaussian : Lorentzian ratio between 80:20 and 90:10.   After peak-fitting many binary oxides, we observed that the FWHM of the C(1s), O(1s) and the main metal signal of the binary oxide were usually in range 1.0-1.4 eV. We used this observation as an indicator of charge compensation quality. If one of the peaks fell with this range (1.0-1.4 eV), then all other spectra were expected to represent spectra without charge induced broadening. If all three of the main spectra were found to have FWHM > 1.5 eV, then we understood that charge compensation was not adequate. In response, we repeated some measurements until at least one of the main signals had FWHM < 1.5 eV, by moving the mesh-screen closer to the surface of the sample or by increasing the flood gun voltage by 1-3 eV.

Charge Compensation of Non-Conductive Compounds

Charge compensation of non-conductive materials was handled by using the patented SSI mesh-screen together with a low voltage flood gun of electrons which used an acceleration voltage adjusted to 2-4 eV, unless otherwise noted. The mesh-screen device uses an 85% transmission electroformed mesh made of nickel metal that is supported above the surface of the sample by mounting the mesh on a conductive metal frame that is grounded to the sample mount. To achieve good charge compensation the mesh-screen was positioned so the distance between the mesh and the surface of the sample is between 0.5-1.0 mm. When the distance between the mesh-screen and the surface of the sample is greater than 1.2 mm, the usefulness of the mesh-screen flood gun system was null. This mesh-screen method has been found to useful on a wide variety of XPS systems that use monochromatic X-rays and a source of electrons that are from a flood source or a poorly focused source of low voltage electrons.

The mesh-screen is understood to function as an electron cut-off lens with some tendency to allow incoming flood gun electrons to focus on the area being irradiated with monochromatic X-ray beam because the X-ray beam does not have a uniform flux density of the area of the beam. In effect, the mesh-screen produces a nearly uniform electric potential at the surface of the sample and allows incoming flood-gun electrons to pass through whenever they are needed.

The mesh-screen was used above every sample except for a few that were analyzed before the mesh-screen method was invented. Because the electrical nature of many of the samples was unknown until we attempted to collect data, nearly all samples were covered by the mesh-screen device. When the mesh-screen covers a conductive sample there is a very slight drop in counts because the mesh-screen captured or deflected some of the photo-emitted electrons. If ion etching is done with the mesh in place, then a slight amount of nickel appears on the ion etched sample.

Abbreviations Used

Due to the limited space provided to describe each sample in each electronic data-file, it was necessary to use various abbreviations. The abbreviations are:

TOA = take-off-angle for the electrons (the angle between the surface plane and the main axis of the electron collection lens)
FG = flood gun
mesh = mesh-screen used for charge control
1mm = 1 mm height used for the mesh-screen
semi-con = semi-conductive behavior
Tech = technical grade purity
pellet = sample pressed into pellet form by pellet press used to make infrared KBr pellets,

INSTRUMENT AND ANALYSIS CONDITIONS USED TO COLLECT XPS SPECTRA

A. Instrument Details

Manufacturer:	Surface Science Instruments (SSI)
Model:	S-Probe (upgraded from M-Probe model 2703)
Operation Software:	1.36.05 (Compiled in MS-DOS "C" v6.0)
Analyzer Type:	Fixed Analyzer Transmission (FAT), which is the same as: Fixed Pass Energy = Constant Analyzer Energy (CAE) 180° Hemi-spherical (truncated)
Input Lens Field of View:	30° for sample normal to lens axis (1" diameter port) (always larger than X-ray beam; retarding potential scanned)
X-ray Type:	Al° K_{α} monochromatic (one 2" diameter, thin, natural SiO_2 wafer glued onto a Zerodur substrate and heated to 65° C)
X-ray Source:	10 kV, 1.5-22.0 mA (depending on spot size used)
X-ray Energy Defined as:	1486.7 eV (8.3393 Å), Bragg angle = 78.5°
Excitation Source Window:	0.6 µ aluminum in S-Probe (10µ Mylar in X-Probe)
Angle of X-ray Incidence:	$\alpha = 71°$ (relative to sample normal)
Electron Emission Angle:	$\beta = 0°$ (relative to sample normal)
Angle between X-ray Axis and Electron Analyzer Axis:	$\phi = 71°$ (fixed, non-variable)
Pass Energies of Analyzer:	150 V for Resolution 4 setting 100 V for Resolution 3 setting 50 V for Resolution 2 setting 25 V for Resolution 1 setting
Type & Size of Input Slit:	Fixed (2 mm X 35 mm) with magnetic compression
Type & Size of Output Slit:	None (dispersion limited by hemisphere voltages)
Electron Collection Lens Field of View:	~ 1 mm^2 for $\beta = 0°$ at 1,000 eV KE
Electron Collection Lens Efficiency:	7% over 2π steradians
Sample Surface to Tip of Electron Collection Lens Distance:	~33 mm

Crystal to Sample Surface Distance: ~190 mm
Crystal to X-ray Anode Distance: ~190 mm
True Background Noise: <10 electrons/second at -50 eV (shot noise limited)
Detector Type: SSI Position Sensitive Detector, resistive anode encoder,
40 mm X 40 mm, electronically defined as 128 active channels with max ct rate of 1,000,000 cps
Dead Time: zero (unless ion etching pure element while collecting data)
Base Pressure: 4 x 10^{-10} torr
Normal Operating Pressure: 1.6 x 10^{-9} torr
X-ray FWHM Diffracted by natural SiO_2: ~0.25 eV
Power Settings: 200 Watts in a 250 x1100µ X-ray beam
100 Watts in a 150 x 800µ X-ray beam
45 Watts in an 80 x 350µ X-ray beam
15 Watts in a 40 x 250µ X-ray Beam
X-ray Induced Current: 1.1 x 10^{-9} amps for a 600µ spot in X-Probe
Approximate True X-ray Power: ~6 x 10^{-6} W in a 600µ spot
Approximate True X-ray Irradiance: ~8 W/m^2
Approximate True X-ray Photon Flux: ~7 x 10^{9} photons/sec

B. Experimental Details

Electron Take-Off-Angle: 90° relative to sample surface (unless otherwise reported)
Pass Energies Used: Wide scans were done at PE = 150 eV
Narrow scans were normally done at PE = 50 eV
Valence band scans were done at PE=150 eV
X-ray Beam Size Used: (S-Probe system) Wide scans: 250 x 1500 µ ellipse (at 90° TOA)
250 x 1100 µ ellipse (at 35° TOA)
Narrow Scans: 250 x 1500 µ ellipse (at 90° TOA)
150 x 1000 µ ellipse (at 90° TOA)
SSI Mesh-Screen: An 85% transmission (20 µ diameter wire with 200 µ spacing) nickel metal mesh screen was adhered to a small 25 mm x 25 mm x 1.5 mm (W x L x H) aluminum plate with a 20 mm x 20 mm aperture.

The mesh-screen was placed over all insulating samples
So that the distance between the sample surface
and the mesh-screen was <1.0 mm but >0.5 mm.

Dwell Time (counting time): 200 milliseconds/channel
Data Transfer Time: 4 milliseconds
Max. Number of Channels: 5,000 (channels = data points)
Scan Time for One Wide Scan: ~ 3.5 minutes (using 1024 data points)
Scan Time for One Narrow Scan: ~100 seconds (using 256 data points)
Energy Range: -100 to +1400 eV (BE range)
Typical Step Size: 0.1 eV/step (i.e. 0.1 eV/data point)

C. Data Processing Details

Baseline Subtraction: None, unless S/BG gave a small display. When the baseline was removed, the intensity of the lowest point was subtracted from all points.
Data Smoothing: None (the 128 channel PSD system producing a smoothing effect)
Energy Shifting: All non-conductive samples were charge referenced so that the hydrocarbon carbon (1s) signal appeared at 285.0 eV

D. Sample Details

The "Description" given on the first page of each data set reports: the empirical chemical formula for the oxide, the hydroxide or carbonate, the reported bulk purity, source, a production lot number, the electron take-off-angle (TOA), the height of mesh-screen above the surface, the electrical behavior of the sample under analysis conditions, sample color, sample preparation, sample size, known melting point in degrees Centigrade, density in grams/cubic-centimeters, and a note on solubility.

Sources of Commercially Pure Binary Oxide, Carbonate and Hydroxide Samples

Most of the commercially pure binary oxides were purchased from the Aldrich Chemical Co. Most of the packages from the Aldrich Chemical Co. included an "Analytical Information" sheet which reported an ICP or AA analysis summary, a production lot number, the Aldrich product number, sample purity (e.g. 99+%), sample appearance (color and physical form), date of chemical analysis, formula weight and a label on the bottle that reported the melting point, toxicity, a Chemical Abstracts registry number and density. The samples from Aldrich were generally quite pure. Other oxide samples were obtained from either Cerac Inc. (USA) or Rare Metallics Co., Ltd. (Japan). These samples tended to have mixed oxides. The packages from Cerac Inc. included a "Certificate of Analysis" with an ICP or AA analysis summary, a production lot number, a product number, purity (e.g. 99+%), and mesh size. The packages from Rare Metallics Co. did not include analytical data reports, but instead had stock numbers and a purity statement. Two samples (i.e. SiO_2 natural crystal and Al_2O_3 as a fused plate) were obtained from in-house sources and do not have any purity reports.

Powdered Samples - Pressed into 3 mm Diameter Pellets

Until analyzed, all finely powdered samples were kept un-opened, in their original glass or plastic containers, which were packaged inside of plastic-lined aluminum bags and stored in an electrically controlled dehumidifier. Just prior to analysis, each bottle was opened in the normal air of the room, where the XPS system was kept, and a small 50-100 mg portion of the powdered sample was removed via a clean Nichrome spatula and placed in the compression chamber of a hand-operated, stainless steel pellet press (Qwik Handi-Press) that is normally used to produce pellets for infrared analyses. All finely powdered samples were compressed without any treatments. The resulting pellets varied in thickness from 0.3 - 0.8 mm. The "Qwik Handi-Press" was manufactured by the Barnes Analytical Division of Spectra-Tech Inc. (652 Glenbrook Road, Stamford, Connecticut, 06906, FAX#: 203-357-0609). Part # 0016-111 to 0016-121 contains 1, 3, and 7 mm die sets. Our hand-press was purchased through the Aldrich Chemical Co.

To avoid iron and/or chromium contamination from the anvil, a small piece of freshly cleaned aluminum foil was placed over the sample in the compression chamber. This aluminum foil is standard kitchen grade foil which was gently rubbed with a cotton swap lightly soaked with iso-propanol (IPA) and allowed to dry in air. Those powders, that were clumped together, were very gently ground into a powder just prior to compression. To avoid unnecessary heat-induced oxidation, those samples which were hard and granular were very gently and slowly hand ground into a fine powder using an agate marble mortar and pestle. As soon as each sample was removed from the compression chamber, it was mounted on top of a fresh drop of silver (Ag°) paint placed in the center of a 5 mm diameter brass boat that was 1.3 mm in height. Silver paint was used so that conductive oxides could behave as true conductors thereby providing true electron binding energies for those oxides that were indeed conductive. This arrangement kept the mesh-screen at a suitable distance from the sample surface. In general, each oxide was exposed to room air for <15 min.

Benefits of Pressing Powders into Pellets

A comparison of the electron counts obtained from powdered samples pressed onto double-sided adhesive tape and positioned at a 35° electron take-off-angle with the electron counts obtained from hand-pressed glossy or semi-glossy pellets positioned at a 90° electron take-off-angle (TOA) revealed that the pellet form at a 90° electron TOA produces 3-5 times higher electron counts than a powdered sample pressed onto double-sided tape at a 35° electron TOA. By pressing the finely powdered oxides into pellets, it was also found the surface charging behavior of these glossy or semi-glossy samples was very easy to control with the mesh-screen flood-gun device.

Problems Caused by Pressing Powdered Samples into Pellets

By pressing finely powdered oxides into pellets, the surface of the resulting pellets were usually smooth enough to appear glossy or semi-glossy. A few samples were found to be contaminated with iron or chromium which indicated that the oxide had undergone a pressure induced reaction with the stainless steel anvil. Very strong hand pressure was indeed found to cause some oxides to react with the stainless steel anvil, but medium hand pressure did not produce the undesired iron and chromium contamination. Other forms of accidental contamination (chlorine or previously analyzed oxides) were caused by insufficient cleaning of the stainless steel anvil, which was normally cleaned with a chlorine-containing metal polishing solution (Pikal) and rinsed with distilled water and isopropanol. All analyses that showed any unexpected contamination were repeated.

Solution to Pressure Induced Contamination of Pellets

Extensive experiments on different methods to avoid contamination while producing pellets revealed that contamination is minimized or avoided by using freshly cleaned aluminum foil as a "buffer" between the oxide powders and the metals in the steel anvil components. The aluminum foil, which is sold as a kitchen wrap material, is cleaned with 100% isopropanol (isopropyl alcohol) just prior to use. The foil is cut to a size that is readily fits inside the pellet press device.

We have also used "glycine" weighing paper which is commonly used as a paper to hold powders when weighing them. This weighing paper is common in chemical laboratories and can be substituted for the aluminum foil whenever the pressing results with the aluminum foil produce undesired binding of the foil to the sample. The glycine paper method sometimes introduces very small amounts of contaminants which produce very weak N (1s) and C (1s) signals.

E. Energy Resolution Details

Table 1: Experimentally Observed Relation between Energy Resolution and Analysis Conditions

Signal and Material used to Define Effective Energy Resolution (treatment)	Energy Resolution FWHM (eV)	Pass Energy	X-ray Spot Size
Si ($2p_{3/2}$) (fractured edge of crystal)	0.38 eV	10 eV	40 x 250μ
Si ($2p_{3/2}$) (fractured edge of crystal)	0.43 eV	25 eV	80 x 350μ
Au ($4f_{7/2}$) (foil - ion etched clean)	0.64 eV	10 eV	250 x 1000μ
Au ($4f_{7/2}$) (foil - ion etched clean)	0.79 eV	25 eV	250 x 1000μ
Au ($4f_{7/2}$) (foil - ion etched clean)	0.86 eV	50 eV	250 x 1000μ
Au ($4f_{7/2}$) (foil - ion etched clean)	1.40 eV	150 eV	250 x 1000μ
Ag ($3d_{5/2}$) (foil - ion etched clean)	0.42 eV	10 eV	40 x 250μ
Ag ($3d_{5/2}$) (foil - ion etched clean)	0.64 eV	25 eV	40 x 250μ
Ag ($3d_{5/2}$) (foil - ion etched clean)	0.75 eV	50 eV	40 x 250μ
Ag ($3d_{5/2}$) (foil - ion etched clean)	1.00 eV	100 eV	40 x 250μ
Ag ($3d_{5/2}$) (foil - ion etched clean)	1.30 eV	150 eV	40 x 250μ
Cu ($2p_{3/2}$) (foil - ion etched clean)	0.85 eV	10 eV	250 x 1000μ
Cu ($2p_{3/2}$) (foil - ion etched clean)	0.94 eV	25 eV	250 x 1000μ
Cu ($2p_{3/2}$) (foil - ion etched clean)	1.06 eV	50 eV	250 x 1000μ
Cu ($2p_{3/2}$) (foil - ion etched clean)	1.60 eV	150 eV	250 x 1000μ
Cu ($2p_{3/2}$) (foil - ion etched clean)	0.85 eV	10 eV	150 x 800μ
Cu ($2p_{3/2}$) (foil - ion etched clean)	0.96 eV	25 eV	150 x 800μ
Cu ($2p_{3/2}$) (foil - ion etched clean)	1.05 eV	50 eV	150 x 800μ
Cu (3s) (foil - ion etched clean)	2.35 eV	50 eV	250 x 1000μ

Table 2: Theoretical Analyzer Resolution versus Pass Energy Setting

Theoretical Analyzer Resolution	Pass Energy	Effective Detector Width
0.25 eV	25 eV	3.5 eV
0.50	50	7.0
1.00	100	14.0
1.50	150	21.0

F. Energy Scale Reference Energies and Calibration Details

From May 1986 to January 1993 (Based on HP energy calibration)

Energy Scale Reference Energies:	932.47 eV for Cu ($2p_{3/2}$) signal
	122.39 eV for Cu (3s) signal
	83.96 eV for Au ($4f_{7/2}$) signal
Binding Energy Uncertainty:	< ±0.08 eV
Digital-to-Analog (DAC) Conversion Setting:	163.88

After January 1993 (Based on NPL reference energies published in 1990)

Energy Scale Reference Energies:	932.67 eV for Cu ($2p_{3/2}$) signal
	122.45 eV for Cu (3s) signal
	83.98 eV for Au ($4f_{7/2}$) signal
Observed Reference Energy:	75.01 eV for Cu (3p3) signal
Binding Energy Uncertainty:	< ±0.05 eV
Digital-to-Analog (DAC) Conversion Setting:	163.87

Note: NPL has recently revised reference energies to be 932.62 eV for Cu ($2p_{3/2}$) and 83.96 eV for Au ($4f_7$/2) for monochromatic systems using an electron take-off-angle of 45° (Ref. 8)

Reference Energies of Adventitious Hydrocarbon Contaminants

From May 1986 to January 1993 the electron binding energy of adventitious hydrocarbons was assumed to occur at 284.6 eV based on SSI and C. D. Wagner's research and recommendations.

Publications by P. Swift in the journal of Surface and Interface Analysis **4**, p.47 (1982), S. Kohiki and K. Oki in the Journal of Electron Spectroscopy and Related Phenomena **33**, p.375-380 (1984), and G. Barth, R. Linder and C. E. Bryson, III in the journal of Surface and Interface Analysis **11**, p.307-311 (1988) have shown that the electron binding energy for various hydrocarbon contaminants and polymers is not necessarily a constant number.

Research by this author indicates that the electron binding energy for adventitious hydrocarbons lies somewhere between 284.4 and 287.0 eV and is dependent on the electronic nature of the surface. By taking a simple average of all available binding energies, the author has found that 284.9 eV is average binding energy for hydrocarbons captured from UHV onto the surface of recently ion etched metals where the surface is many hours old (>8 hr). For naturally-formed native oxides, the average binding energy is 285.2 eV. Binary oxides, for metals located at the far left of the periodic table (columns 1-4) tend to have higher C (1s) binding energies (285.3-286.7 eV), while most of the transition metal oxides center around 285.0 eV. Near the far right of the periodic table, the C (1s) binding energy rises to a 285.2-286.5 eV range (columns 12-14).

In routine practice, this author prefers to use the 285.0 eV number to compare data with previous publications. Factors that may cause this rather large range of electron binding energies for adventitious hydrocarbon contamination include: (a) variations in surface dipole moment at the vacuum-surface interface of the oxide material, which is known to be much larger in length and intensity than the surface dipole moment of a pure metal, and also, in the case of naturally formed native oxide films, (b) the thickness of the native oxide, (c) any physical or chemical treatments, (d) the thickness of the adventitious hydrocarbon layer, and (e) the electrical behavior of the instrument used to analyze the sample. The type of instrument being used may cause different shifts in the observed binding energy of the adventitious hydrocarbon contamination because the source may or may not generate different amounts of low energy secondary electrons from the window that protects the X-ray source. The heat from the source and contamination that de-gases from a just turned on source can also influence observed binding energies. Electron flood guns may or may not influence the binding energy as well.

Instrument Stability and Long Term Calibration

Each of the three SSI XPS systems, that we have used, was calibrated 2-3 times per week until its ability to maintain accurate voltage settings was defined. Once it was determined that the systems could maintain reliable voltage settings for 1-3 months, it was decided that good calibration could be maintained by checking and, if necessary, correcting the pass energies of the system on a 2-4 week basis. Each of the three SSI XPS instruments that we have used, have been checked or calibrated on a routine basis every 2-4 weeks by using SSI's reference energies. By using this method over several years time, it was found that the maximum uncertainty (error in pass energies) was normally < ±0.10 eV, but a few times rose to ±0.15 eV or less. In a very rare case, the uncertainty rose to 0.20 eV. Long term use of the SSI systems has shown that the DAC circuit does not change enough to be observed unless the room temperature changes by more than 10 degrees Centigrade. If the room temperature changes within a few hours time by more than 10 degrees or the temperature of the DAC chip is changed by more than 10 degrees, then a >0.1 eV shift, which is much, much smaller than the reliability of almost all literature data, can be observed. Variables, which seem to cause pass energy settings to change slightly, include building line-voltages, ion etching conditions, and the addition or removal of some electrical device.

G. Electron Counting and Instrument Response Function Details

Instrument Response Functions (for the X-Probe System only)

Instrument Response Function: $Q(E) = E^{+0.27}$ for 150 eV PE (ref.3)
Instrument Response Function: $Q(E) = E^{+1.0}$ for 50 eV PE (ref.3)

Signal/Background Ratios for Ion Etched Silver using a 250x1000 µ Spot*

Pass Energy	25 eV	50 eV	100 eV	150 eV
S/BG ratio**	>140	>110	>70	>50

* Using a 90° electron take-off-angle and a smooth Ag°/Mylar film.

** The S/BG ratio is a simple numerical ratio of electrons counts at the peak maximum relative to the average electron counts observed at approximately 10 eV lower BE.

Voltage Settings of the Electron Collection Lens

Pass Energy*	29.6-29.8	54.7-54.9	105.1-105.3	155.9-156.2
Detector Widths	3.743	7.486	14.954	22.297
Sensitivity Exponent	-0.1	0.3	0.7	1.1
V1 Offset	30	55	105	155
V1 Slope	0.600	0.611	0.676	0.709

*These pass energies include corrections for instrument work function. True pass energies were set to 25, 50, 100, and 150 eV ±0.1 eV.

H. Effects of Poorly Focusing the Distance between the Sample and the Electron Lens

If the focus distance between the sample surface and the electron collection lens is poorly adjusted, then the number of electron counts drops very quickly. A 0.5 mm error in focus produces a >300% decrease in counts, but does not produce any observable error in binding energies. A 0.1mm error in focus produces a 15% decrease in peak area counts and is easily observed as a horizontal displacement in the static (un-scanned mode) XPS signal as observed on the standard CRT display of the detector signal. Such a decrease in signal intensity causes the operator to correct the focus error to maximize the electron count rate and maintain good laboratory practice and self-consistency. In this manner, the operator minimized the chance of obtaining false BE readings and has accurately reproduced a nearly absolute focus point which greatly increases the quantitative accuracy of any unknown sample and the accuracy of the measured binding energies. Experiments with Bragg angle alignment of the crystal indicated that the maximum error due to an unusual bad alignment of the crystal would be <0.1 eV. To observe an error greater than 0.1 eV, the electron counts were found to decrease by >50%.

I. Quantization Details and "RSF Exponents"

By default, the SSI system uses a 0.7 number as the RSF exponent factor for each pass energy setting which is used in an equation that modifies theoretically calculated atomic photo-ionization cross-sections (John H. Scofield) to generate relative sensitivity factors that are valid for this XPS systems and which can be used to generate valid atomic percentages. This correction corrects for the overall instrument response function which includes the transmission function. For signals in the 0-700 eV range, the 0.7 RSF exponent factors produces a ±10% accuracy in quantitative results for XPS signals obtained with 150 eV pass energy. For signals that occur at higher binding energies, it is necessary to change the RSF exponent factor to a 1.1-1.5 value.

To obtain a useful RSF exponent factor for an SSI system, it is possible to use freshly ion etched poly-crystalline copper foil to test the validity of the sensitivity exponent factor for larger BE ranges and different pass energies. By integrating the peak areas of the Cu($2p_{1/2}$), Cu($2p_{3/2}$), Cu(3s), Cu(3p) and Cu(3d) signals it is possible to perform trial and error choices of the RSF exponent until a useful number is determined. When a useful number is entered into the software routine, the software generates fictional atomic percentages for each of the integrated copper signals which, when optimized, generates a 20 atom % value with an uncertainty of ±1-2 atom % for all five signals. If the RSF exponent factor is wrong then the atomic percentages will generate numbers such as 10%, 11%, 26%, 24%, and 29% or perhaps 31%, 28%, 14%, 13%, and 14%.

This trial-and-error approach may require 1-2 hours time and can be done by using wide scan survey spectra data or more preferably narrow scan spectra for each of the pass energies. This method, in effect, assumes that all five of the relative sensitivity factors (RSFs) for copper are reasonably correct which was confirmed by analyzing various natural crystals and pure polymers.

This method, in effect, assumes that the pure copper sample is a standard material that is composed of 5 components which are present in 20 atomic % abundances. Once a useful RSF exponent factor is found it will generate a 20 atom % result for each of the five copper signals. After a useful RSF exponent factor is found, it is tested by analyzing freshly exposed bulk regions of crystalline materials such as SiO_2, Al_2O_3, and NaCl. The high and low BE signals of the NaCl crystal are especially useful to test the validity of the sensitivity exponents.

As further checks, the freshly exposed bulk of common polymers (e.g. Mylar or PMMA) or a thin film of high purity silicone oil can also be analyzed. Teflon has repeatedly given slightly larger than desirable error by comparison to the other materials listed above. For that reason Teflon is a less desirable material to test the sensitivity exponents.

J. Test of the Reliability of Relative Sensitivity Factors (RSFs)

Crude testing of Scofield's RSF numbers was performed by measuring the atomic percentage of each signal for a pure element. This testing used the software's automatic peak area integration software that is reasonably accurate. The results indicate that some of the relative sensitivity factors for some of the weaker signals may be more uncertain. If, however, all factors are taken into account, then Scofield's numbers are reliable to a 90-95% accuracy level for truly homogeneous materials.

K. Traceability Details

The definition of traceability reported by Martin P. Seah and Cedric J. Powell in the J. Vac. Soc. Technol. Vol 8, p.736 (1990) publication is: "The property of a result of a measurement whereby it can be related to appropriate standards, generally international or national standards, through an unbroken chain of comparisons."

Traceability of Reference Binding Energies (Calibration)

At the time that these spectra were collected, there were no international standards for binding energies or reference energies. Recently, many people in the world have been using NPL's reference energies, which have become "de facto" standards. After further refinement and round-robin testing, the NPL values have become ISO values.

Many workers and researchers are unfortunately still using various numbers provided by the instrument makers. The author of this book was using Surface Science Instruments (SSI) Co. reference energies until December 1992, and then switched to NPL binding energies (binding energies (BEs)) in January 1993. SSI reference energies originally came from Hewlett-Packard (HP) and their high precision voltage systems. SSI and HP both used high precision voltage meters from HP to calibrate their ESCA machines (i.e. X, M, and S-Probe and HP-5950 A-type and B-type, resp.).

In a recent effort to improve the accuracy of binding energies (BEs) obtained from pure elements, the S-Probe pass energies were checked and corrected, if needed, almost every work-day for two months to obtain high precision and high accuracy binding energies (BEs) for the pure elements that are metals. This study used the NPL reference energies with Cu ($2p_{3/2}$) at 932.67 eV with +/- 0.02 uncertainty and Au ($4f_{7/2}$) 83.98 eV with +/-0.02 uncertainty by using 0.02 eV/pt. steps for the calibrations. To determine the "true" BE of each of the pure elements, which were scraped clean in air and then ion etched in vacuum, a 0.05 eV/pt. step-size was used. A repetitive ion etching (depth profile) style was used to collect wide scan, valence (Fermi edge) band, and narrow scans of the main signals for each metal at 50, 25 and 10 eV pass energies. Each repetitive experiment run lasted about 4 hours. If NPL BE numbers are accepted as "de facto" international standards, then the ultimate traceability of binding energies (BEs) in this data set can be related to NPL BE numbers for Cu ($2p_{3/2}$) and Au ($4f_{7})_{/2}$. Because the refined NPL values are now ISO standard values, the traceability of the reference energies used in this data set are traceable to ISO standards.

Transfer of Traceability from Pure Metals to Non-conductive Binary Oxides

A question that should be posed is traceability to the non-conductive binary oxide binding energies. For the binary oxides in this volume, traceability begins with NPL's binding energies (BEs) for pure copper and gold as state above. Traceability then transfers to pure element binding energies (BEs) which is based on NPL reference binding energies (BEs). Traceability then transfers to pure element binding energies (BEs) based on SSI's reference binding energies (BEs), and then the naturally formed native oxide data published in Volume 1 of our XPS Handbook series where binding energies (BEs) were measured from pure element signals and also the naturally formed native oxide signals.

Naturally formed native oxides typically have thin oxide films (10-80Å) which, in general, behave as good or true electrical conductors, which allows a direct measure of the true binding energy of many, but not all, binary oxides. To determine if traceability can indeed be transferred to true binary oxides, it was necessary to study the behavior of the naturally formed native oxides by applying various flood gun settings with the samples grounded and insulated. The results from that study can be used to transfer traceability to the experimentally observed binding energies (binding energies (BEs)) of pure binary oxides. The most difficult transfer of traceability occurs for the naturally formed native oxide systems. If the flood gun study was not done, then it is difficult to transfer traceability in a reliable manner from a conductive metal to one of its corresponding non-conductive binary oxides.

Traceability of Instrument Response (Throughput) Function

Copper, gold and silver data obtained from the M-Probe system were submitted to Martin P. Seah at the NPL for a round robin test on transmission function; the results of which were published in the journal of Surface and Interface Analysis, p.243 (1993). In that publication, M-Probe data, which we contributed, were attributed to group #35. That paper reported that instrument has a $Q(E) = E^{0.27}$

for a Res 4 pass energy (PE=150eV) and a Q (E) = $E^{1.0}$ for the Res 2 pass energy (PE=50 V). If the NPL method is accepted as a "de-facto" standard, even though it is not an internationally recognized standard, then the transmission function and quantitation results of the S-Probe system are traceable to the "metrology spectrometer" at NPL.

Traceability of Relative Sensitivity Factors (RSFs) used for Quantization

Scofield's theoretically calculated photo-ionization cross-sections are internationally used as the "de-facto" standard theoretical RSFs, except in Russia and a few other places, where other RSF numbers are preferred but are, in effect, after renormalization almost identical to Scofield’s RSFs. The SSI system uses a very simple equation that modifies normalized values of Scofield's photo-ionization cross-section values to generate relative sensitivity factors. That equation corrects the instrument response function for differences due to pass energy, differences due to transmission function, and the inelastic mean free path versus kinetic energy dependency.

Traceability of Sample Purity

The purity of the commercially pure (99%) binary oxides is linked to the ICP or AA analyses performed by the Aldrich Chemical Co. and their methods for calibrating their instruments.

L. Reference Papers Describing Capabilities of X-Probe, M-Probe, and S-Probe XPS Systems

1. Robert L. Chaney, *Surface and Interface Analysis,* **10,** 36-47 (1987) [re: X-Probe]
2. Noel H. Turner, *Surface and Interface Analysis,* **18,** 47-51 (1992) [re: Quantization]
3. M. P. Seah, *Surface and Interface Analysis,* **20,** 243-266 (1993) [re: Response Function]
4. L.T. Weng et al, *Surface and Interface Analysis,* **20,** 179-192 (1993) [re: Response Function]
5. L.T. Weng et al, *Surface and Interface Analysis,* **20,** 193-205 (1993) [re: Response Function]
6. B. Vincent Crist, *Surface Science Spectra*, **1**, 292-296 (1993) [re: KBr spectra]
7. B. Vincent Crist, *Surface Science Spectra*, **1**, 376-380 (1993) [re: Ar/C spectra]
8. M. P. Seah, I.S. Gilmore, and G. Beamson, *Surface and Interface Analysis,* **26,** 642-649 (1998)

XPS Spectra
of
Commercially Pure Binary Oxides
and a few Common Carbonates and Hydroxides

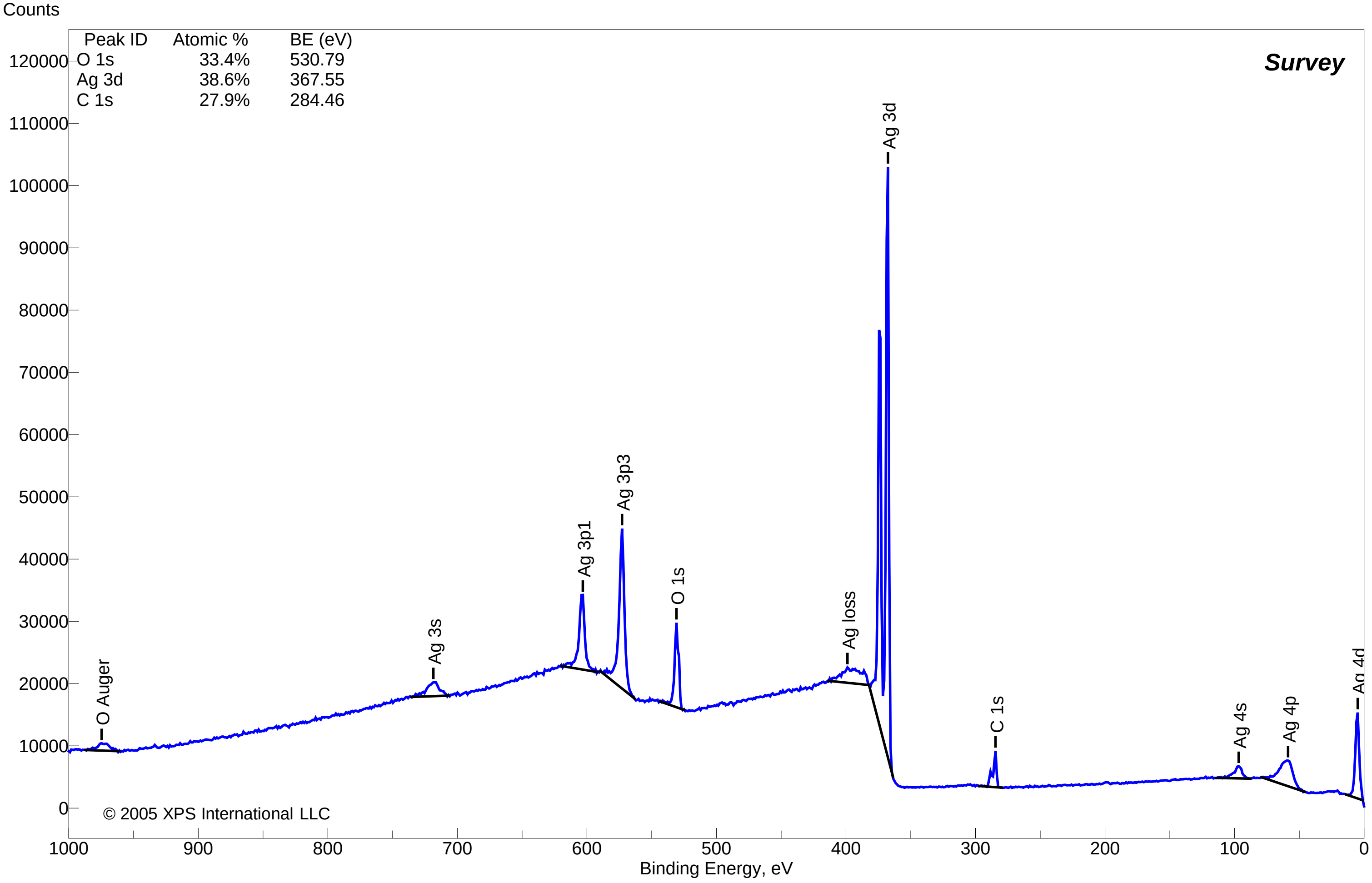
Silver (II) Oxide (FW = 123.87)
Surface Composition Table

Description: AgO (99%) from Aldrich Lot# 00108JV, pressed into 3 mm pellet, analyzed at 90 deg TOA, conductive gray-black powder pressed into 5 mm pellet, mp >100 C dec., d. 7.44, sol. in ammonia (dec.)

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
Ag 4d	4.9	4.9	1.55	1.5	62,729	
Ag 4p	58.7	58.7	1.36	1.5	63,032	
Ag 4s	96.8	96.8	0.64	1.5	19,754	
C 1s	284.5	284.5	1.00	1.5	24,842	27.9%
Ag 3d	367.5	367.5	18.04	1.5	556,356	38.6%
Ag loss	398.8	398.8	1.80	1.5	59,988	
O 1s	530.8	530.8	2.93	1.5	61,714	33.4%
Ag 3p3	572.8	572.8	8.06	1.5	162,297	
Ag 3p1	603.1	603.1	4.03	1.5	78,803	
Ag 3s	718.5	718.5	2.93	1.5	32,609	
O Auger	974.6	974.6	0.00	1.5	14,615	
Ag Auger	1134.7	1134.7	0.00	1.1	19,283	
Ag Auger	1189.0	1189.0	0.00	1.1	4,809	
Ag Auger	1225.6	1225.6	0.00	1.1	3,524	

Silver (II) Oxide (FW = 123.87)

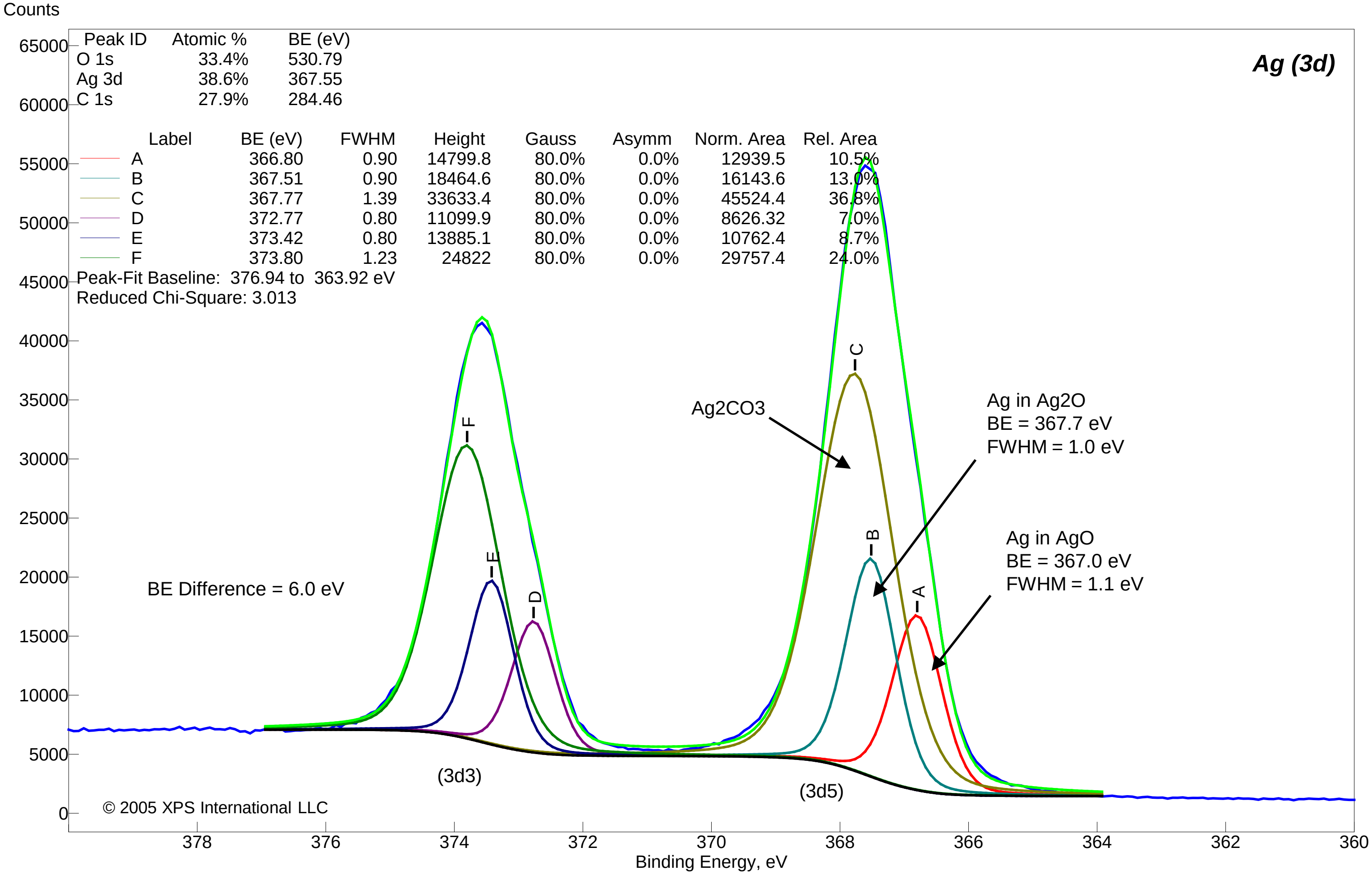
Sample Description: AgO (99%) from Aldrich lot# 00108JV (contaminated with Ag2O), conductive pressed into 3 mm pellet, analyzed at 90 deg TOA



Peak ID	Atomic %	BE (eV)
O 1s	33.4%	530.79
Ag 3d	38.6%	367.55
C 1s	27.9%	284.46

Silver (II) Oxide (FW = 123.87)

Sample Description: AgO (99%) Aldrich lot# 00108JV (contaminated with Ag2O)
3 mm pellet, CONDUCTIVE, 90 DEG TOA



Peak ID	Atomic %	BE (eV)
O 1s	33.4%	530.79
Ag 3d	38.6%	367.55
C 1s	27.9%	284.46

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	366.80	0.90	14799.8	80.0%	0.0%	12939.5	10.5%
B	367.51	0.90	18464.6	80.0%	0.0%	16143.6	13.0%
C	367.77	1.39	33633.4	80.0%	0.0%	45524.4	36.8%
D	372.77	0.80	11099.9	80.0%	0.0%	8626.32	7.0%
E	373.42	0.80	13885.1	80.0%	0.0%	10762.4	8.7%
F	373.80	1.23	24822	80.0%	0.0%	29757.4	24.0%

Peak-Fit Baseline: 376.94 to 363.92 eV
Reduced Chi-Square: 3.013

Ag (3d)

Ag2CO3

Ag in Ag2O
BE = 367.7 eV
FWHM = 1.0 eV

Ag in AgO
BE = 367.0 eV
FWHM = 1.1 eV

BE Difference = 6.0 eV

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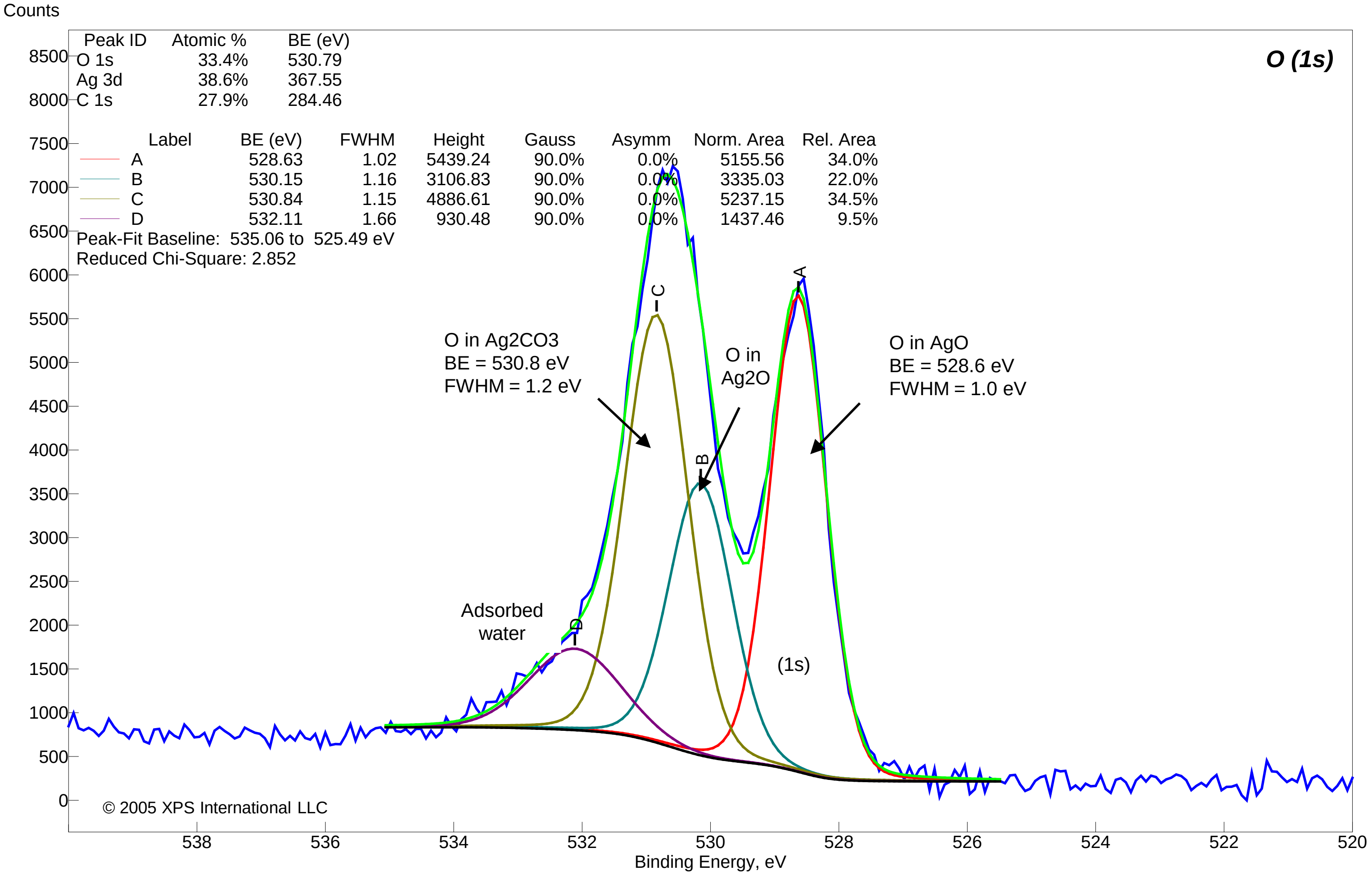
Silver (II) Oxide (FW = 123.87)

Sample Description: AgO (99%) Aldrich lot# 00108JV (contaminated with Ag_2O)
3 mm pellet, CONDUCTIVE, 90 DEG TOA



Peak ID	Atomic %	BE (eV)
O 1s	33.4%	530.79
Ag 3d	38.6%	367.55
C 1s	27.9%	284.46

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	528.63	1.02	5439.24	90.0%	0.0%	5155.56	34.0%
B	530.15	1.16	3106.83	90.0%	0.0%	3335.03	22.0%
C	530.84	1.15	4886.61	90.0%	0.0%	5237.15	34.5%
D	532.11	1.66	930.48	90.0%	0.0%	1437.46	9.5%

Peak-Fit Baseline: 535.06 to 525.49 eV
Reduced Chi-Square: 2.852

O in Ag_2CO_3
BE = 530.8 eV
FWHM = 1.2 eV

O in
Ag_2O

O in AgO
BE = 528.6 eV
FWHM = 1.0 eV

Adsorbed
water

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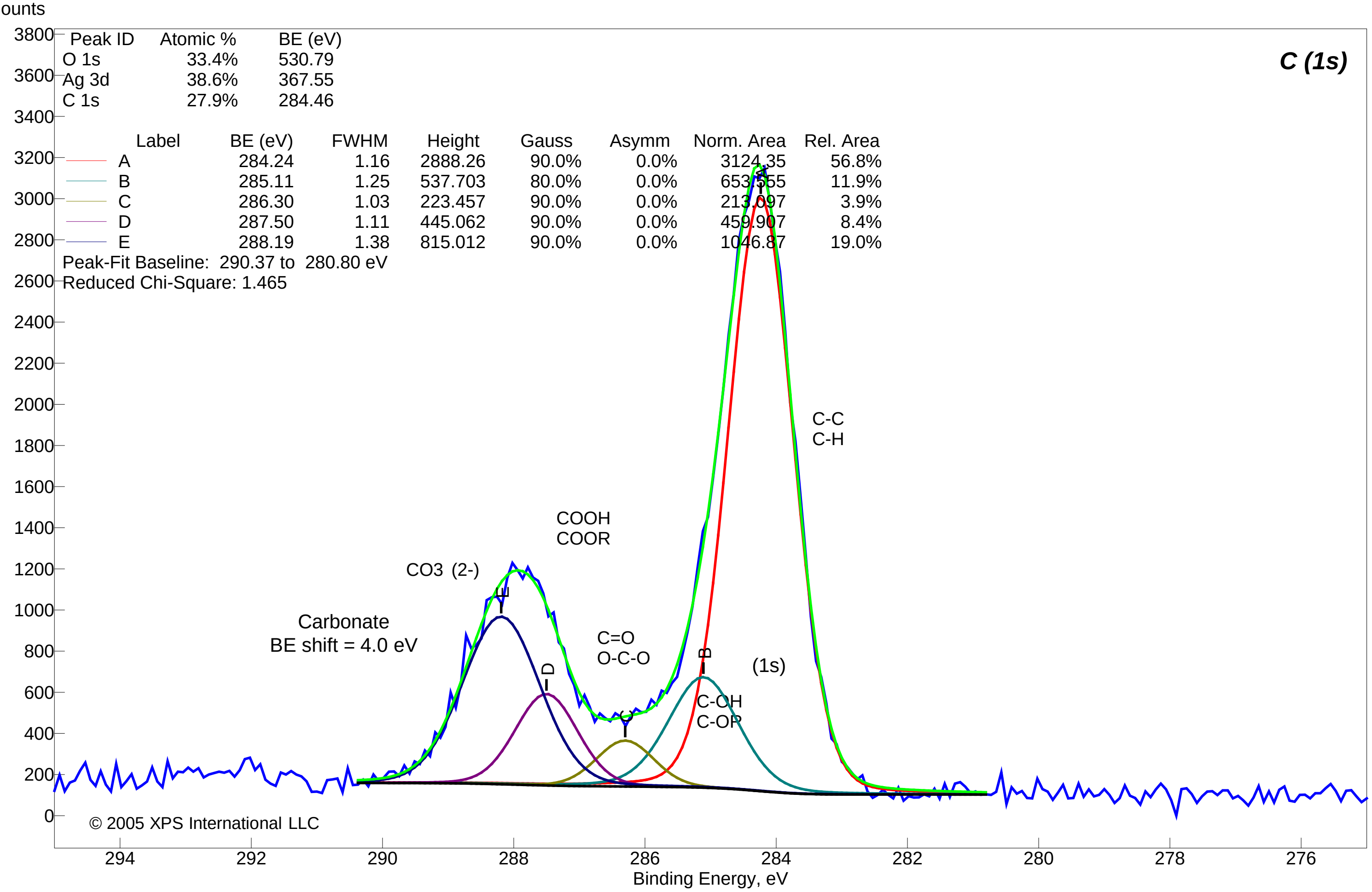
Silver (II) Oxide (FW = 123.87)

Sample Description: AgO (99%) Aldrich lot# 00108JV (contaminated with Ag2O)
3 mm pellet, CONDUCTIVE, 90 DEG TOA



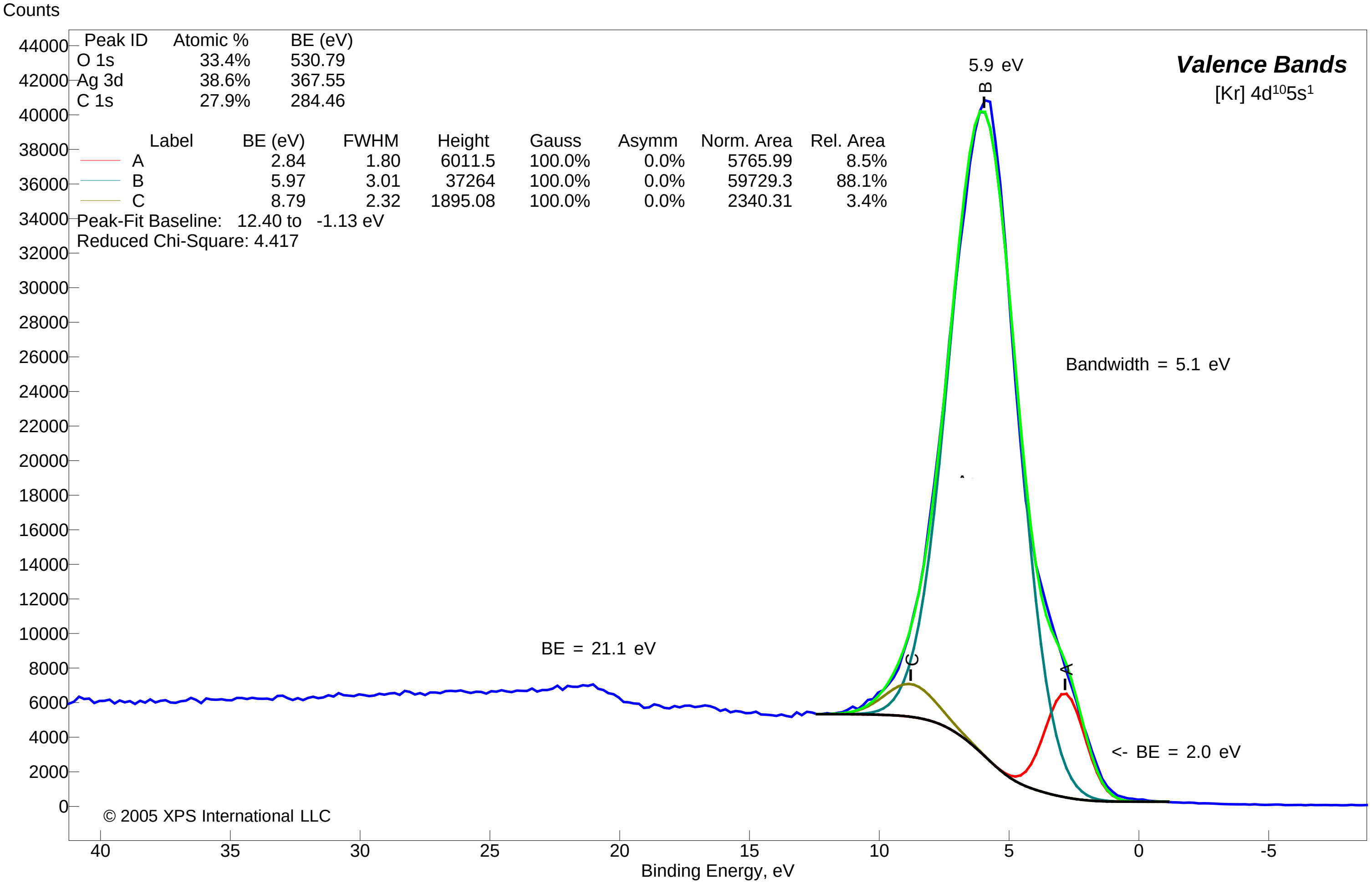
Peak ID	Atomic %	BE (eV)
O 1s	33.4%	530.79
Ag 3d	38.6%	367.55
C 1s	27.9%	284.46

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	284.24	1.16	2888.26	90.0%	0.0%	3124.35	56.8%
B	285.11	1.25	537.703	80.0%	0.0%	653.555	11.9%
C	286.30	1.03	223.457	90.0%	0.0%	213.097	3.9%
D	287.50	1.11	445.062	90.0%	0.0%	459.907	8.4%
E	288.19	1.38	815.012	90.0%	0.0%	1046.87	19.0%

Peak-Fit Baseline: 290.37 to 280.80 eV
Reduced Chi-Square: 1.465

Silver (II) Oxide (FW = 123.87)

Sample Description: AgO (99%) Aldrich lot# 00108JV (contaminated with Ag_2O)
3 mm pellet, CONDUCTIVE, 90 DEG TOA



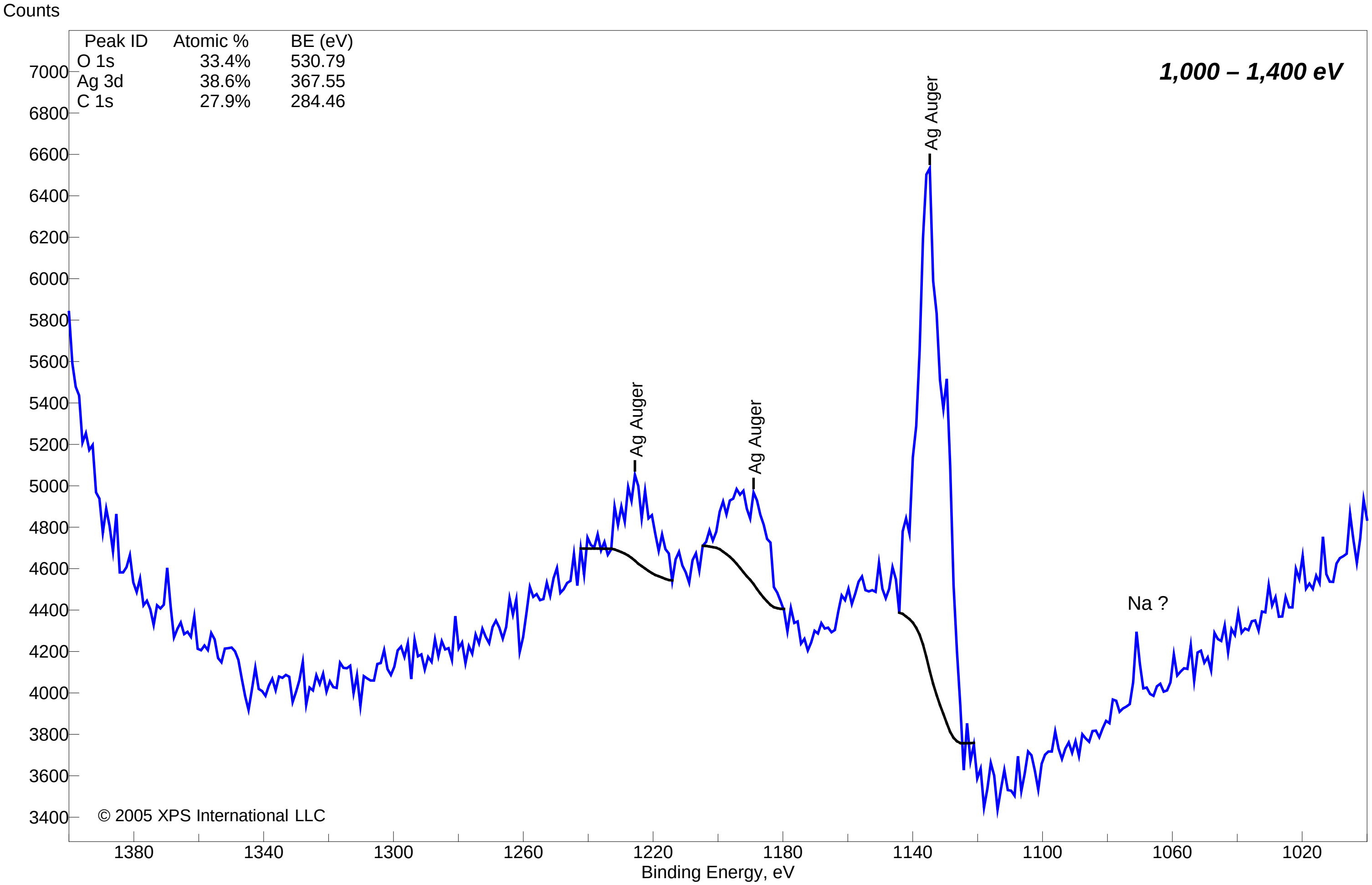
Peak ID	Atomic %	BE (eV)
O 1s	33.4%	530.79
Ag 3d	38.6%	367.55
C 1s	27.9%	284.46

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	2.84	1.80	6011.5	100.0%	0.0%	5765.99	8.5%
B	5.97	3.01	37264	100.0%	0.0%	59729.3	88.1%
C	8.79	2.32	1895.08	100.0%	0.0%	2340.31	3.4%

Peak-Fit Baseline: 12.40 to -1.13 eV
Reduced Chi-Square: 4.417

Silver (II) Oxide (FW = 123.87)

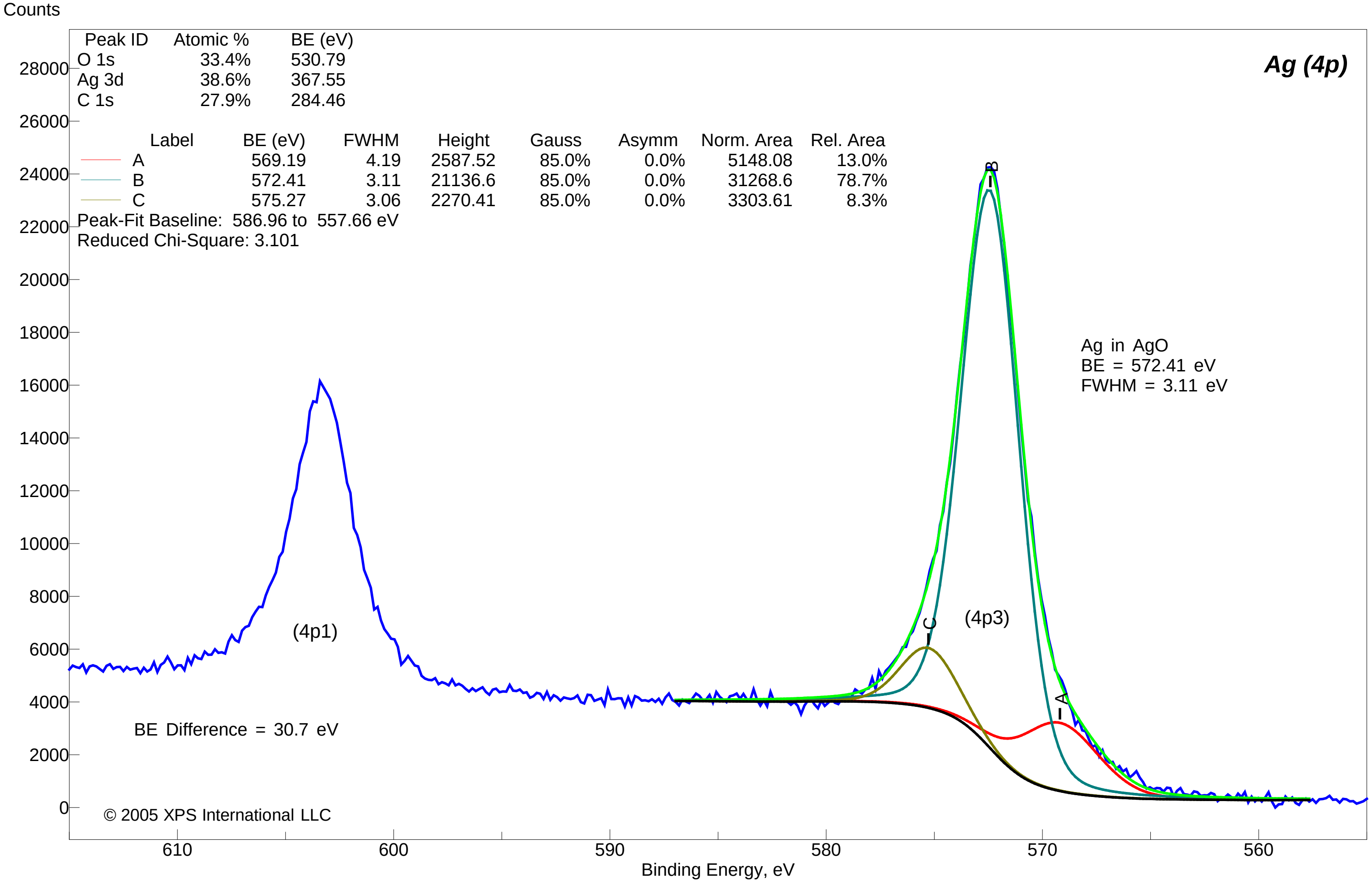
Sample Description: AgO (99%) Aldrich lot# 00108JV (contaminated with Ag2O)
3 mm pellet, CONDUCTIVE, 90 DEG TOA



Peak ID	Atomic %	BE (eV)
O 1s	33.4%	530.79
Ag 3d	38.6%	367.55
C 1s	27.9%	284.46

Silver (II) Oxide (FW = 123.87)

Sample Description: AgO (99%) Aldrich lot# 00108JV (contaminated with Ag2O)
3 mm pellet, CONDUCTIVE, 90 DEG TOA



Peak ID	Atomic %	BE (eV)
O 1s	33.4%	530.79
Ag 3d	38.6%	367.55
C 1s	27.9%	284.46

	Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
—	A	569.19	4.19	2587.52	85.0%	0.0%	5148.08	13.0%
—	B	572.41	3.11	21136.6	85.0%	0.0%	31268.6	78.7%
—	C	575.27	3.06	2270.41	85.0%	0.0%	3303.61	8.3%

Peak-Fit Baseline: 586.96 to 557.66 eV
Reduced Chi-Square: 3.101

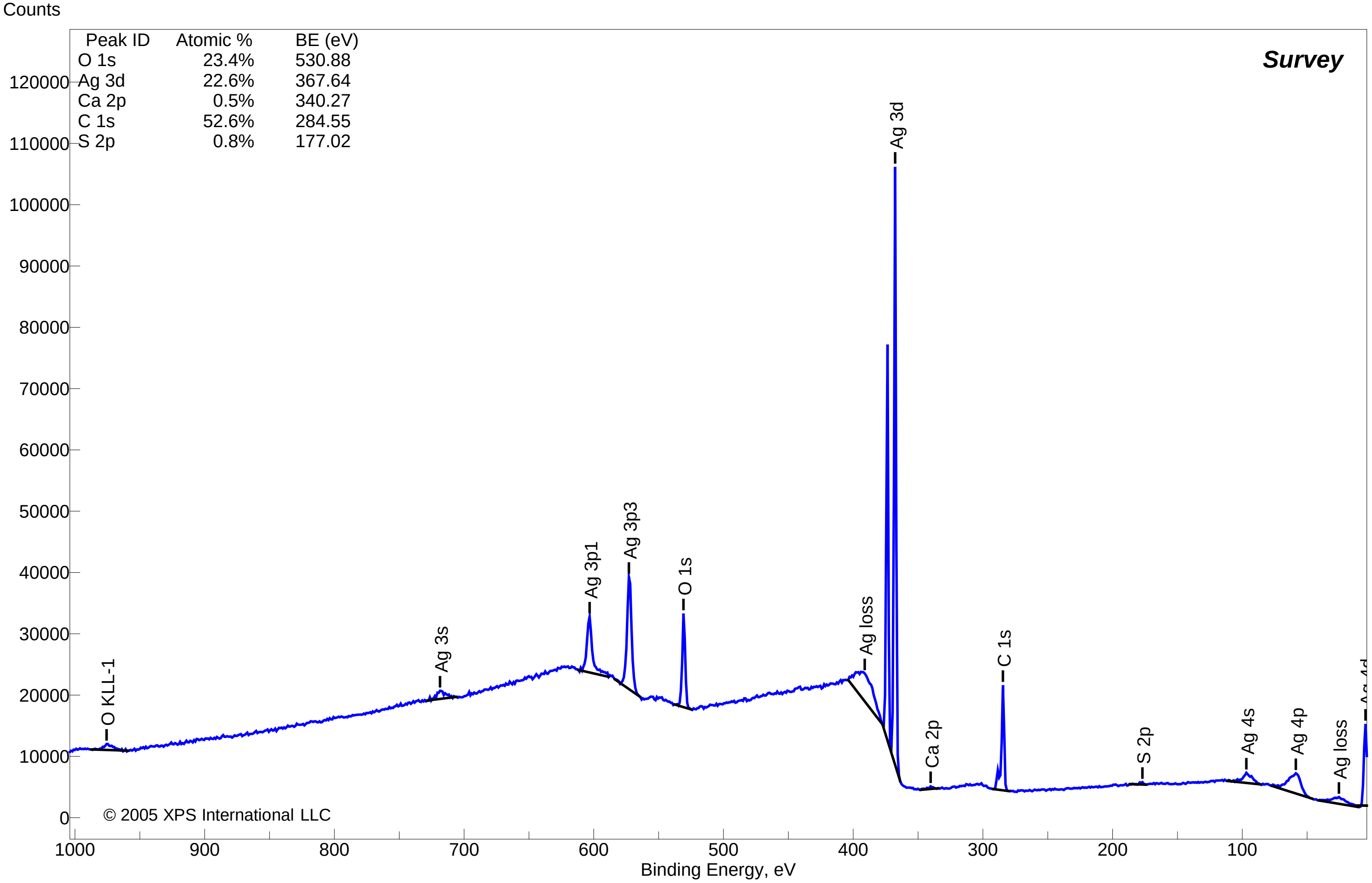
Silver (I) Oxide (FW = 231.74)
Surface Composition Table

Description: Ag_2O (99.99%) from Aldrich Lot# 00105CV, analyzed at 35 deg TOA, mesh at 1mm, conductive black powder pressed into 5 mm pellet, mp 230, d. 7.14, sol in dil. HNO_3 and ammonia

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
Ag 4d	5.6	5.0	1.55	1.4	5580.7	
Ag loss	26.1	25.5	0.15	1.4	2430.6	
Ag 4p	59.3	58.7	1.36	1.4	6388.2	
Ag 4s	97.5	96.9	0.64	1.4	2398.0	
S 2p	177.6	177.0	1.68	1.4	210.5	0.8%
C 1s	285.1	284.5	1.00	1.4	7338.6	52.6%
Ca 2p	340.9	340.3	5.07	1.4	337.9	0.5%
Ag 3d	368.2	367.6	18.00	1.4	51467.1	22.6%
Ag loss	391.7	391.1	0.00	1.4	11949.7	
O 1s	531.6	530.9	2.93	1.4	6937.9	23.4%
Ag 3p3	573.5	572.9	8.06	1.4	13040.6	
Ag 3p1	603.8	603.2	4.03	1.4	7758.5	
Ag 3s	719.2	718.6	2.93	1.4	1785.8	
O KLL-1	976.3	975.7	0.70	1.4	1379.4	

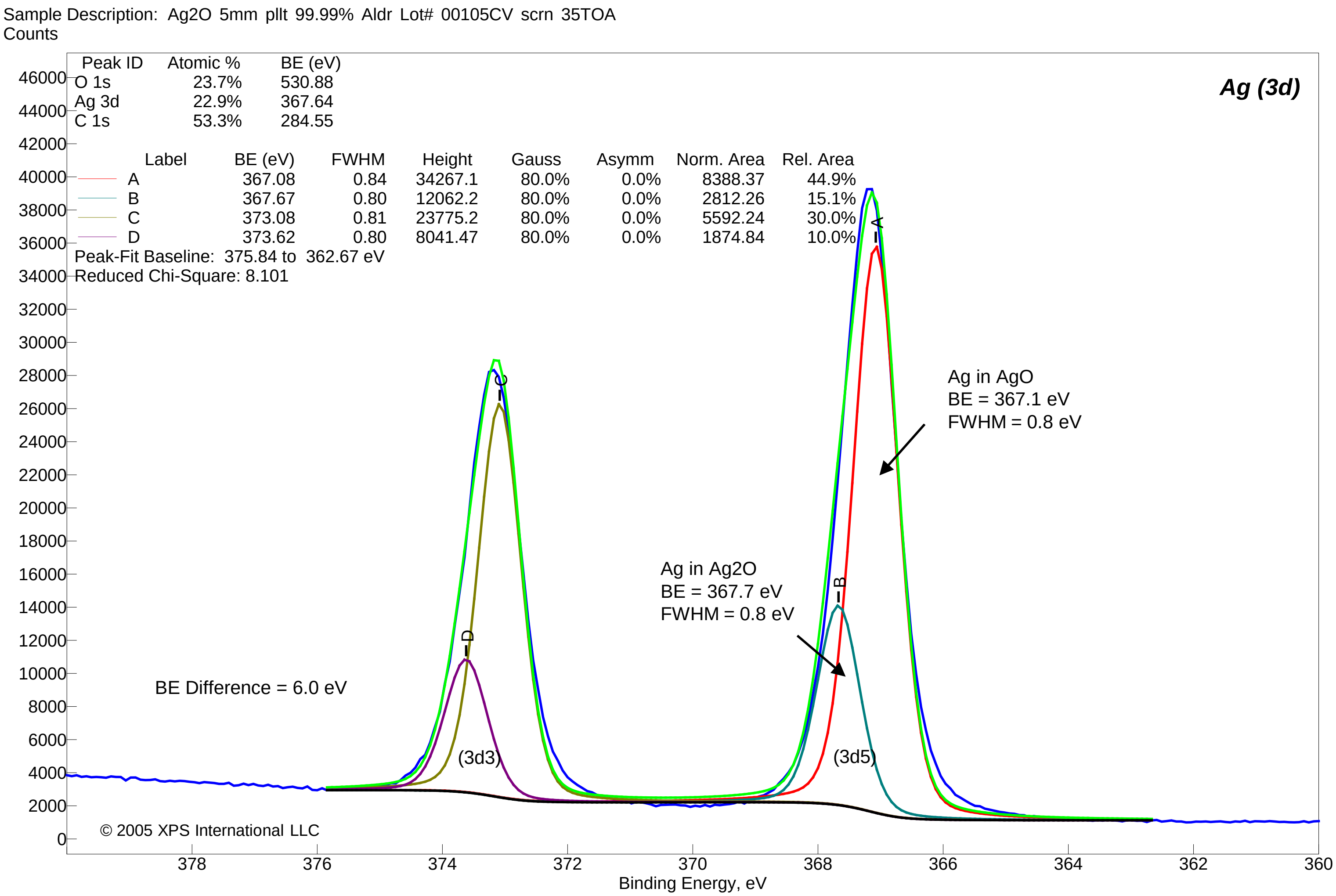
Silver (I) Oxide (FW = 231.74)

Sample Description: Ag2O (99.99%) from Aldrich Lot# 00105CV
pressed into 5 mm pellet, analyzed at 35 deg TOA, mesh-screen at 1 mm height



Peak ID	Atomic %	BE (eV)
O 1s	23.4%	530.88
Ag 3d	22.6%	367.64
Ca 2p	0.5%	340.27
C 1s	52.6%	284.55
S 2p	0.8%	177.02

Silver (I) Oxide (FW = 231.74)



Sample Description: Ag2O 5mm pllt 99.99% Aldr Lot# 00105CV scrn 35TOA

Peak ID	Atomic %	BE (eV)
O 1s	23.7%	530.88
Ag 3d	22.9%	367.64
C 1s	53.3%	284.55

	Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
—	A	367.08	0.84	34267.1	80.0%	0.0%	8388.37	44.9%
—	B	367.67	0.80	12062.2	80.0%	0.0%	2812.26	15.1%
—	C	373.08	0.81	23775.2	80.0%	0.0%	5592.24	30.0%
—	D	373.62	0.80	8041.47	80.0%	0.0%	1874.84	10.0%

Peak-Fit Baseline: 375.84 to 362.67 eV

Reduced Chi-Square: 8.101

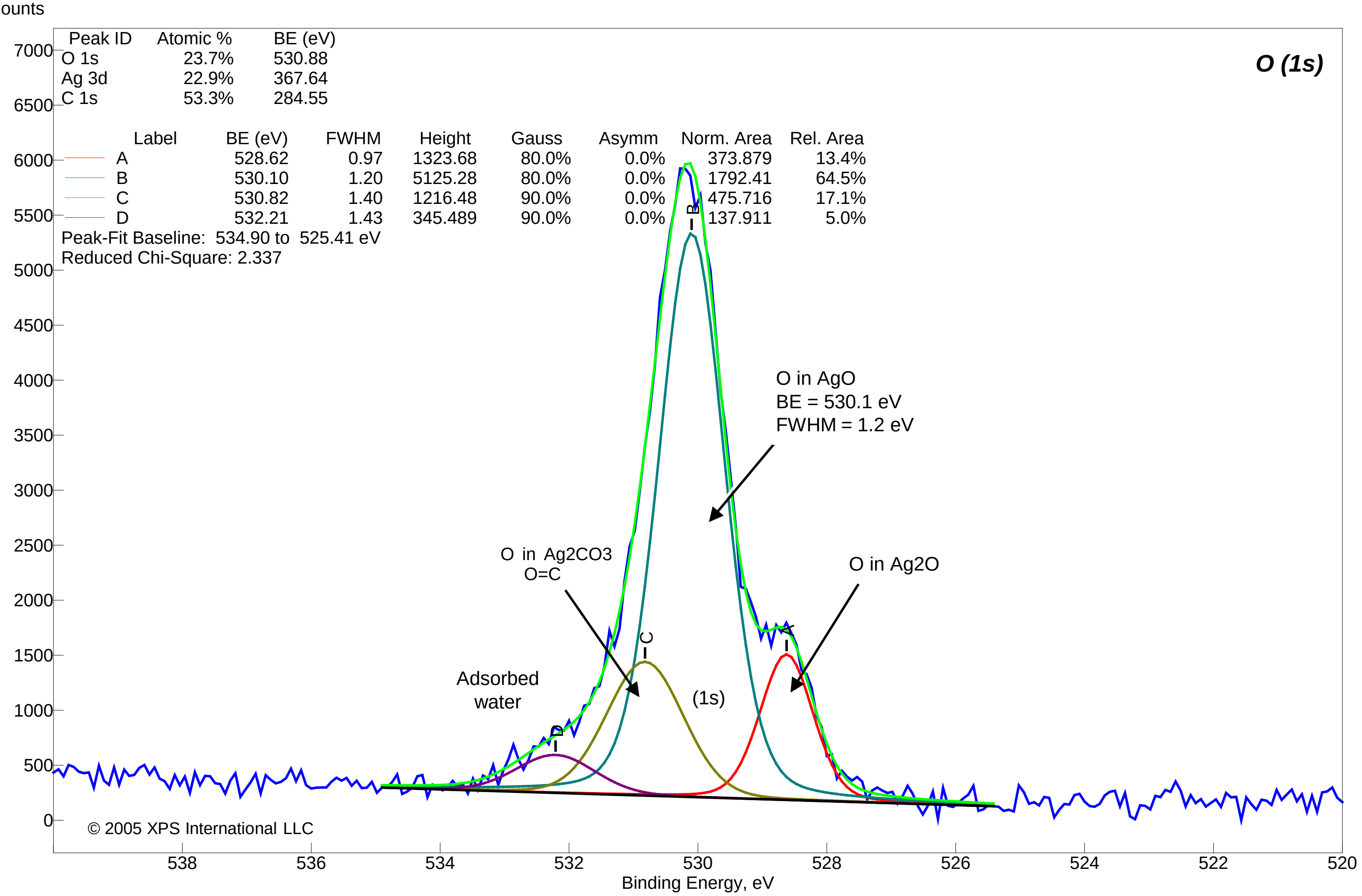
Ag in AgO
BE = 367.1 eV
FWHM = 0.8 eV

Ag in Ag2O
BE = 367.7 eV
FWHM = 0.8 eV

BE Difference = 6.0 eV

Silver (I) Oxide (FW = 231.74)

Sample Description: Ag2O 5mm pllt 99.99% Aldr Lot# 00105CV scrn 35TOA



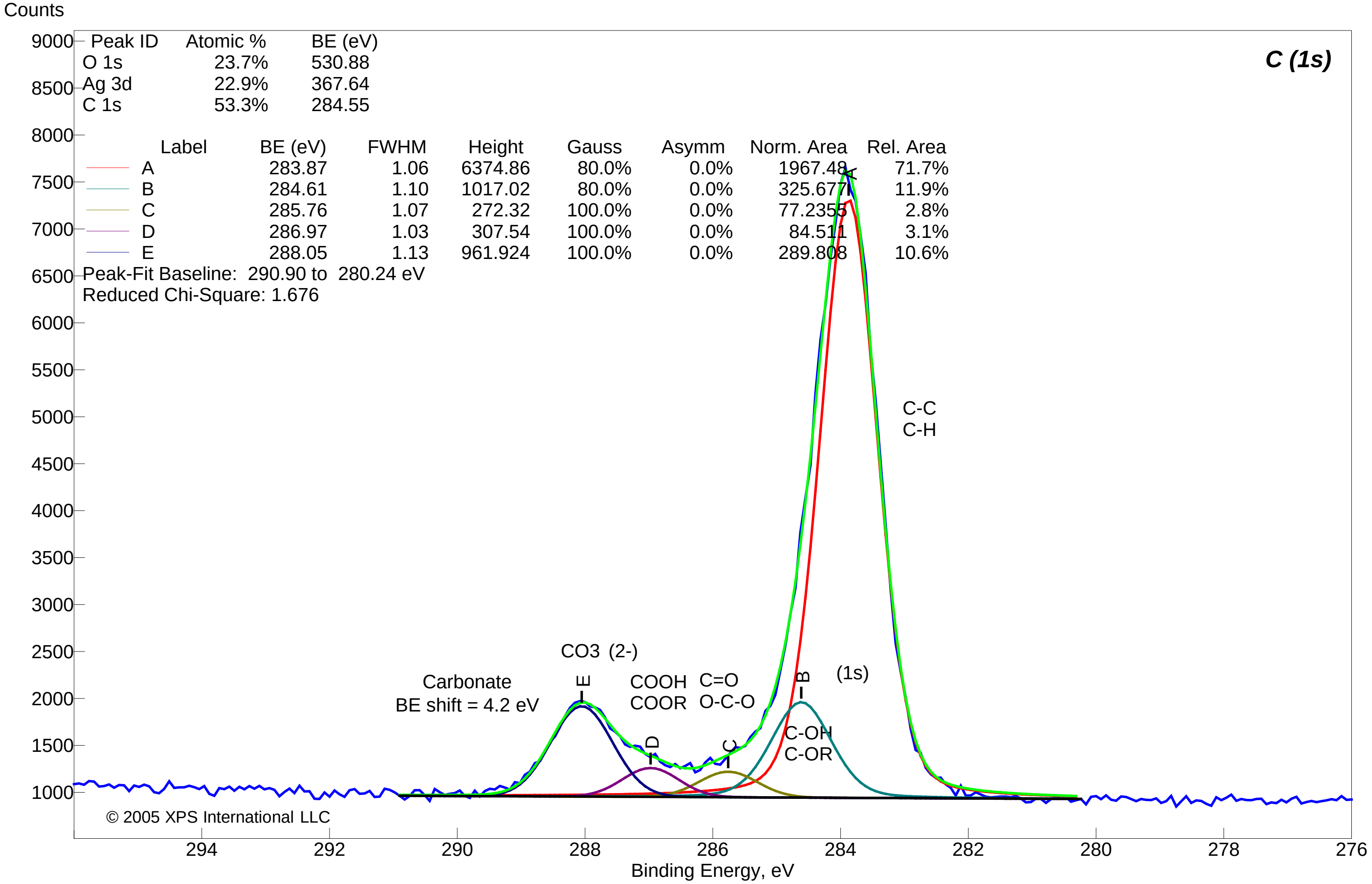
Peak ID	Atomic %	BE (eV)
O 1s	23.7%	530.88
Ag 3d	22.9%	367.64
C 1s	53.3%	284.55

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	528.62	0.97	1323.68	80.0%	0.0%	373.879	13.4%
B	530.10	1.20	5125.28	80.0%	0.0%	1792.41	64.5%
C	530.82	1.40	1216.48	90.0%	0.0%	475.716	17.1%
D	532.21	1.43	345.489	90.0%	0.0%	137.911	5.0%

Peak-Fit Baseline: 534.90 to 525.41 eV
Reduced Chi-Square: 2.337

Silver (I) Oxide (FW = 231.74)

Sample Description: Ag2O 5mm pllt 99.99% Aldr Lot# 00105CV scrn 35TOA



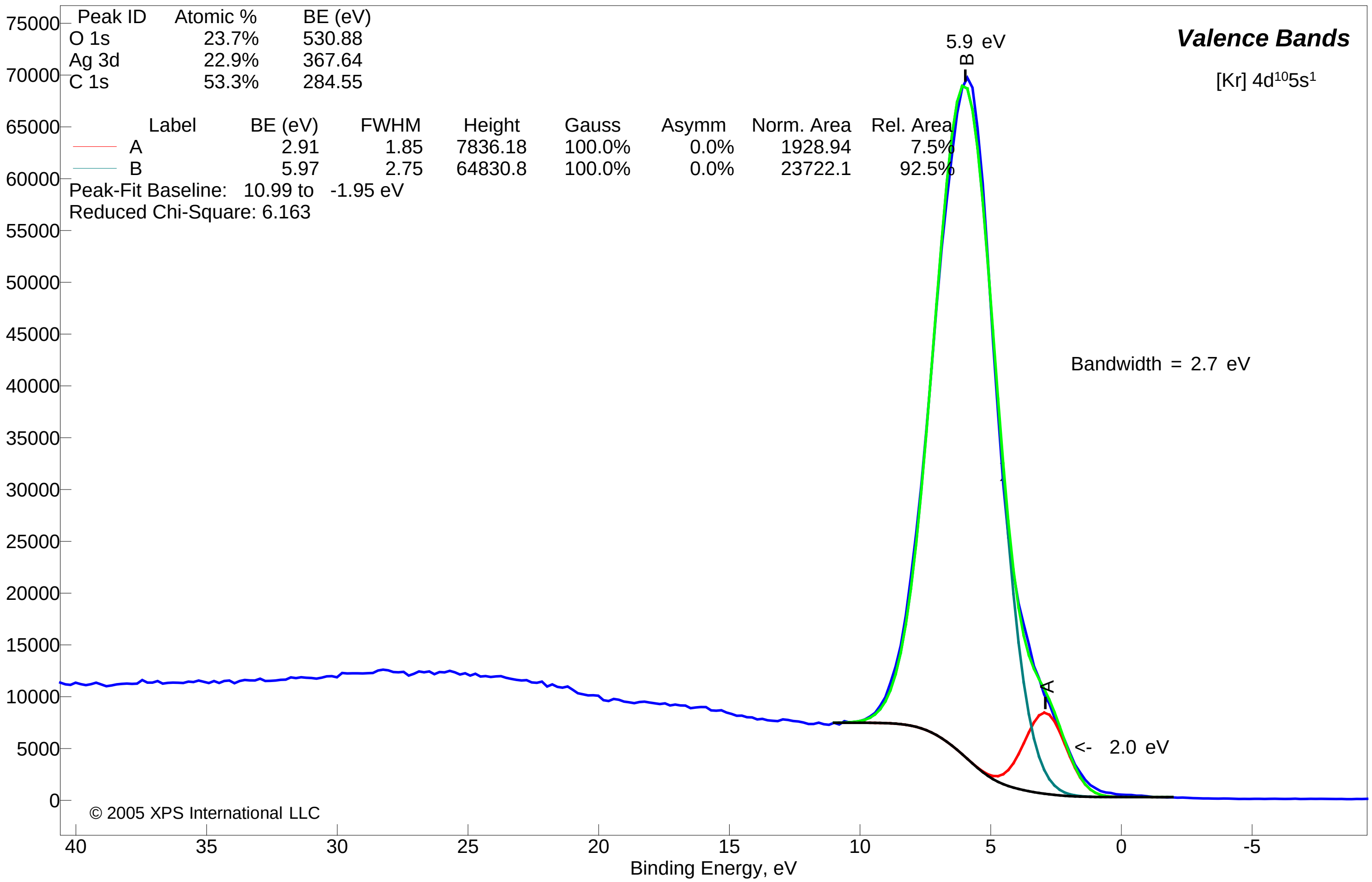
Peak ID	Atomic %	BE (eV)
O 1s	23.7%	530.88
Ag 3d	22.9%	367.64
C 1s	53.3%	284.55

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	283.87	1.06	6374.86	80.0%	0.0%	1967.48	71.7%
B	284.61	1.10	1017.02	80.0%	0.0%	325.677	11.9%
C	285.76	1.07	272.32	100.0%	0.0%	77.2355	2.8%
D	286.97	1.03	307.54	100.0%	0.0%	84.511	3.1%
E	288.05	1.13	961.924	100.0%	0.0%	289.808	10.6%

Peak-Fit Baseline: 290.90 to 280.24 eV
Reduced Chi-Square: 1.676

Silver (I) Oxide (FW = 231.74)

Sample Description: Ag2O 5mm pllt 99.99% Aldr Lot# 00105CV scrn 35TOA



Peak ID	Atomic %	BE (eV)
O 1s	23.7%	530.88
Ag 3d	22.9%	367.64
C 1s	53.3%	284.55

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	2.91	1.85	7836.18	100.0%	0.0%	1928.94	7.5%
B	5.97	2.75	64830.8	100.0%	0.0%	23722.1	92.5%

Peak-Fit Baseline: 10.99 to -1.95 eV
Reduced Chi-Square: 6.163

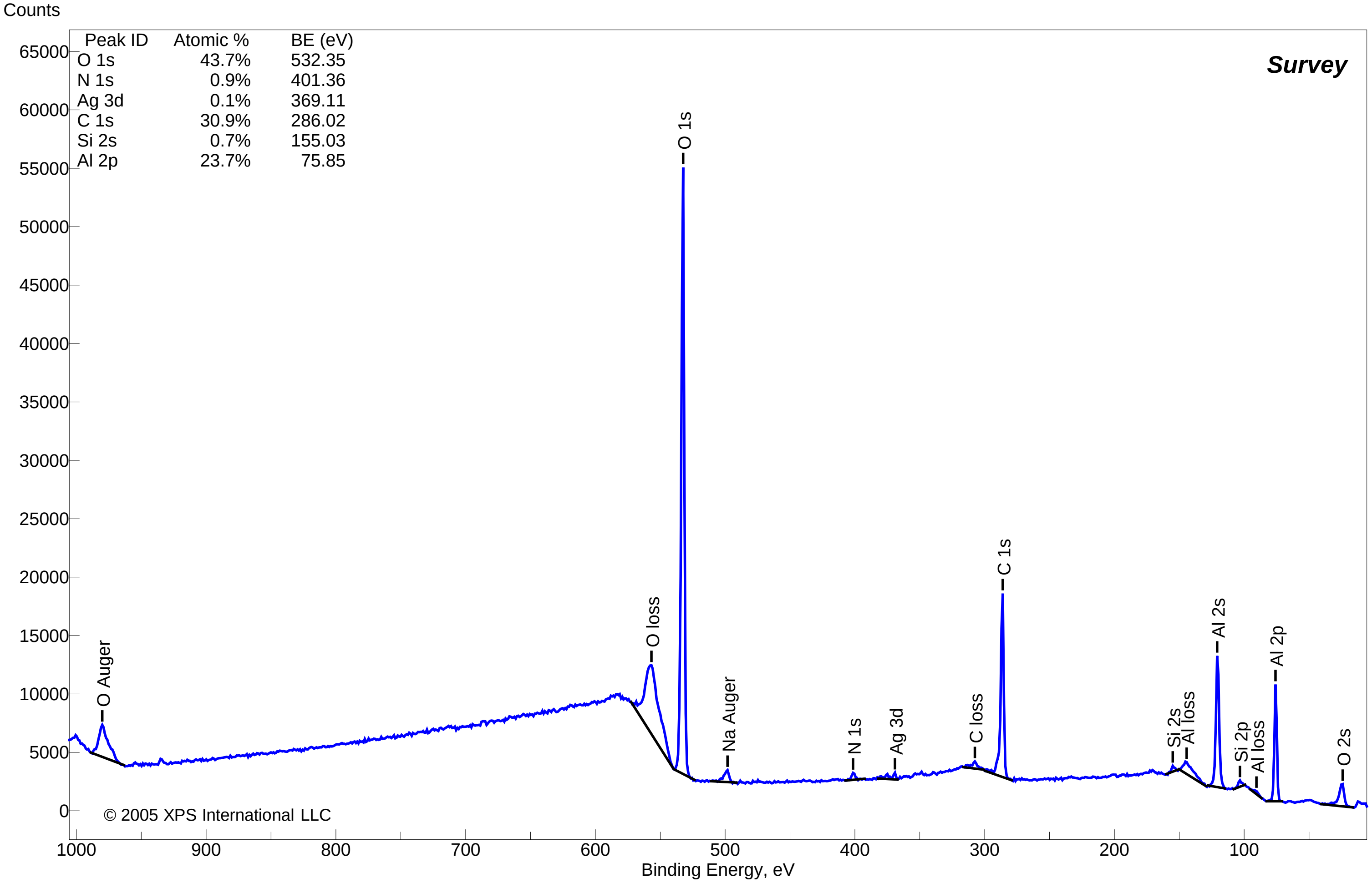
Aluminum (III) Oxide (FW = 101.96)
Surface Composition Table

Description: Al_2O_3 (99%), analyzed at 90 deg TOA, mesh at 1mm, non-conductive fused into clear glass 1 mm thick, mp 2040 C, d 3.97

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
O 2s	24.0	19.9	0.14	1.2	12,578	
Al 2p	75.9	71.8	0.54	1.2	28,737	23.7%
Al loss	90.5	86.4	0.00	1.5	1,485	
Si 2p	103.2	99.1	0.82	1.5	2,122	
Al 2s	120.8	116.7	0.75	1.2	42,744	
Al loss	144.3	140.2	0.00	1.2	11,965	
Si 2s	155.0	150.9	0.96	1.2	1,481	0.7%
C 1s	286.0	281.9	1.00	1.2	57,477	30.9%
C loss	307.5	303.4	0.00	1.2	4,508	
Ag 3d	369.1	365.0	18.04	1.2	4,186	0.1%
N 1s	401.4	397.3	1.80	1.2	2,528	0.9%
Na Auger	498.1	494.0	3.40	1.2	6,270	
O 1s	532.4	528.3	2.93	1.2	180,659	43.7%
O loss	556.8	552.7	0.00	1.2	95,458	
O Auger	980.1	976.0	0.00	1.2	29,773	

Aluminum (III) Oxide (FW = 101.96)

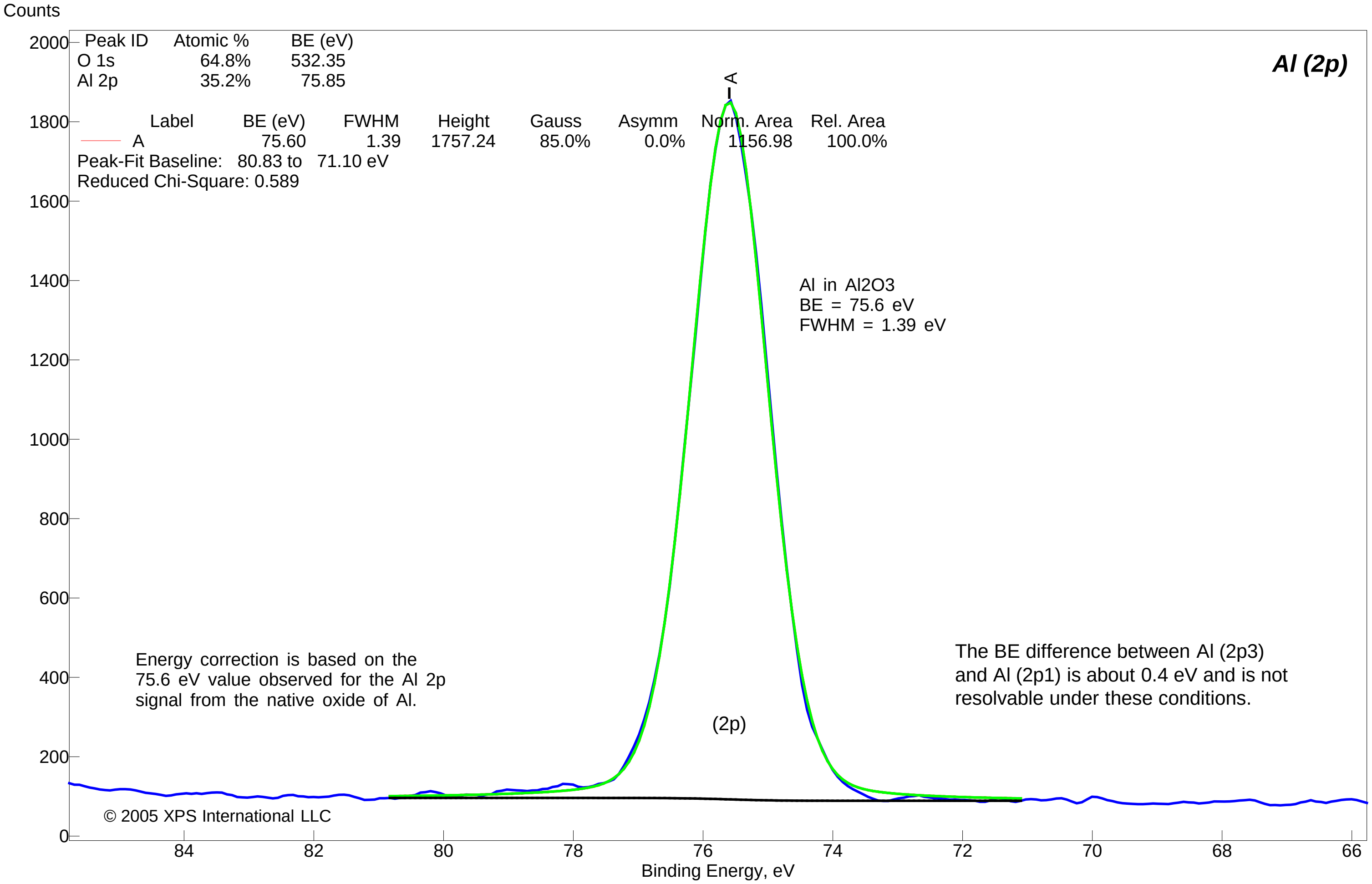
Sample Description: Al2O3 (99%) fused into glass 1mm thick
analyzed as received at 90 deg TOA , mesh-screen at 1mm



Peak ID	Atomic %	BE (eV)
O 1s	43.7%	532.35
N 1s	0.9%	401.36
Ag 3d	0.1%	369.11
C 1s	30.9%	286.02
Si 2s	0.7%	155.03
Al 2p	23.7%	75.85

Aluminum (III) Oxide (FW = 101.96)

Sample Description: Fused Al2O3
(as rec'd, surface of 1 mm thick plate, screen, 90 DEG TOA)



Peak ID	Atomic %	BE (eV)
O 1s	64.8%	532.35
Al 2p	35.2%	75.85

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	75.60	1.39	1757.24	85.0%	0.0%	1156.98	100.0%

Peak-Fit Baseline: 80.83 to 71.10 eV
Reduced Chi-Square: 0.589

Al in Al2O3
BE = 75.6 eV
FWHM = 1.39 eV

Energy correction is based on the 75.6 eV value observed for the Al 2p signal from the native oxide of Al.

The BE difference between Al (2p3) and Al (2p1) is about 0.4 eV and is not resolvable under these conditions.

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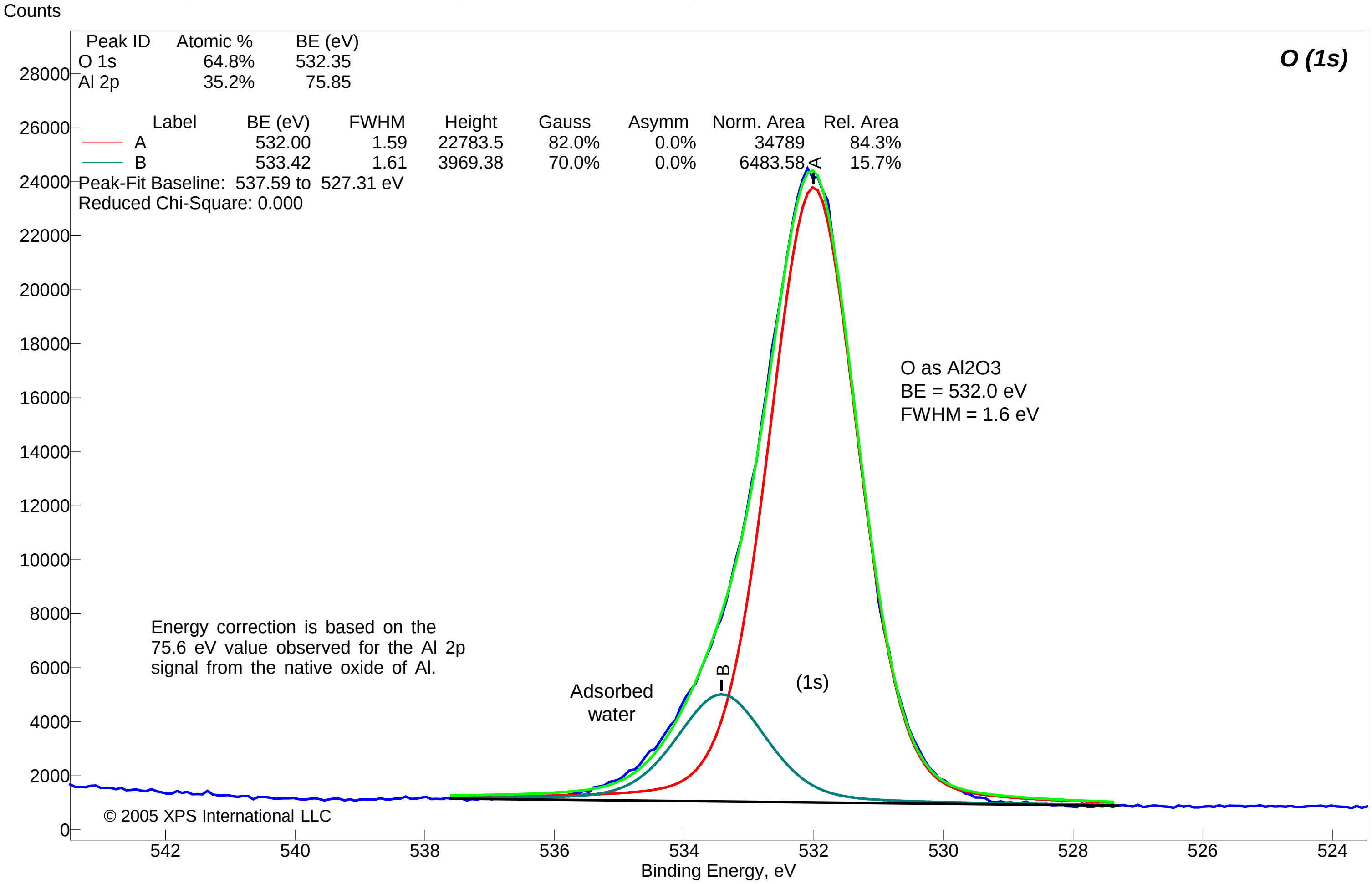
Aluminum (III) Oxide (FW = 101.96)

Sample Description: Fused Al2O3
(as rec'd, surface of 1 mm thick plate, screen, 90 DEG TOA)



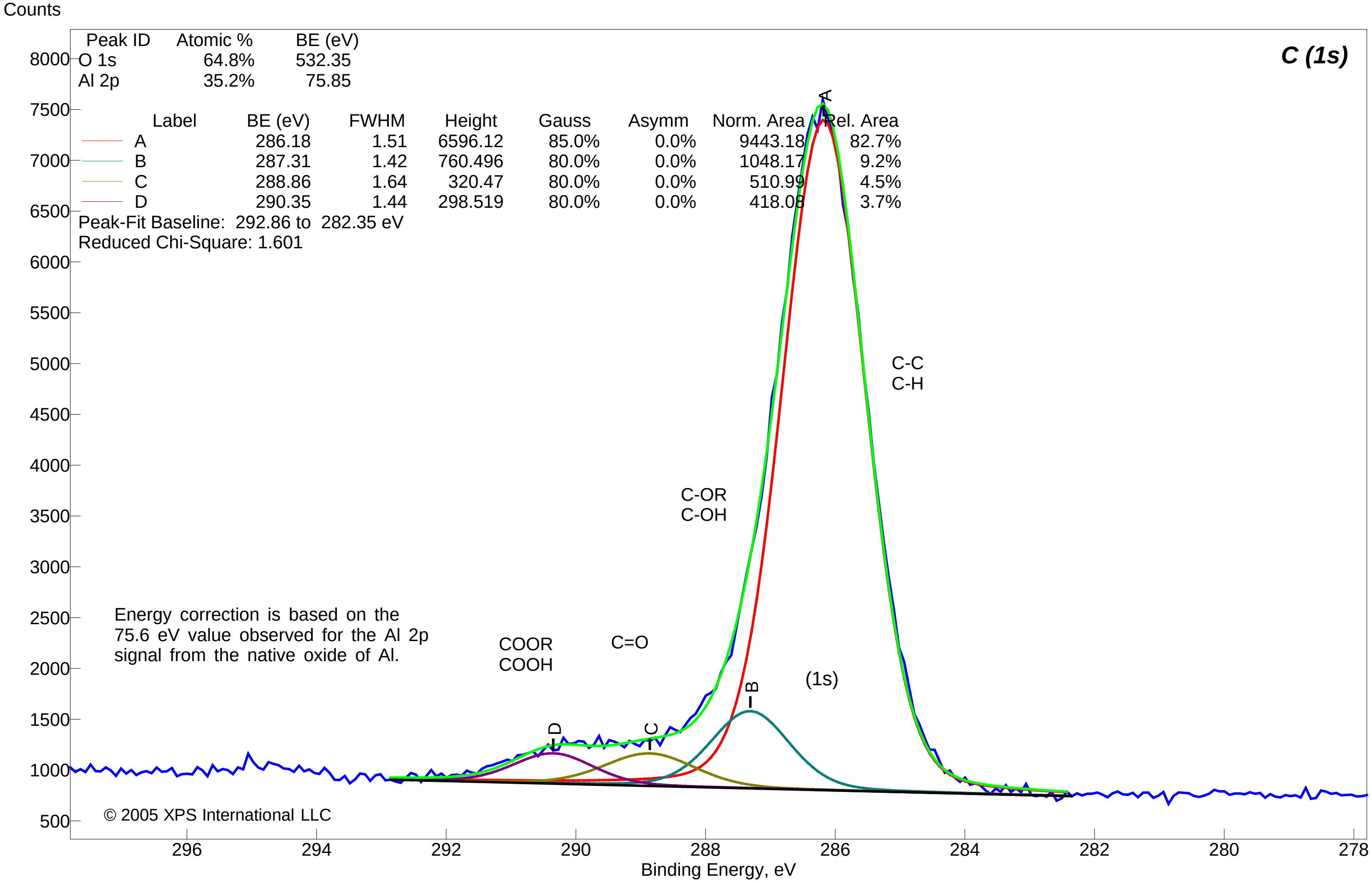
Peak ID	Atomic %	BE (eV)
O 1s	64.8%	532.35
Al 2p	35.2%	75.85

	Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
—	A	532.00	1.59	22783.5	82.0%	0.0%	34789	84.3%
—	B	533.42	1.61	3969.38	70.0%	0.0%	6483.58	15.7%

Peak-Fit Baseline: 537.59 to 527.31 eV
Reduced Chi-Square: 0.000

Aluminum (III) Oxide (FW = 101.96)

Sample Description: Fused Al2O3
(as rec'd, surface of 1 mm thick plate, screen, 90 DEG TOA)



Peak ID	Atomic %	BE (eV)
O 1s	64.8%	532.35
Al 2p	35.2%	75.85

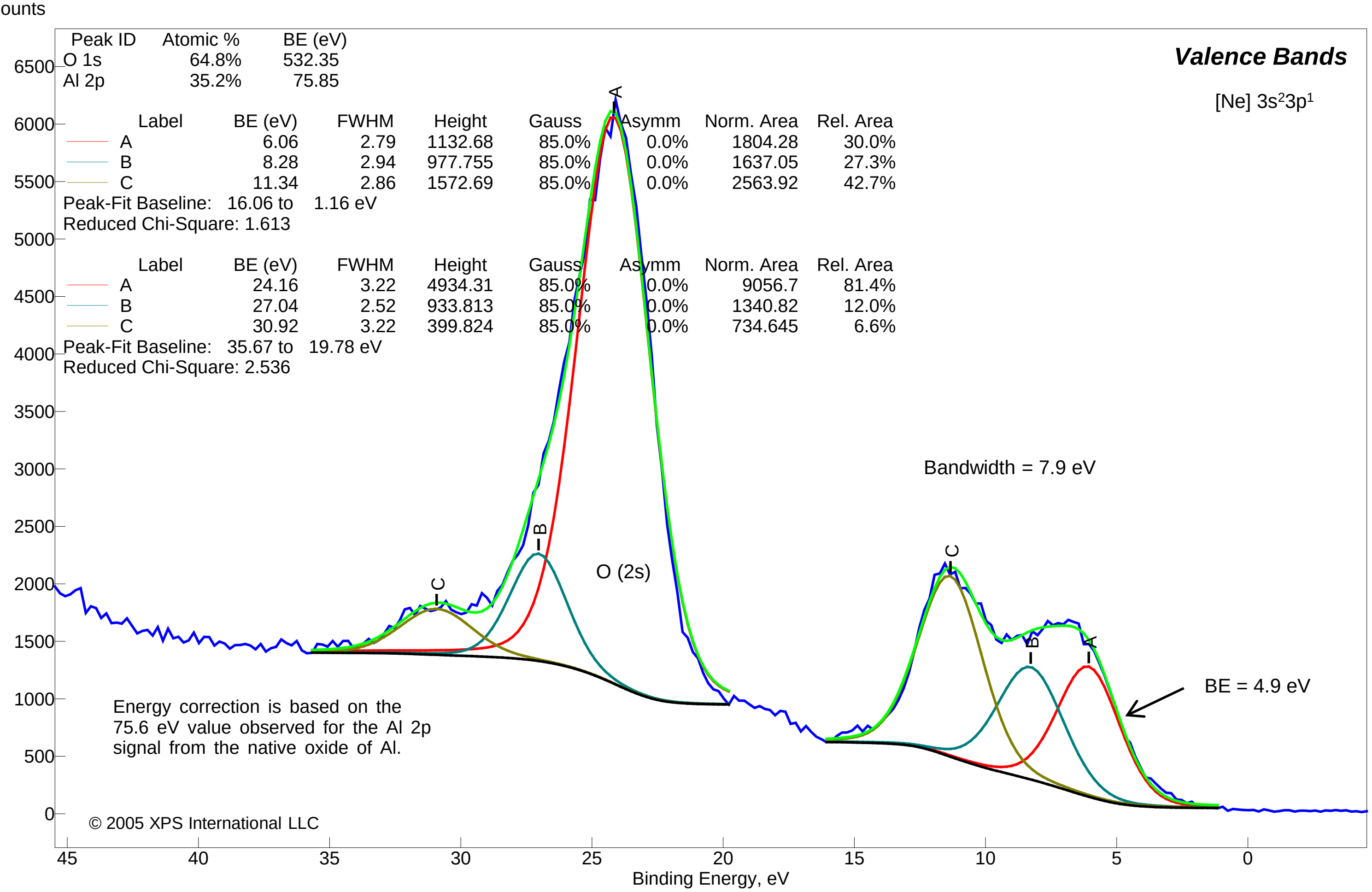
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	286.18	1.51	6596.12	85.0%	0.0%	9443.18	82.7%
B	287.31	1.42	760.496	80.0%	0.0%	1048.17	9.2%
C	288.86	1.64	320.47	80.0%	0.0%	510.99	4.5%
D	290.35	1.44	298.519	80.0%	0.0%	418.08	3.7%

Peak-Fit Baseline: 292.86 to 282.35 eV
Reduced Chi-Square: 1.601

Energy correction is based on the 75.6 eV value observed for the Al 2p signal from the native oxide of Al.

Aluminum (III) Oxide (FW = 101.96)

Sample Description: Fused Al2O3
(as rec'd, surface of 1 mm thick plate, screen, 90 DEG TOA)



Peak ID	Atomic %	BE (eV)
O 1s	64.8%	532.35
Al 2p	35.2%	75.85

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	6.06	2.79	1132.68	85.0%	0.0%	1804.28	30.0%
B	8.28	2.94	977.755	85.0%	0.0%	1637.05	27.3%
C	11.34	2.86	1572.69	85.0%	0.0%	2563.92	42.7%

Peak-Fit Baseline: 16.06 to 1.16 eV
Reduced Chi-Square: 1.613

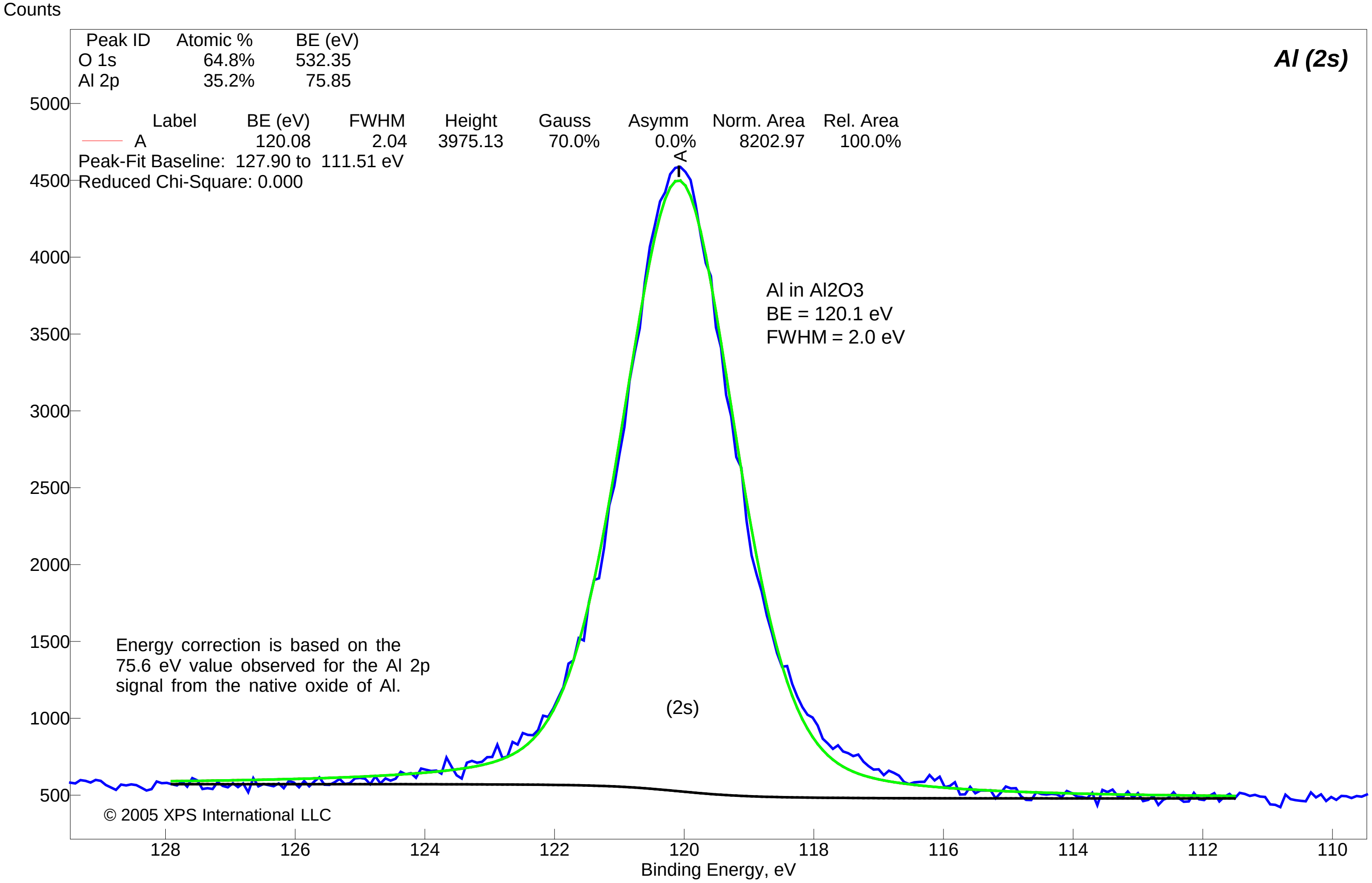
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	24.16	3.22	4934.31	85.0%	0.0%	9056.7	81.4%
B	27.04	2.52	933.813	85.0%	0.0%	1340.82	12.0%
C	30.92	3.22	399.824	85.0%	0.0%	734.645	6.6%

Peak-Fit Baseline: 35.67 to 19.78 eV
Reduced Chi-Square: 2.536

Energy correction is based on the 75.6 eV value observed for the Al 2p signal from the native oxide of Al.

Aluminum (III) Oxide (FW = 101.96)

Sample Description: Fused Al2O3
(as rec'd, surface of 1 mm thick plate, screen, 90 DEG TOA)



Peak ID	Atomic %	BE (eV)
O 1s	64.8%	532.35
Al 2p	35.2%	75.85

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	120.08	2.04	3975.13	70.0%	0.0%	8202.97	100.0%

Peak-Fit Baseline: 127.90 to 111.51 eV
Reduced Chi-Square: 0.000

Al in Al2O3
BE = 120.1 eV
FWHM = 2.0 eV

Energy correction is based on the 75.6 eV value observed for the Al 2p signal from the native oxide of Al.

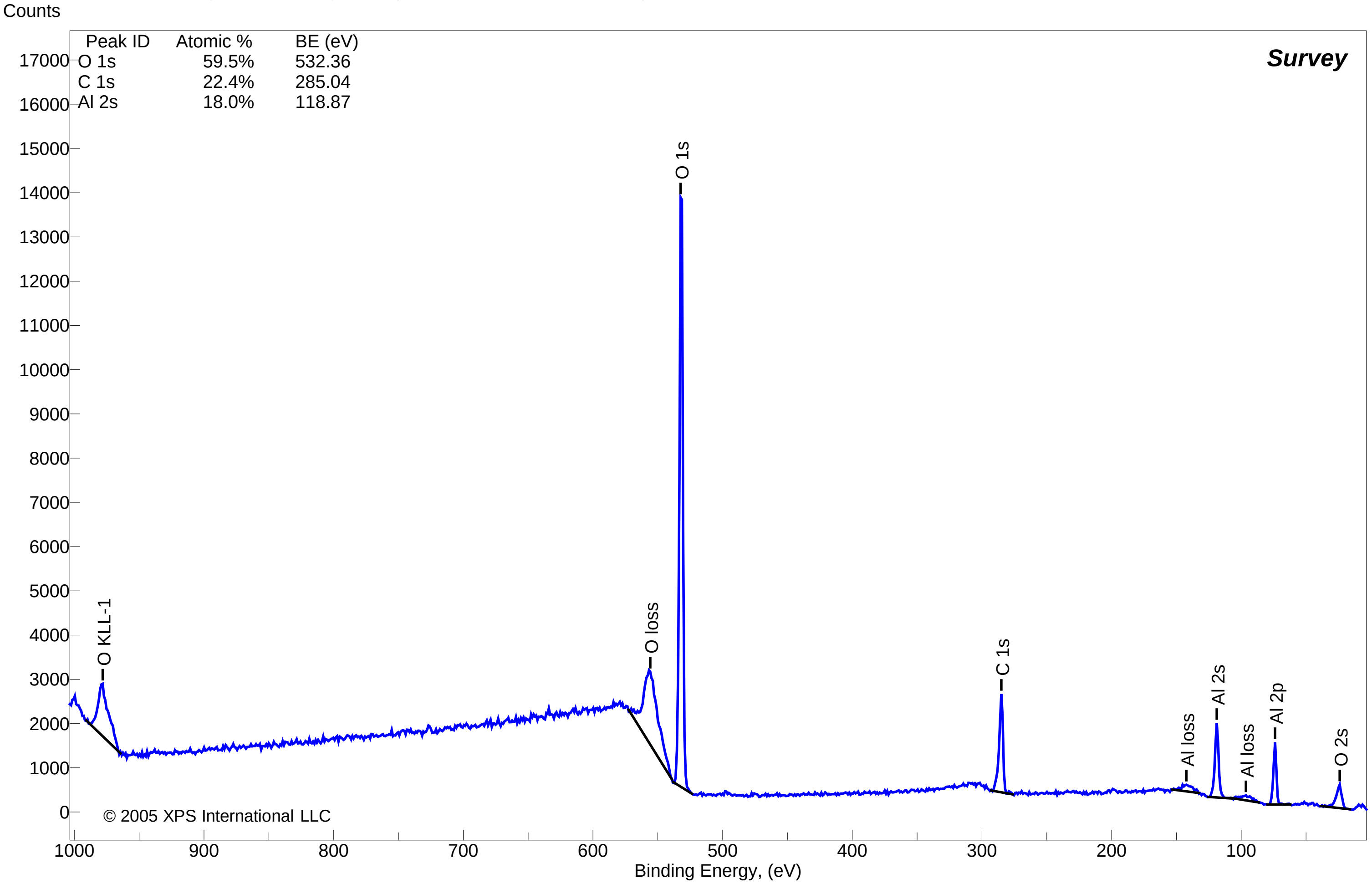
Aluminum (III) Hydroxide (FW = 78.00)
Surface Composition Table

Description: $Al(OH)_3$ (Tech.) from Perfect Parts Chem. Co., analyzed at 35 deg TOA, no mesh, non-conductive white powder pressed onto double sided tape, dec to Al2O3 >300 C, sol in aq. alkaline soln, HCl, H_2SO_4

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
O 2s	24.0	20.2	0.14	0.6	3,409	
Al 2p	73.9	70.1	0.54	0.6	4,885	
Al loss	96.4	92.6	0.00	0.6	1,419	
Al 2s	118.9	115.1	0.75	1.5	7,230	18.0%
Al loss	142.3	138.5	0.00	0.6	2,350	
C 1s	285.0	281.2	1.00	1.5	9,833	22.4%
O 1s	532.4	528.6	2.93	1.5	54,136	59.5%
O loss	555.8	552.0	0.00	0.6	28,217	
O KLL-1	978.1	974.3	0.70	0.6	13,859	

Aluminum (III) Hydroxide (FW = 78.00)

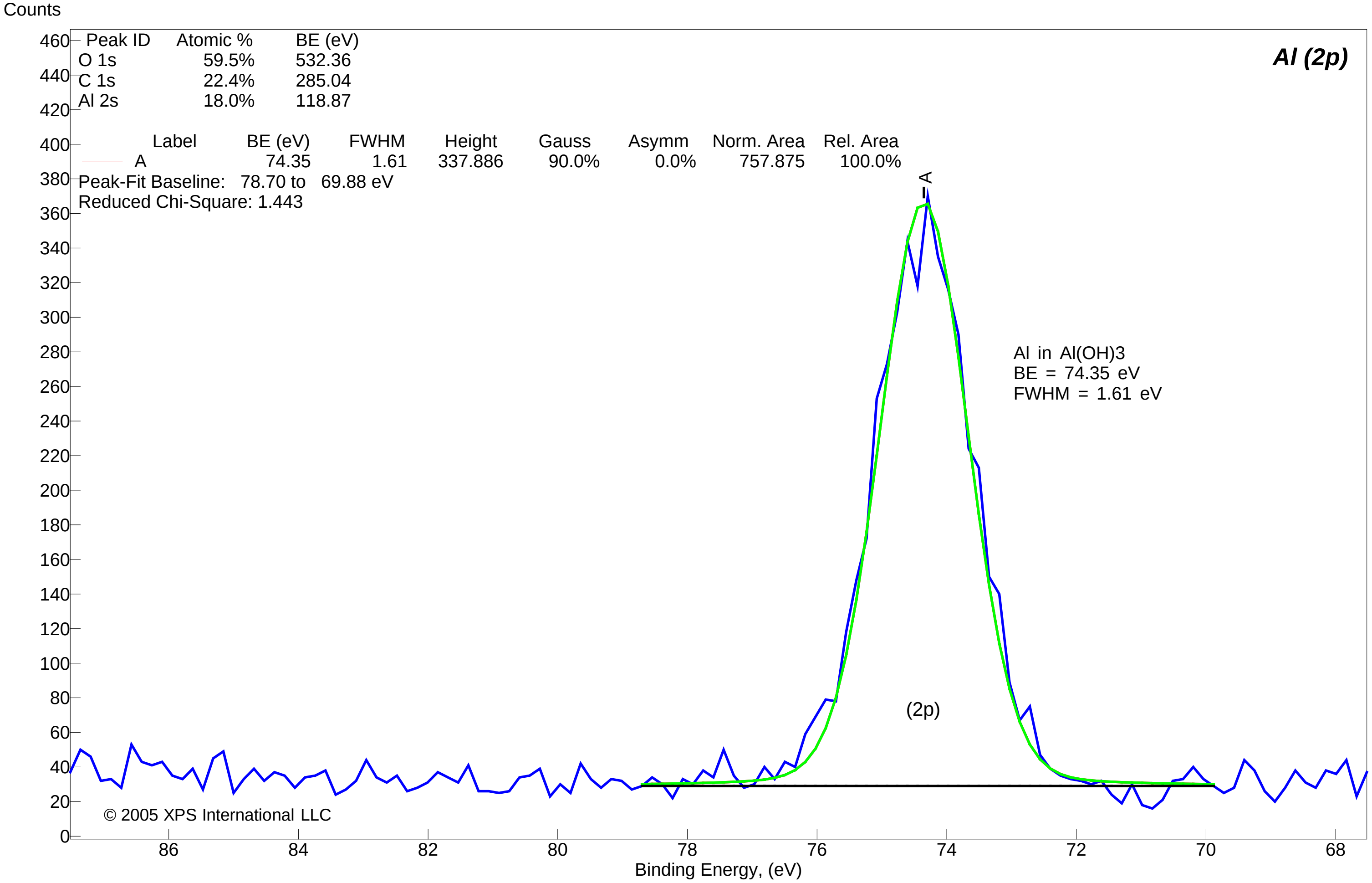
Sample Description: Al(OH)3 (Tech. Grade) from Perfect Parts Chemical Co.
analyzed at 35 deg TOA, pressed onto double sided tape, no mesh-screen



Peak ID	Atomic %	BE (eV)
O 1s	59.5%	532.36
C 1s	22.4%	285.04
Al 2s	18.0%	118.87

Aluminum (III) Hydroxide (FW = 78.00)

Sample Description: ALUMINUM HYDROXIDE (Al(OH)3) powder/tape (no mesh)
TECHNICAL GRADE, PERFECT PARTS CHEMICAL CO.



Peak ID	Atomic %	BE (eV)
O 1s	59.5%	532.36
C 1s	22.4%	285.04
Al 2s	18.0%	118.87

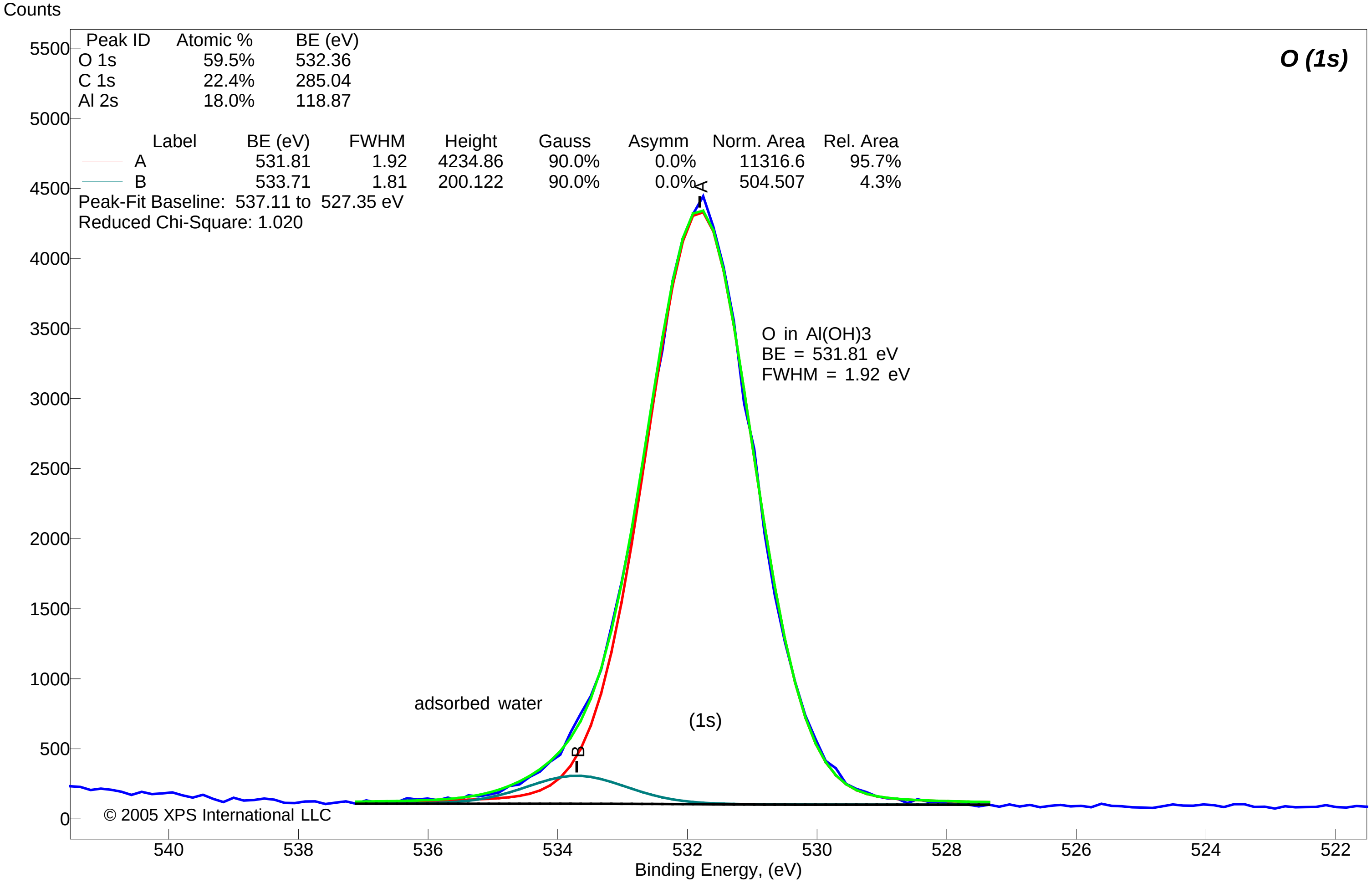
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	74.35	1.61	337.886	90.0%	0.0%	757.875	100.0%

Peak-Fit Baseline: 78.70 to 69.88 eV
Reduced Chi-Square: 1.443

Al in Al(OH)3
BE = 74.35 eV
FWHM = 1.61 eV

Aluminum (III) Hydroxide (FW = 78.00)

Sample Description: ALUMINUM HYDROXIDE (Al(OH)3) powder/tape (no mesh)
TECHNICAL GRADE, PERFECT PARTS CHEMICAL CO.



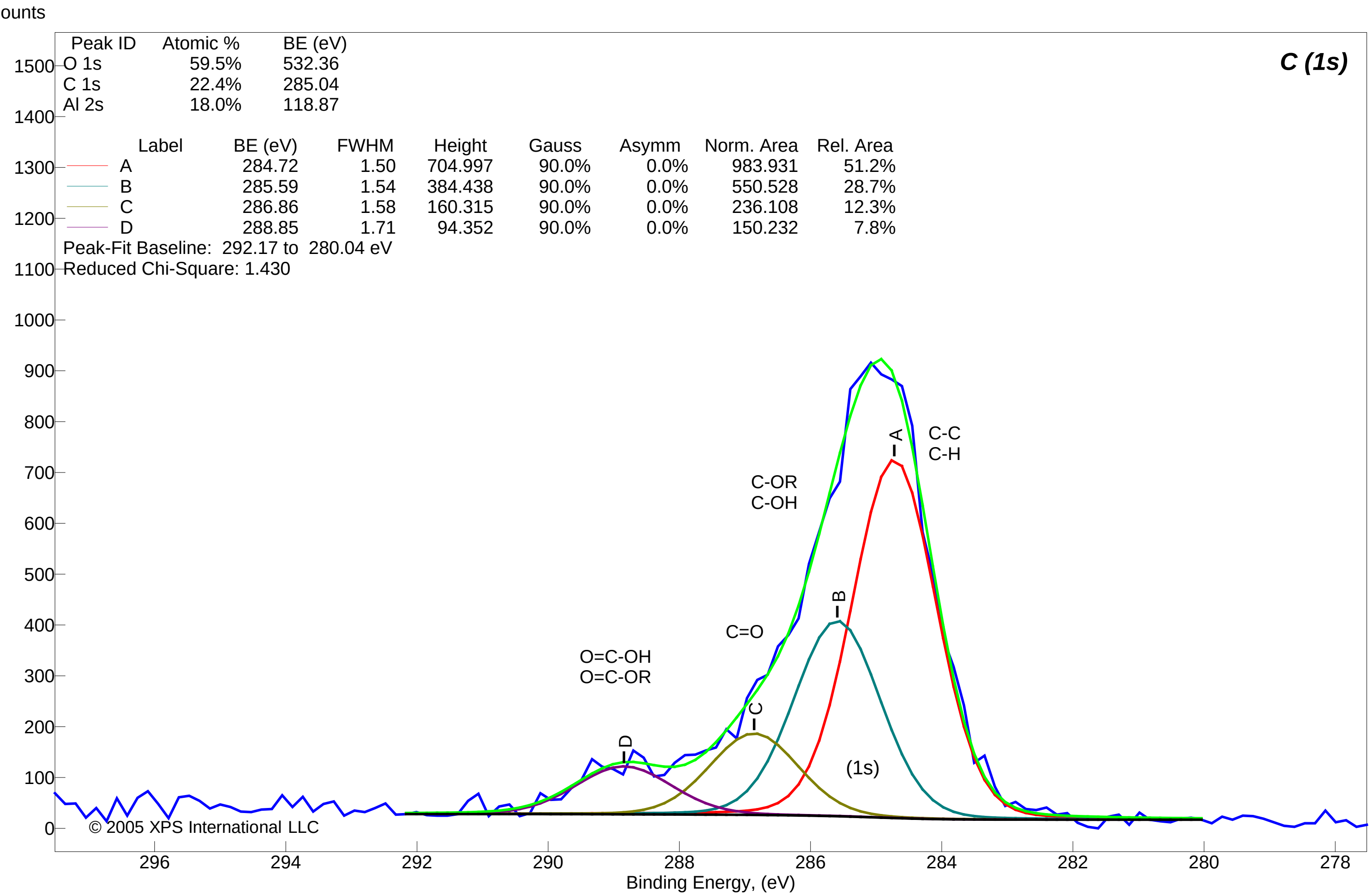
Peak ID	Atomic %	BE (eV)
O 1s	59.5%	532.36
C 1s	22.4%	285.04
Al 2s	18.0%	118.87

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	531.81	1.92	4234.86	90.0%	0.0%	11316.6	95.7%
B	533.71	1.81	200.122	90.0%	0.0%	504.507	4.3%

Peak-Fit Baseline: 537.11 to 527.35 eV
Reduced Chi-Square: 1.020

Aluminum (III) Hydroxide (FW = 78.00)

Sample Description: ALUMINUM HYDROXIDE (Al(OH)3) powder/tape (no mesh)
TECHNICAL GRADE, PERFECT PARTS CHEMICAL CO.



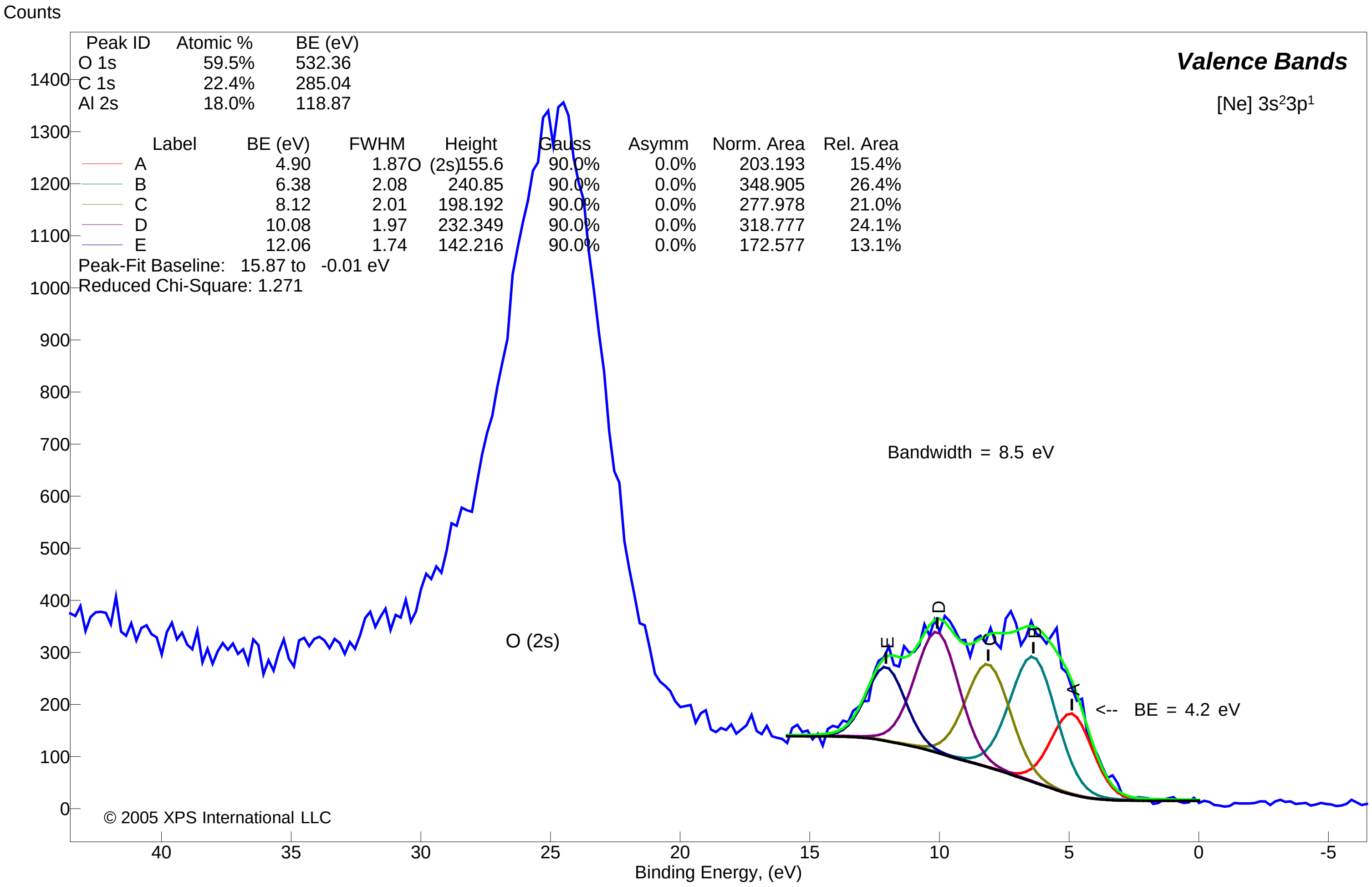
Peak ID	Atomic %	BE (eV)
O 1s	59.5%	532.36
C 1s	22.4%	285.04
Al 2s	18.0%	118.87

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	284.72	1.50	704.997	90.0%	0.0%	983.931	51.2%
B	285.59	1.54	384.438	90.0%	0.0%	550.528	28.7%
C	286.86	1.58	160.315	90.0%	0.0%	236.108	12.3%
D	288.85	1.71	94.352	90.0%	0.0%	150.232	7.8%

Peak-Fit Baseline: 292.17 to 280.04 eV
Reduced Chi-Square: 1.430

Aluminum (III) Hydroxide (FW = 78.00)

Sample Description: ALUMINUM HYDROXIDE (Al(OH)3) powder/tape (no mesh)
TECHNICAL GRADE, PERFECT PARTS CHEMICAL CO.



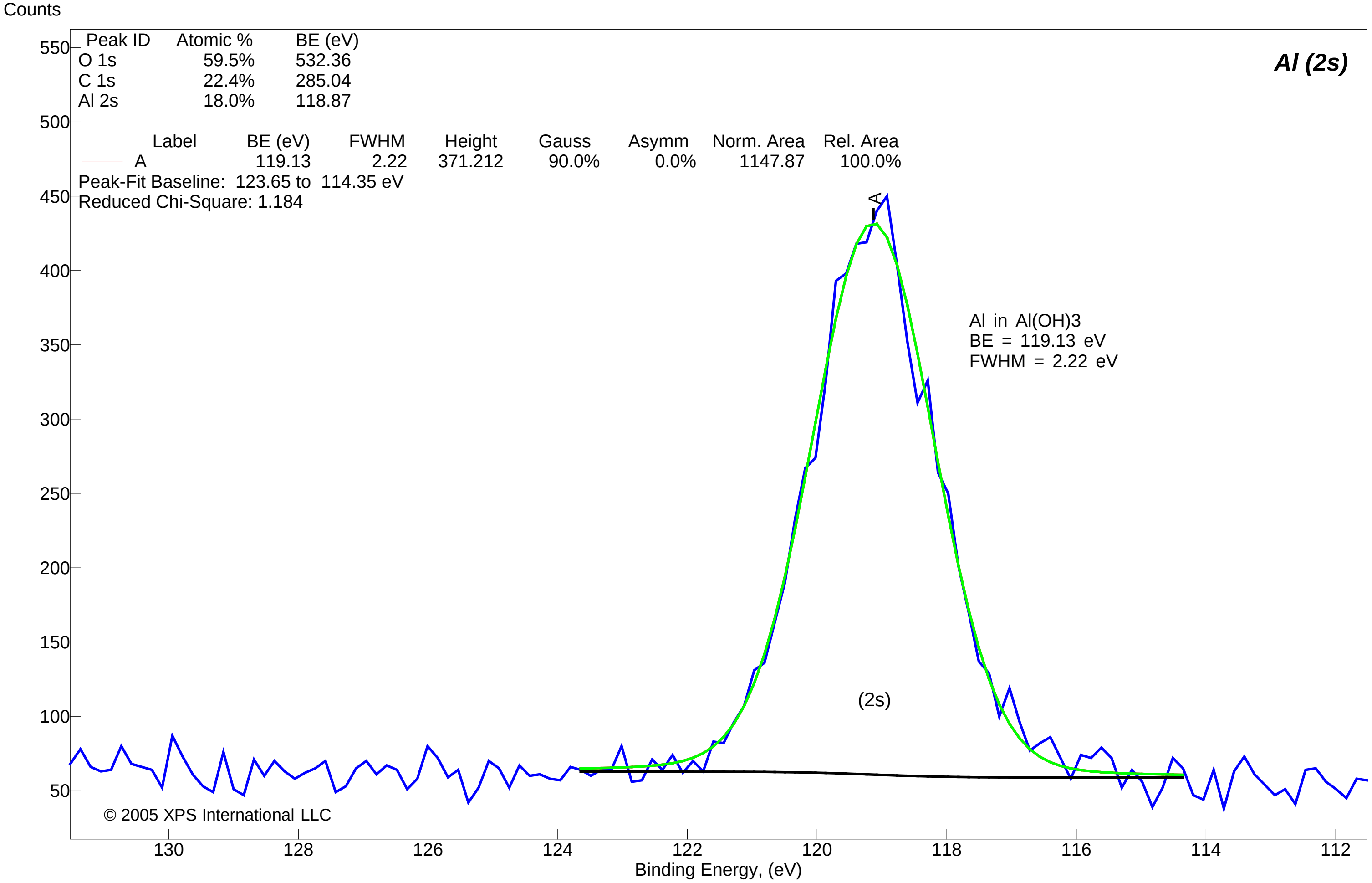
Peak ID	Atomic %	BE (eV)
O 1s	59.5%	532.36
C 1s	22.4%	285.04
Al 2s	18.0%	118.87

	Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
—	A	4.90	1.87	155.6	90.0%	0.0%	203.193	15.4%
—	B	6.38	2.08	240.85	90.0%	0.0%	348.905	26.4%
—	C	8.12	2.01	198.192	90.0%	0.0%	277.978	21.0%
—	D	10.08	1.97	232.349	90.0%	0.0%	318.777	24.1%
—	E	12.06	1.74	142.216	90.0%	0.0%	172.577	13.1%

Peak-Fit Baseline: 15.87 to -0.01 eV
Reduced Chi-Square: 1.271

Aluminum (III) Hydroxide (FW = 78.00)

Sample Description: ALUMINUM HYDROXIDE (Al(OH)3) powder/tape (no mesh)
TECHNICAL GRADE, PERFECT PARTS CHEMICAL CO.



Aluminum (III) Oxy-hydroxide (FW = 59.99)
Surface Composition Table

Description: AlOOH (Diaspore, Al_2O_3-H_2O) a natural mineral, analyzed at 90 deg TOA, mesh at 1 mm, non-conductive white, freshly fractured in air

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
C 2s	24.2	24.2	0.15	1.4	2,945	
Al 2p	75.0	75.0	0.54	1.4	6,323	
Al KLL-1	99.4	99.4	0.22	1.4	2,556	
Al 2s	119.9	119.9	0.75	1.4	9,912	24.8%
Al loss	144.4	144.4	0.00	1.4	4,440	
C 1s	286.1	286.1	1.00	1.4	11,569	26.1%
C loss	303.7	303.7	0.00	1.4	1,695	
O 1s	532.5	532.5	2.93	1.4	46,298	49.1%
O loss	555.9	555.9	0.00	1.4	25,489	
O loss	581.3	581.3	0.00	1.4	1,853	
O KLL-1	979.2	979.2	0.70	1.4	6,850	

AlOOH

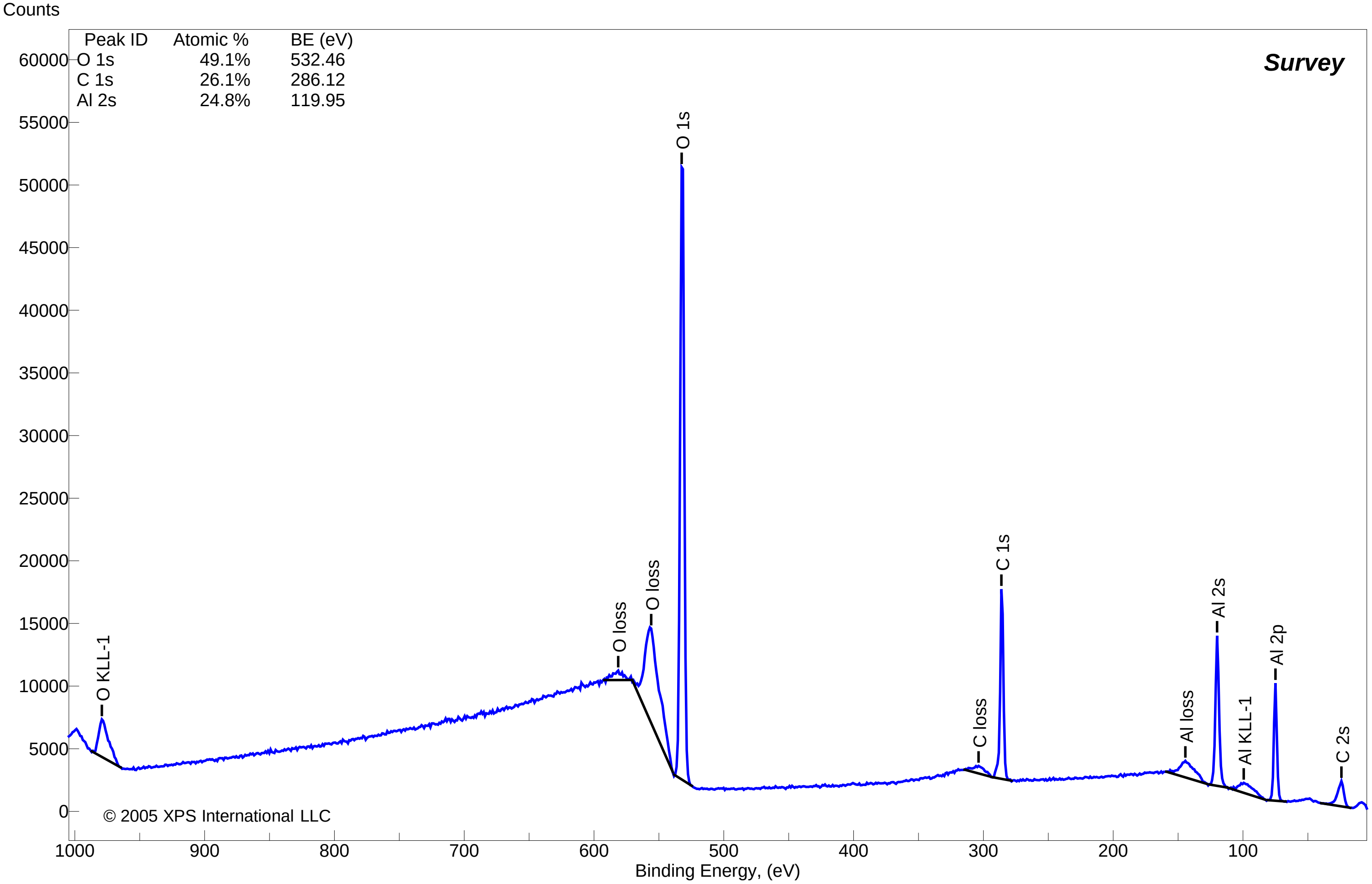
Diaspore

AlOOH

Diaspore

Aluminum (III) Oxy-hydroxide (FW = 59.99)

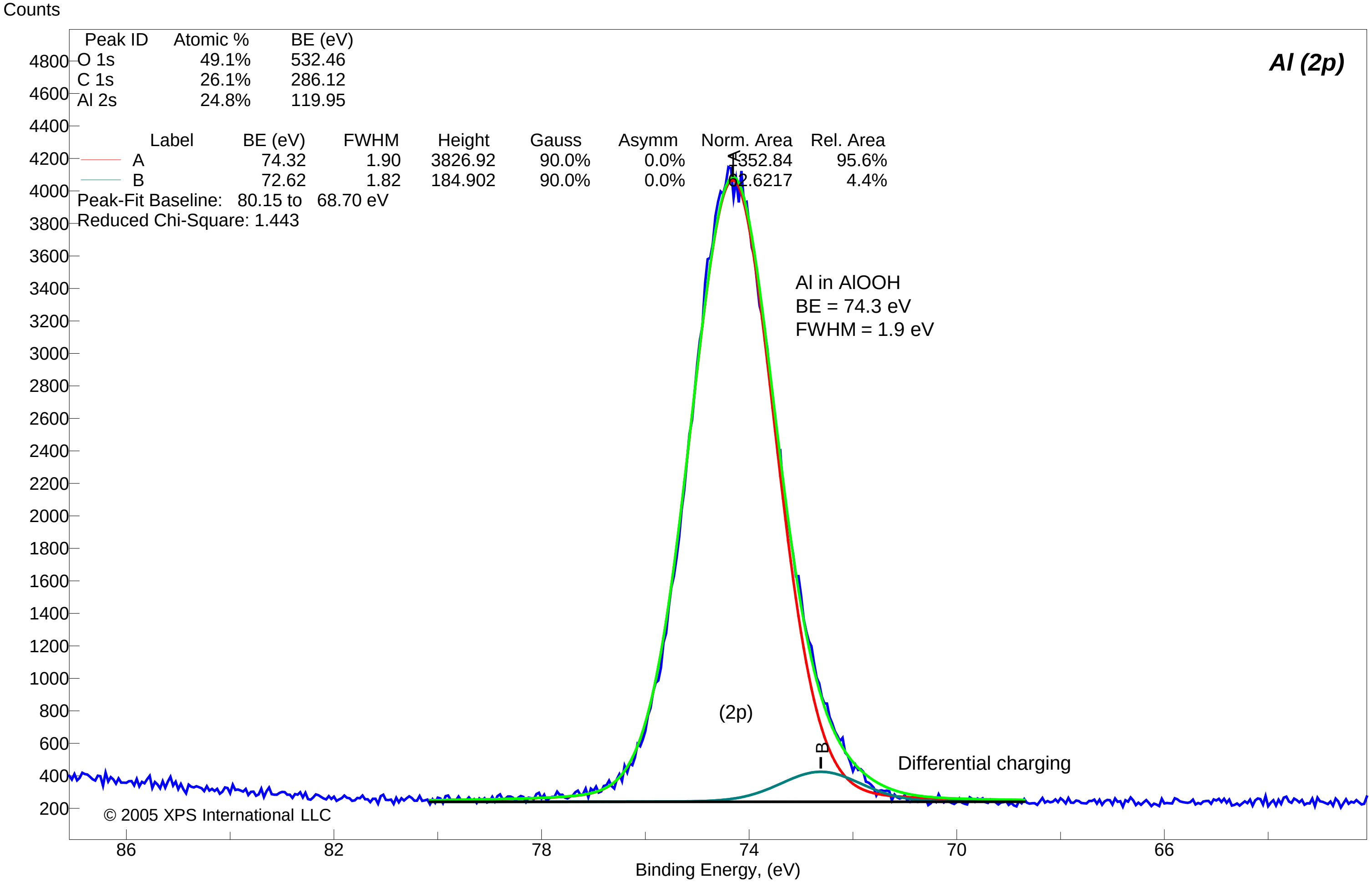
Sample Description: AlOOH (Diaspore, Al2O3-H2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive
white, freshly fractured in air, mp xxx, d xxx



Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

Aluminum (III) Oxy-hydroxide (FW = 59.99)

Sample Description: AlOOH (Diaspore, Al2O3-H2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive white, freshly fractured in air, mp xxx, d xxx



Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	74.32	1.90	3826.92	90.0%	0.0%	1352.84	95.6%
B	72.62	1.82	184.902	90.0%	0.0%	62.6217	4.4%

Peak-Fit Baseline: 80.15 to 68.70 eV
Reduced Chi-Square: 1.443

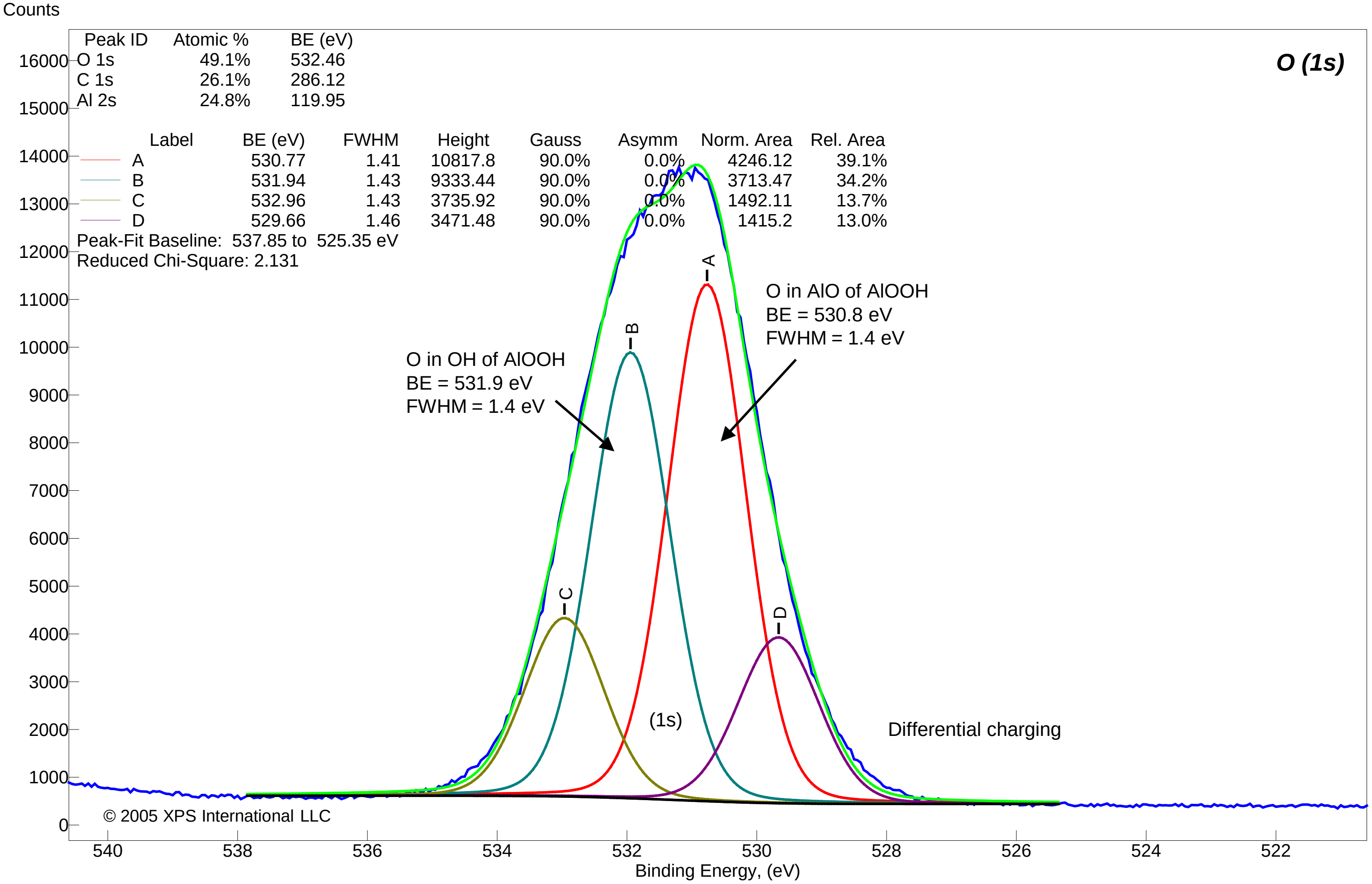
Al (2p)

Al in AlOOH
BE = 74.3 eV
FWHM = 1.9 eV

Differential charging

Aluminum (III) Oxy-hydroxide (FW = 59.99)

Sample Description: AlOOH (Diaspore, Al2O3-H2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive
white, freshly fractured in air, mp xxx, d xxx



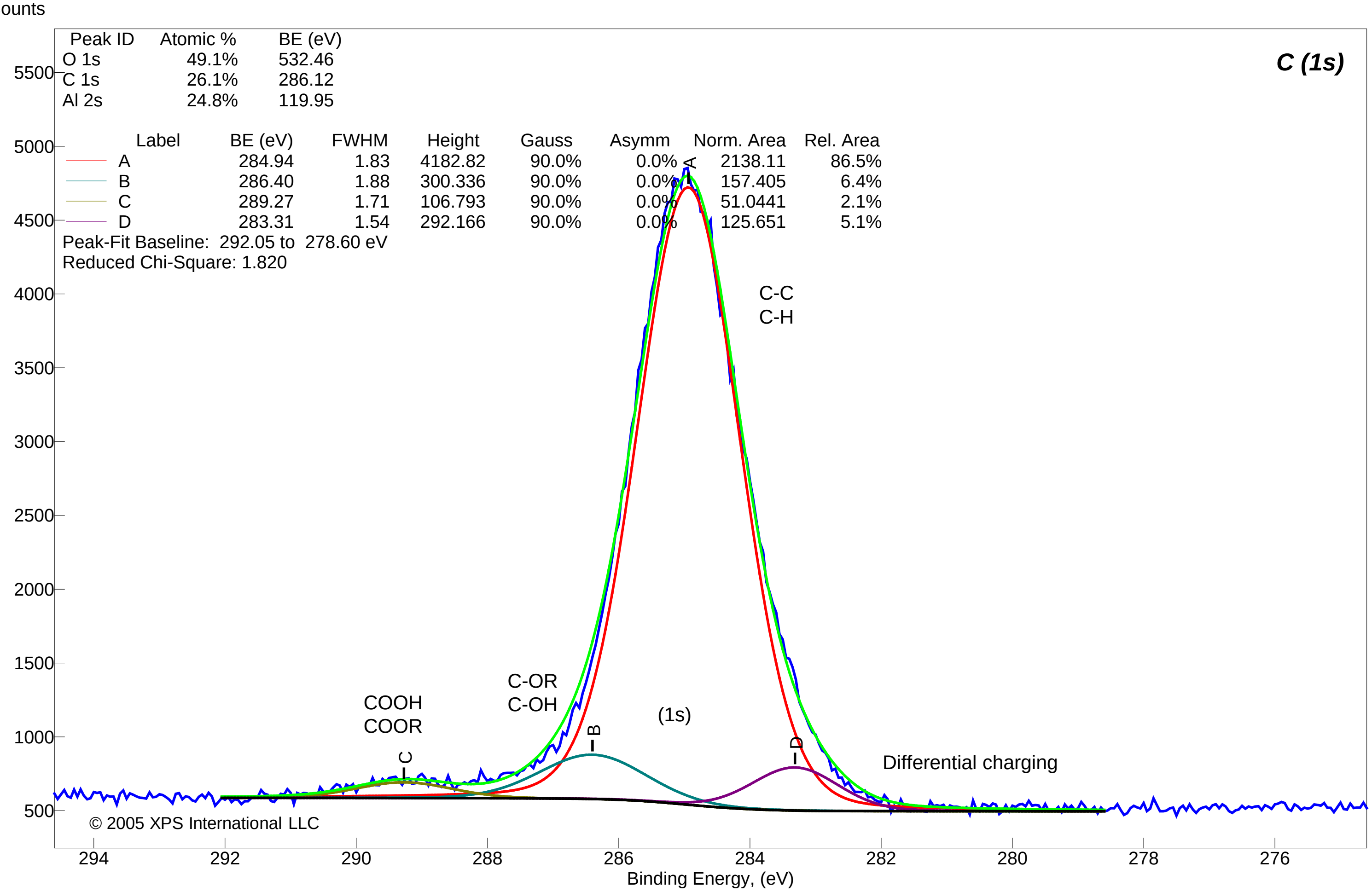
Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	530.77	1.41	10817.8	90.0%	0.0%	4246.12	39.1%
B	531.94	1.43	9333.44	90.0%	0.0%	3713.47	34.2%
C	532.96	1.43	3735.92	90.0%	0.0%	1492.11	13.7%
D	529.66	1.46	3471.48	90.0%	0.0%	1415.2	13.0%

Peak-Fit Baseline: 537.85 to 525.35 eV
Reduced Chi-Square: 2.131

Aluminum (III) Oxy-hydroxide (FW = 59.99)

Sample Description: AlOOH (Diaspore, Al2O3-H2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive white, freshly fractured in air, mp xxx, d xxx



Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	284.94	1.83	4182.82	90.0%	0.0%	2138.11	86.5%
B	286.40	1.88	300.336	90.0%	0.0%	157.405	6.4%
C	289.27	1.71	106.793	90.0%	0.0%	51.0441	2.1%
D	283.31	1.54	292.166	90.0%	0.0%	125.651	5.1%

Peak-Fit Baseline: 292.05 to 278.60 eV
Reduced Chi-Square: 1.820

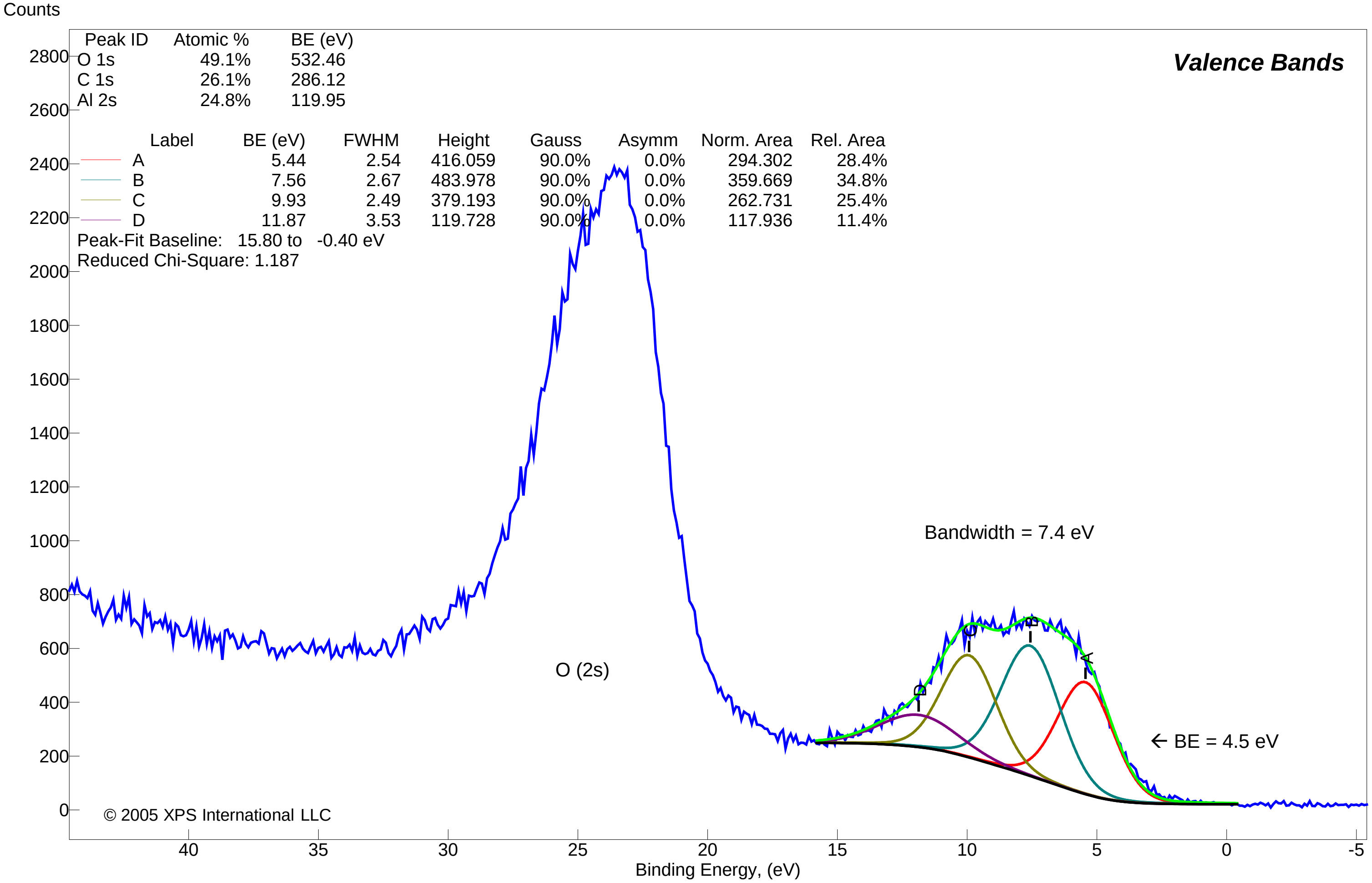
AlOOH

Diaspore

AlOOH
Diaspore

Aluminum (III) Oxy-hydroxide (FW = 59.99)

Sample Description: AlOOH (Diaspore, Al_2O_3-H_2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive white, freshly fractured in air, mp xxx, d xxx



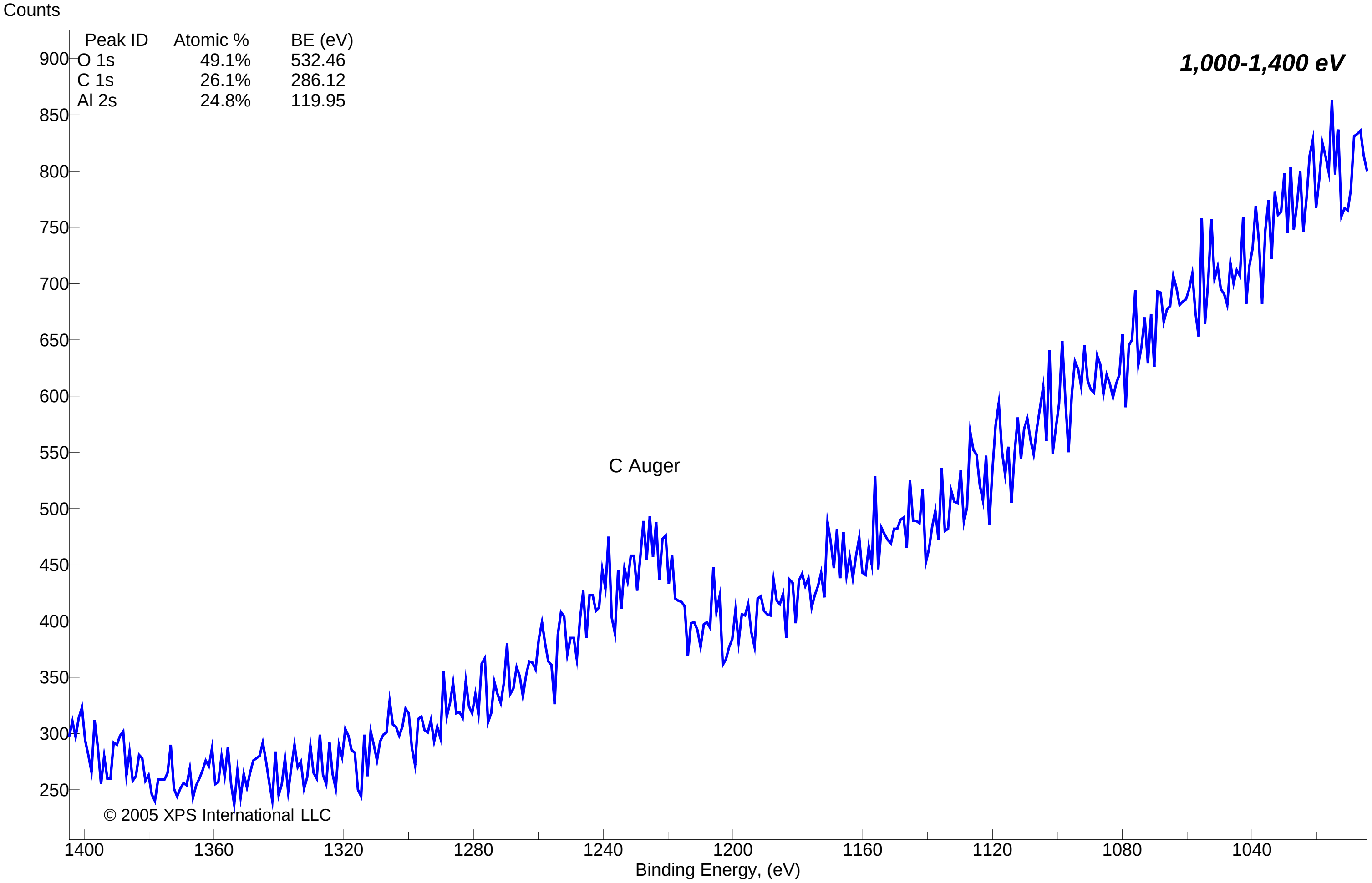
Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	5.44	2.54	416.059	90.0%	0.0%	294.302	28.4%
B	7.56	2.67	483.978	90.0%	0.0%	359.669	34.8%
C	9.93	2.49	379.193	90.0%	0.0%	262.731	25.4%
D	11.87	3.53	119.728	90.0%	0.0%	117.936	11.4%

Peak-Fit Baseline: 15.80 to -0.40 eV
Reduced Chi-Square: 1.187

Aluminum (III) Oxy-hydroxide (FW = 59.99)

Sample Description: AlOOH (Diaspore, Al_2O_3-H_2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive white, freshly fractured in air, mp xxx, d xxx



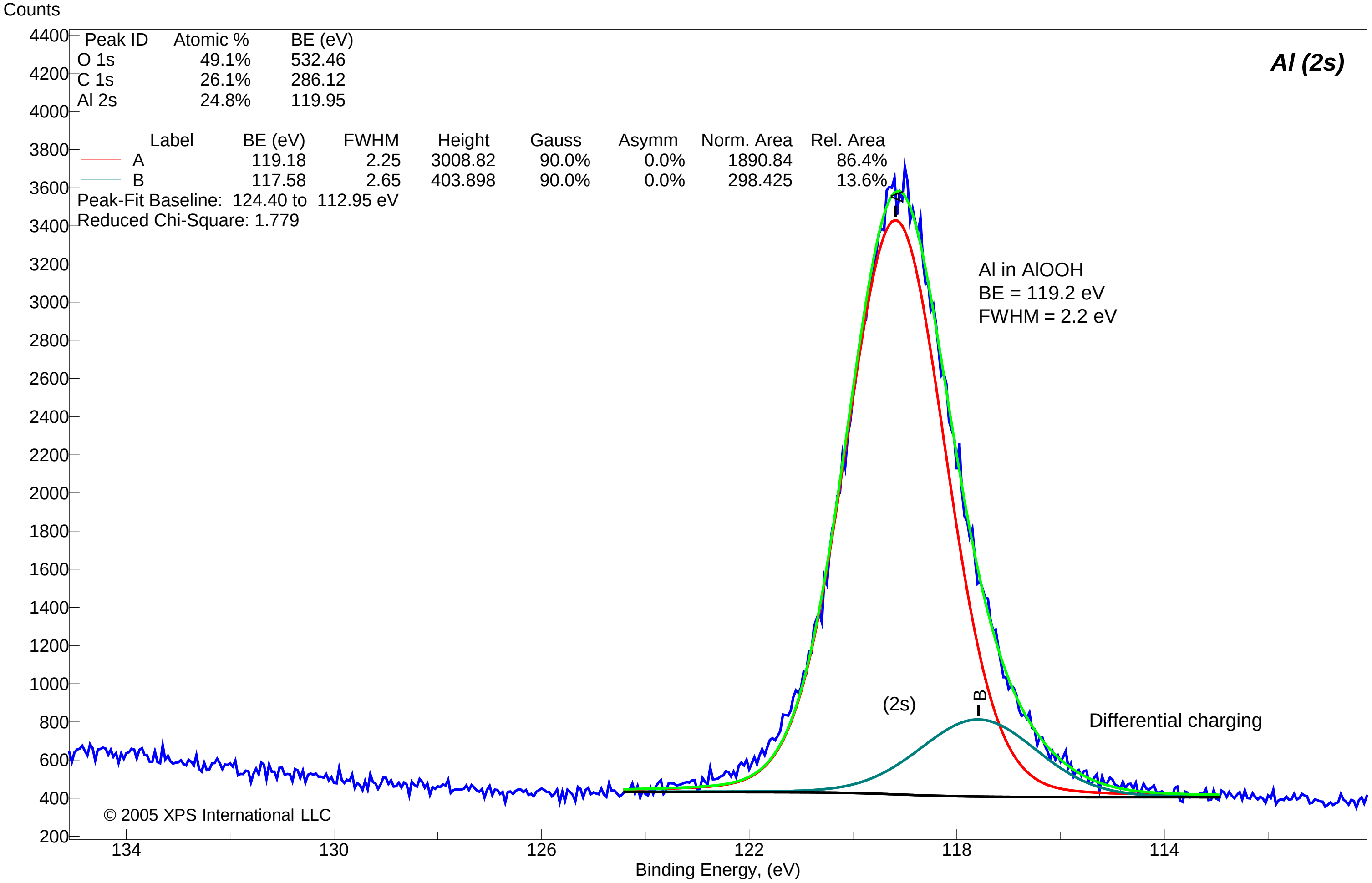
Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

AlOOH
Diaspore

AlOOH
Diaspore

Aluminum (III) Oxy-hydroxide   (FW = 59.99)

Sample Description: AlOOH (Diaspore, Al_2O_3-H_2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive
white, freshly fractured in air, mp xxx, d xxx



Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	119.18	2.25	3008.82	90.0%	0.0%	1890.84	86.4%
B	117.58	2.65	403.898	90.0%	0.0%	298.425	13.6%

Peak-Fit Baseline: 124.40 to 112.95 eV
Reduced Chi-Square: 1.779

Al in AlOOH
BE = 119.2 eV
FWHM = 2.2 eV

(2s)

Differential charging

AlOOH

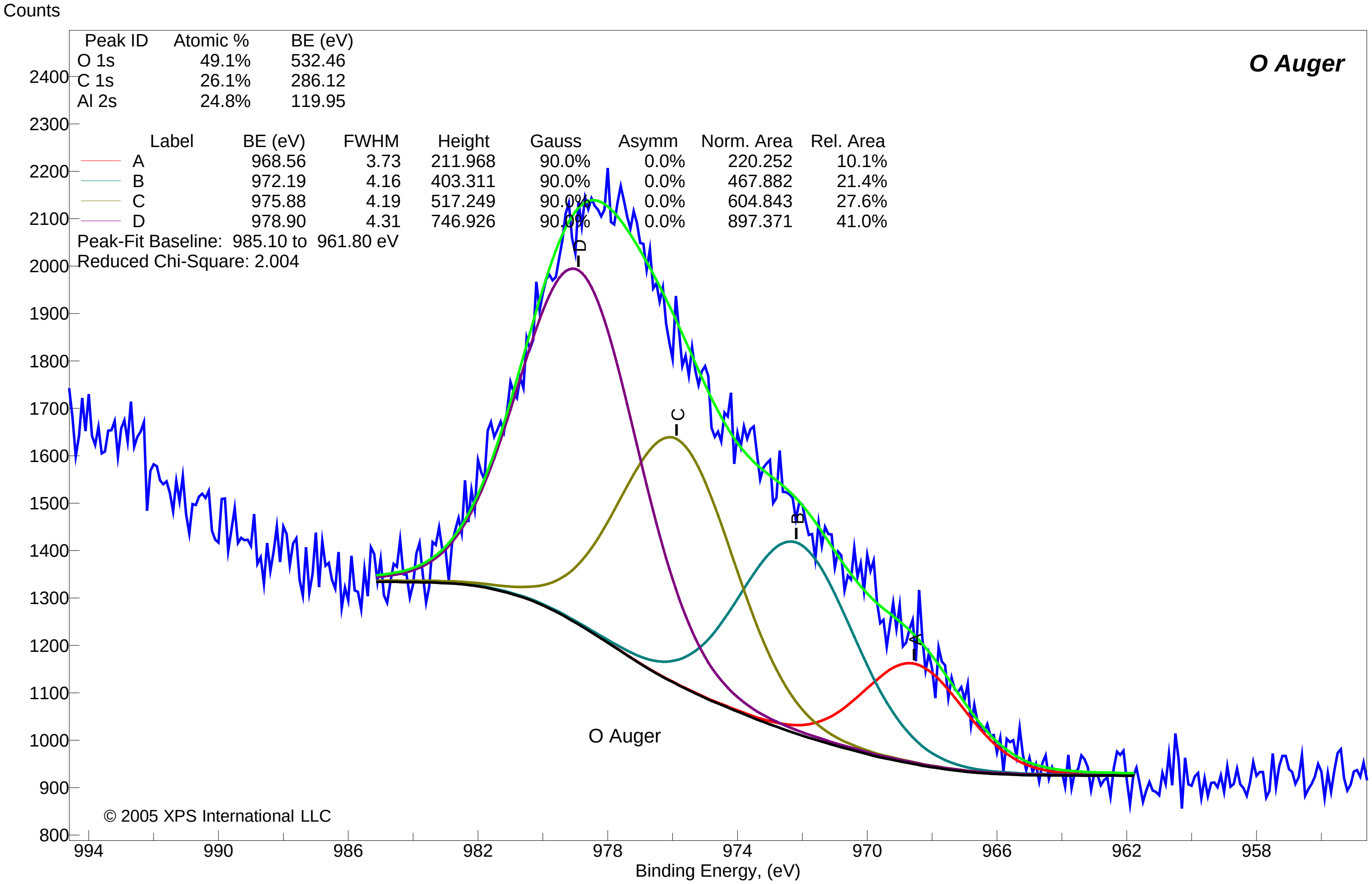
Diaspore

AlOOH

Diaspore

Aluminum (III) Oxy-hydroxide   (FW = 59.99)

Sample Description: AlOOH (Diaspore, Al2O3-H2O), analyzed at 90 deg TOA, mesh at 1 mm, non-conductive
white, freshly fractured in air, mp xxx, d xxx



Peak ID	Atomic %	BE (eV)
O 1s	49.1%	532.46
C 1s	26.1%	286.12
Al 2s	24.8%	119.95

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
— A	968.56	3.73	211.968	90.0%	0.0%	220.252	10.1%
— B	972.19	4.16	403.311	90.0%	0.0%	467.882	21.4%
— C	975.88	4.19	517.249	90.0%	0.0%	604.843	27.6%
— D	978.90	4.31	746.926	90.0%	0.0%	897.371	41.0%

Peak-Fit Baseline: 985.10 to 961.80 eV
Reduced Chi-Square: 2.004

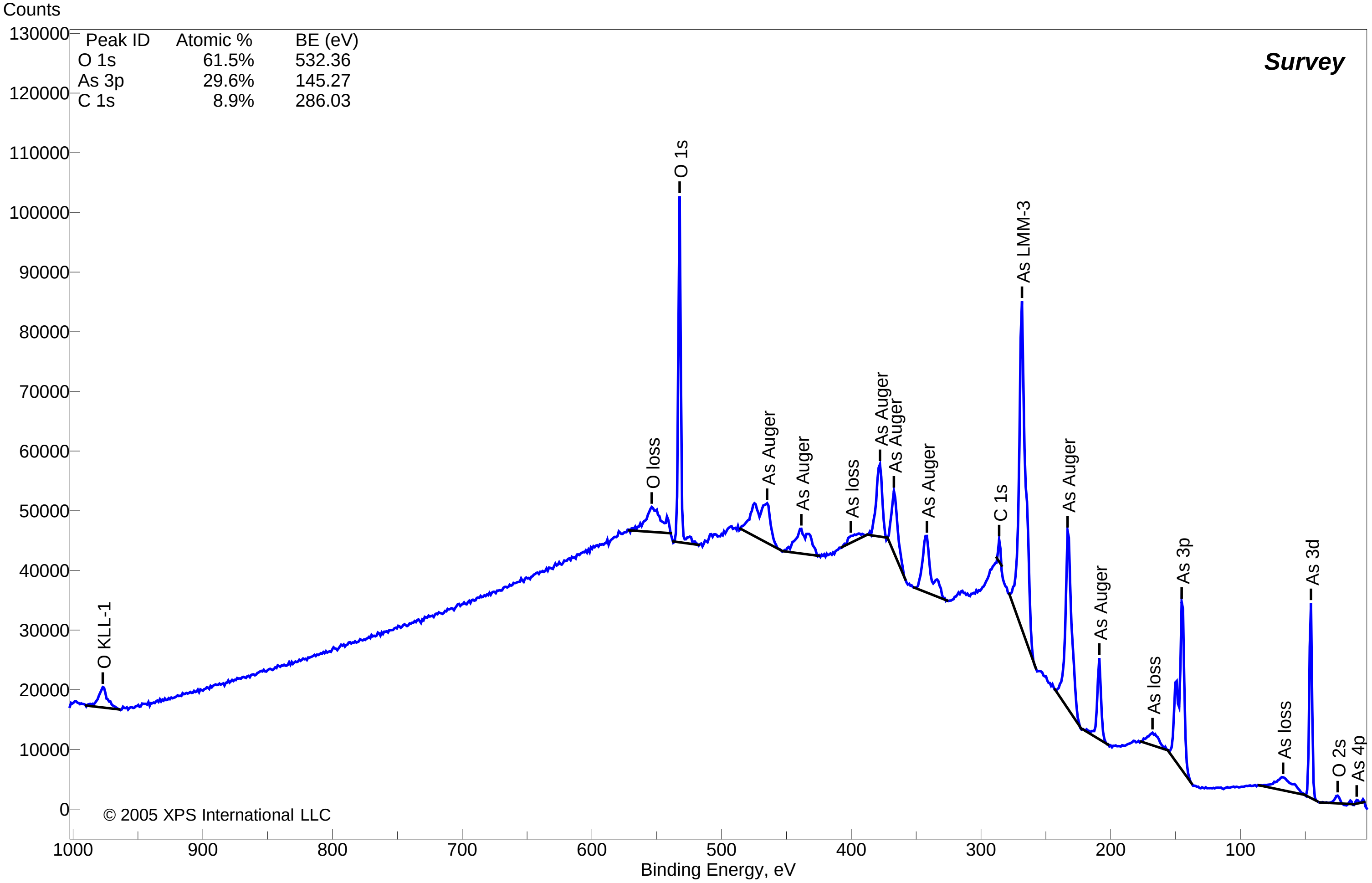
Arsenic (III) Oxide (FW = 197.84)
Surface Composition Table

Description: As_2O_3 (99.995%) from Aldrich Lot# 04445CW, analyzed at 90 deg TOA, mesh at 1mm, non-conductive white powder pressed into 3 mm pellet, mp 312 C, d 3.7, sol in boiling water, HCl, insol. in alcohol

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
As 4p	10.4	10.4	0.12	1.4	1,945	
O 2s	25.0	25.0	0.14	1.4	6,487	
As 3d	45.6	45.6	1.82	1.4	68,690	
As loss	67.1	67.1	0.00	1.4	29,942	
As 3p	145.3	145.3	4.07	1.4	128,540	29.6%
As loss	167.8	167.8	0.00	1.4	17,059	
As Auger	208.8	208.8	0.00	1.4	39,047	
As Auger	233.2	233.2	0.00	1.4	145,382	
As LMM-3	268.4	268.4	0.40	1.4	270,869	
C 1s	286.0	286.0	1.00	1.4	8,106	8.9%
As Auger	341.7	341.7	0.00	1.4	62,610	
As Auger	367.2	367.2	0.00	1.4	48,861	
As Auger	377.9	377.9	0.00	1.4	54,150	
As loss	400.4	400.4	0.00	1.4	10,545	
As Auger	438.5	438.5	0.00	1.4	45,111	
As Auger	464.9	464.9	0.00	1.4	82,310	
O 1s	532.4	532.4	2.93	1.4	119,613	61.5%
O loss	553.9	553.9	0.00	1.4	51,082	
O KLL-1	977.1	977.1	0.70	1.4	25,155	

Arsenic (III) Oxide (FW = 197.84)

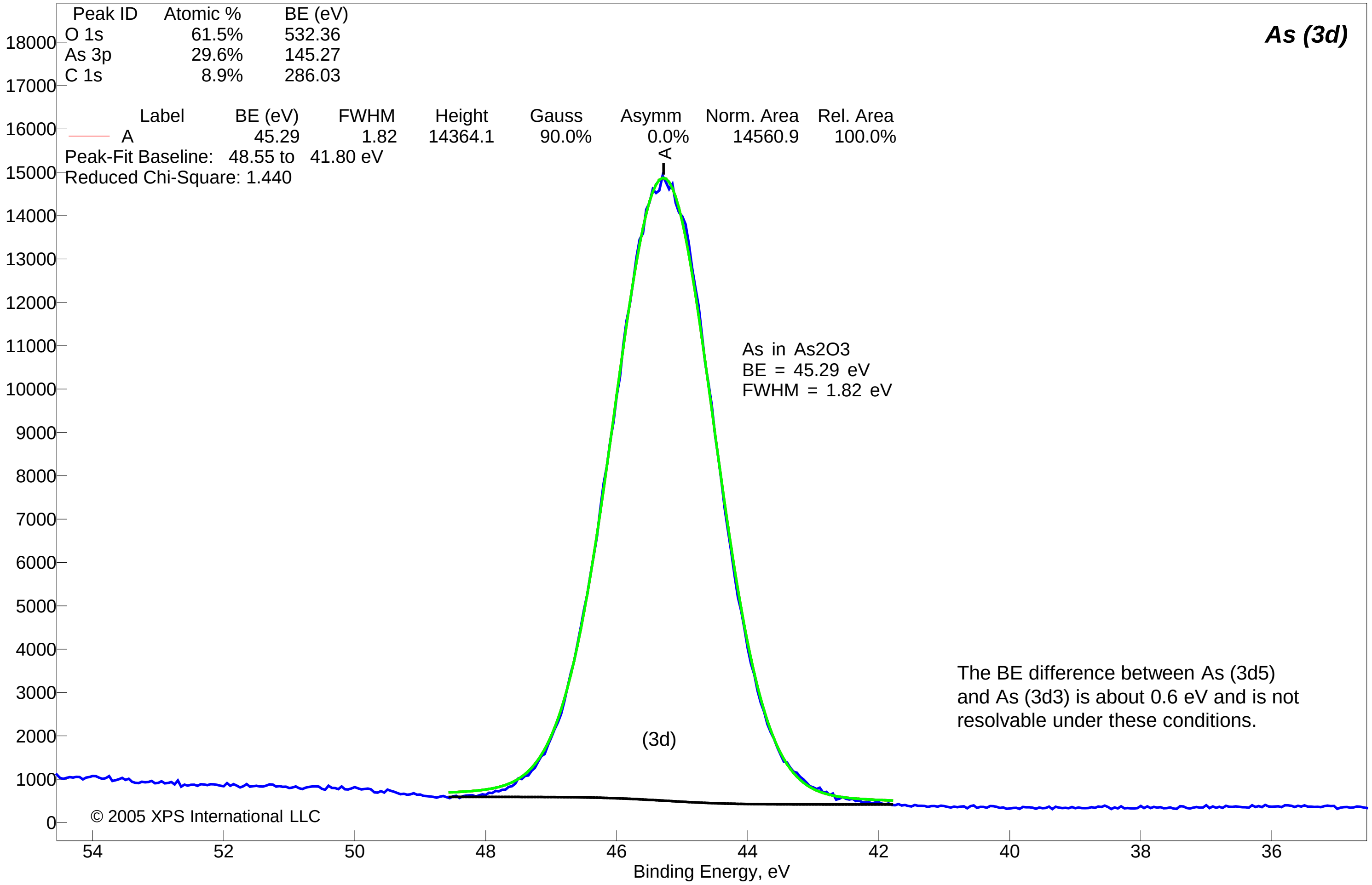
Sample Description: As2O3 (99.995%) from Aldrich lot# 04445CW
pressed into 3 mm pellet, analyzed at 90 deg TOA, mesh-screen at 1 mm height



Peak ID	Atomic %	BE (eV)
O 1s	61.5%	532.36
As 3p	29.6%	145.27
C 1s	8.9%	286.03

Arsenic (III) Oxide (FW = 197.84)

Sample Description: As2O3 99.995% Aldr# 04445CW 3mm plt 90 TOA mesh



Peak ID	Atomic %	BE (eV)
O 1s	61.5%	532.36
As 3p	29.6%	145.27
C 1s	8.9%	286.03

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	45.29	1.82	14364.1	90.0%	0.0%	14560.9	100.0%

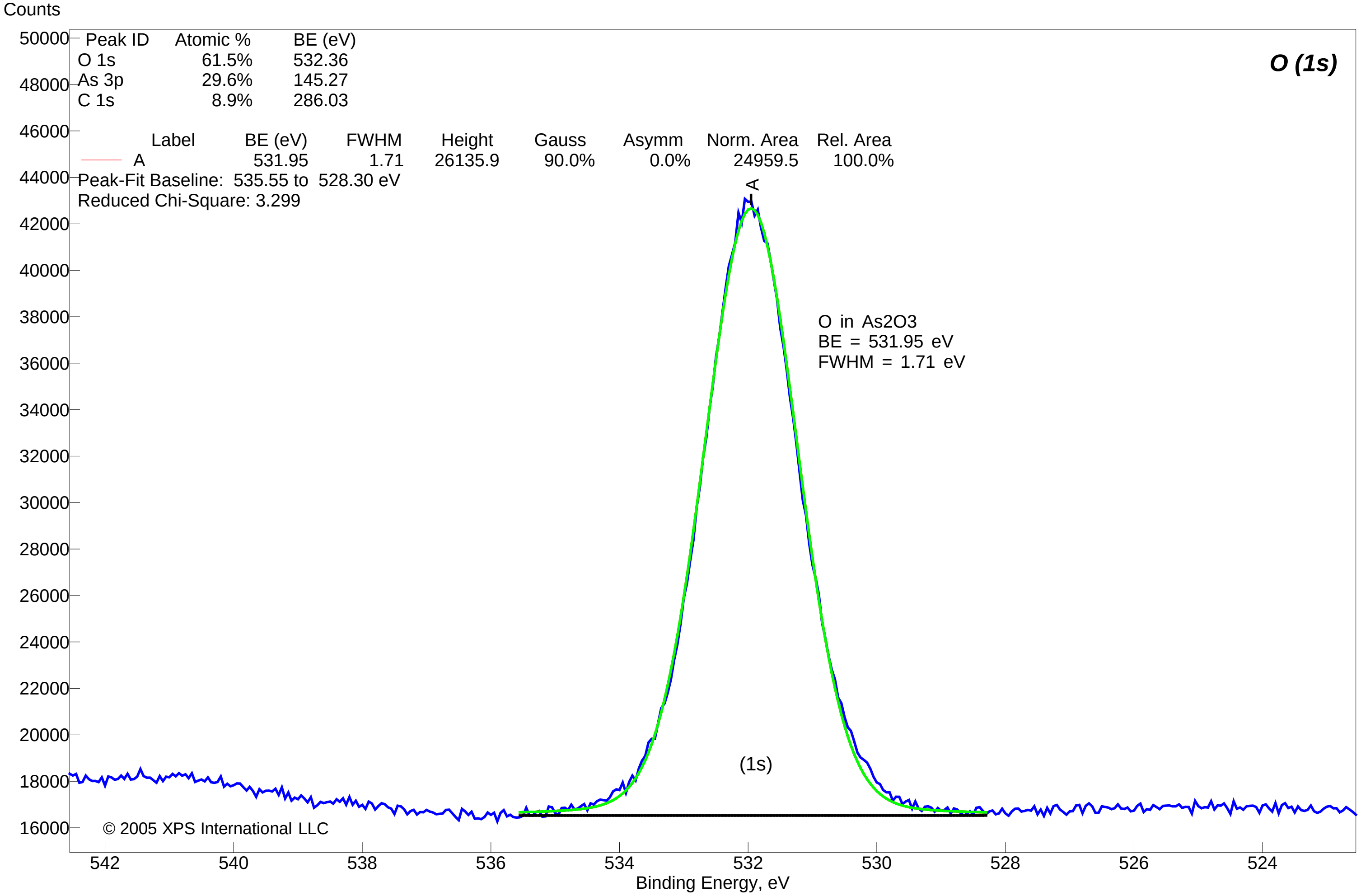
Peak-Fit Baseline: 48.55 to 41.80 eV
Reduced Chi-Square: 1.440

As in As2O3
BE = 45.29 eV
FWHM = 1.82 eV

The BE difference between As (3d5) and As (3d3) is about 0.6 eV and is not resolvable under these conditions.

Arsenic (III) Oxide (FW = 197.84)

Sample Description: As2O3 99.995% Aldr# 04445CW 3mm plt 90 TOA mesh



Peak ID	Atomic %	BE (eV)
O 1s	61.5%	532.36
As 3p	29.6%	145.27
C 1s	8.9%	286.03

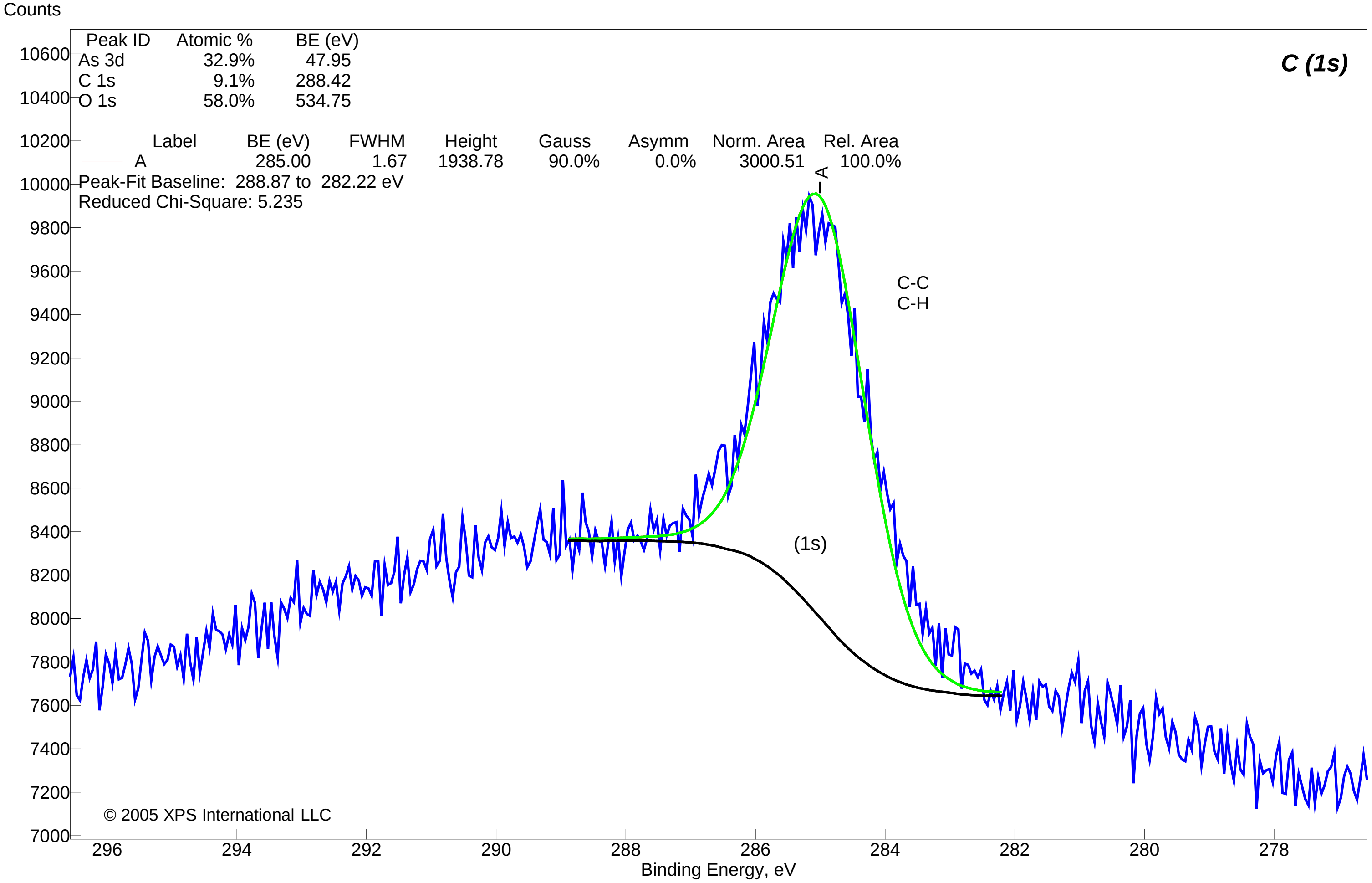
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	531.95	1.71	26135.9	90.0%	0.0%	24959.5	100.0%

Peak-Fit Baseline: 535.55 to 528.30 eV
Reduced Chi-Square: 3.299

O in As2O3
BE = 531.95 eV
FWHM = 1.71 eV

Arsenic (III) Oxide (FW = 197.84)

Sample Description: As2O3 99.995% Aldrich Chem. Co. Lot# 04445CW
3mm pellet, 90 TOA, mesh



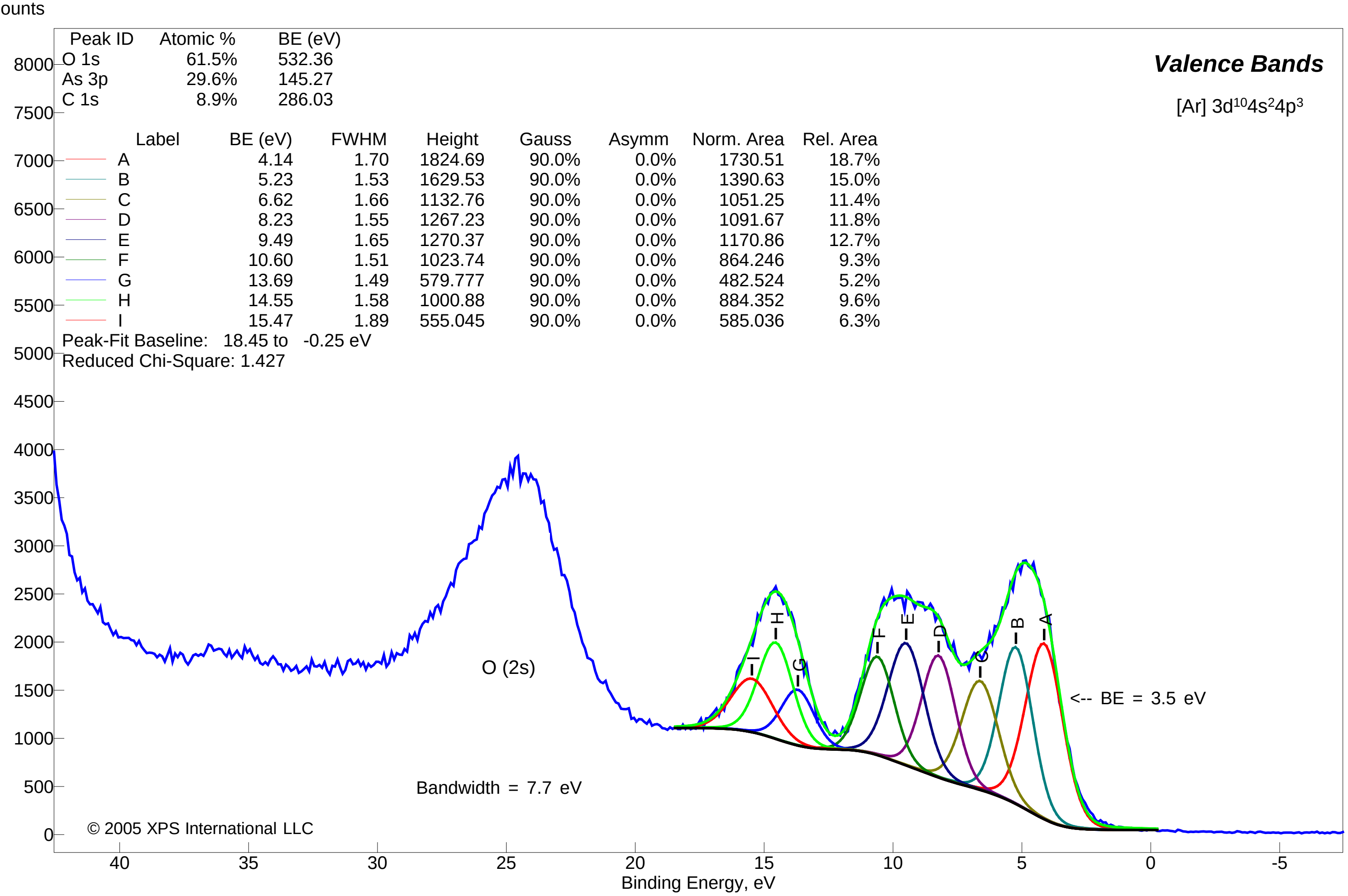
Peak ID	Atomic %	BE (eV)
As 3d	32.9%	47.95
C 1s	9.1%	288.42
O 1s	58.0%	534.75

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	285.00	1.67	1938.78	90.0%	0.0%	3000.51	100.0%

Peak-Fit Baseline: 288.87 to 282.22 eV
Reduced Chi-Square: 5.235

Arsenic (III) Oxide (FW = 197.84)

Sample Description: As2O3 99.995% Aldr# 04445CW 3mm plt 90 TOA mesh



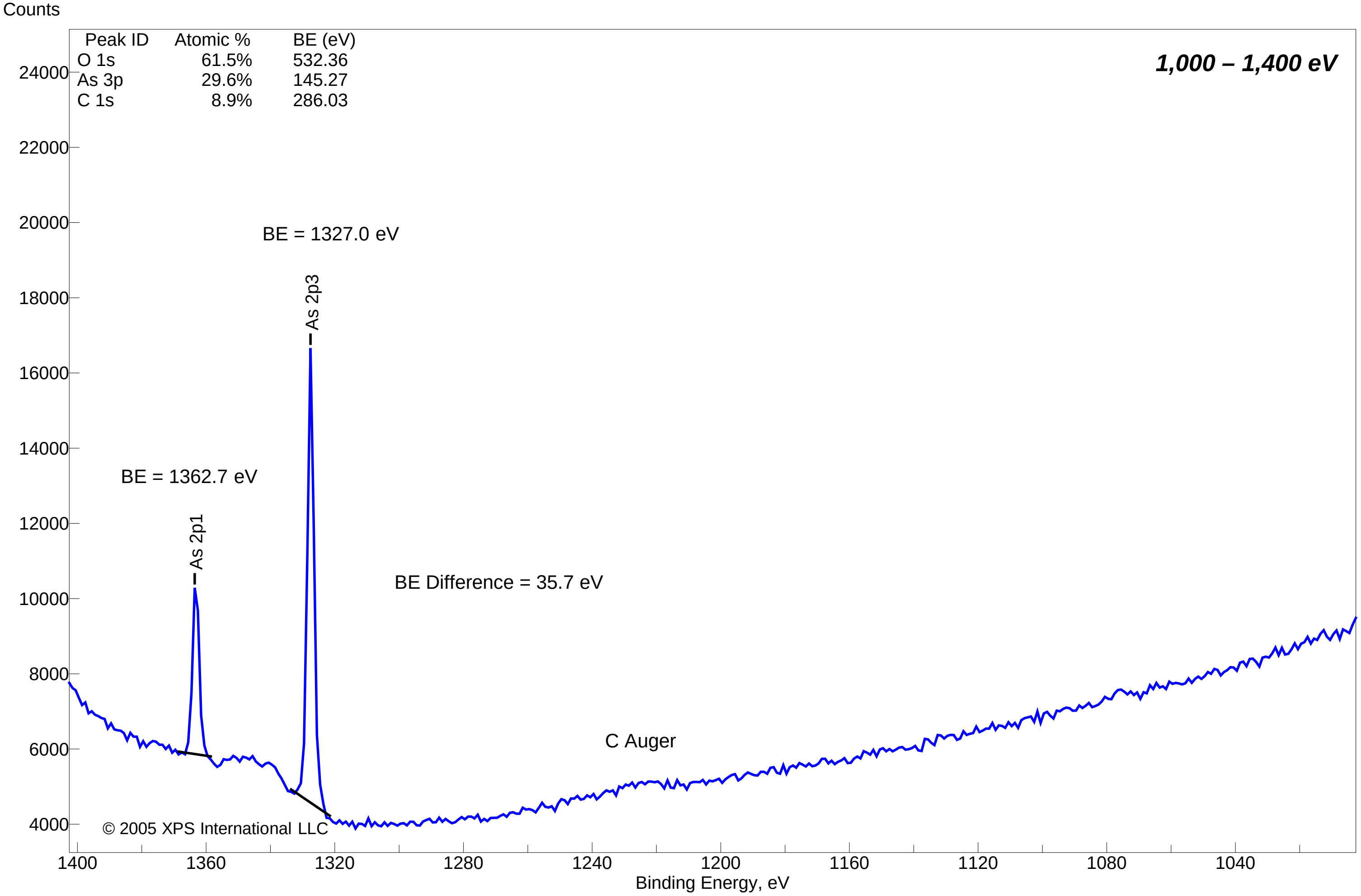
Peak ID	Atomic %	BE (eV)
O 1s	61.5%	532.36
As 3p	29.6%	145.27
C 1s	8.9%	286.03

	Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
—	A	4.14	1.70	1824.69	90.0%	0.0%	1730.51	18.7%
—	B	5.23	1.53	1629.53	90.0%	0.0%	1390.63	15.0%
—	C	6.62	1.66	1132.76	90.0%	0.0%	1051.25	11.4%
—	D	8.23	1.55	1267.23	90.0%	0.0%	1091.67	11.8%
—	E	9.49	1.65	1270.37	90.0%	0.0%	1170.86	12.7%
—	F	10.60	1.51	1023.74	90.0%	0.0%	864.246	9.3%
—	G	13.69	1.49	579.777	90.0%	0.0%	482.524	5.2%
—	H	14.55	1.58	1000.88	90.0%	0.0%	884.352	9.6%
—	I	15.47	1.89	555.045	90.0%	0.0%	585.036	6.3%

Peak-Fit Baseline: 18.45 to -0.25 eV
Reduced Chi-Square: 1.427

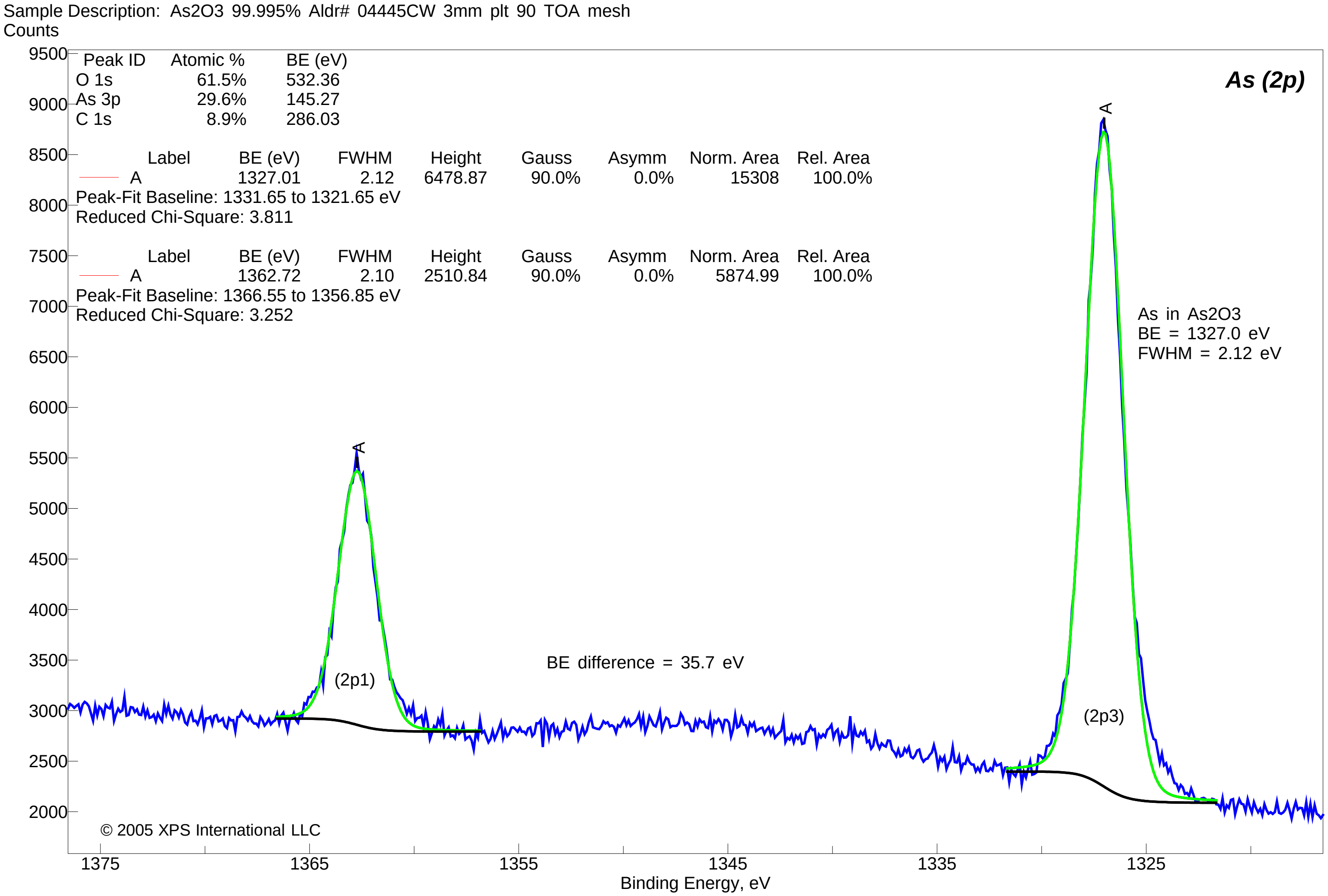
Arsenic (III) Oxide (FW = 197.84)

Sample Description: As2O3 99.995% Aldr# 04445CW 3mm plt 90 TOA mesh



Peak ID	Atomic %	BE (eV)
O 1s	61.5%	532.36
As 3p	29.6%	145.27
C 1s	8.9%	286.03

Arsenic (III) Oxide (FW = 197.84)



Sample Description: As2O3 99.995% Aldr# 04445CW 3mm plt 90 TOA mesh

Peak ID	Atomic %	BE (eV)
O 1s	61.5%	532.36
As 3p	29.6%	145.27
C 1s	8.9%	286.03

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	1327.01	2.12	6478.87	90.0%	0.0%	15308	100.0%

Peak-Fit Baseline: 1331.65 to 1321.65 eV
Reduced Chi-Square: 3.811

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	1362.72	2.10	2510.84	90.0%	0.0%	5874.99	100.0%

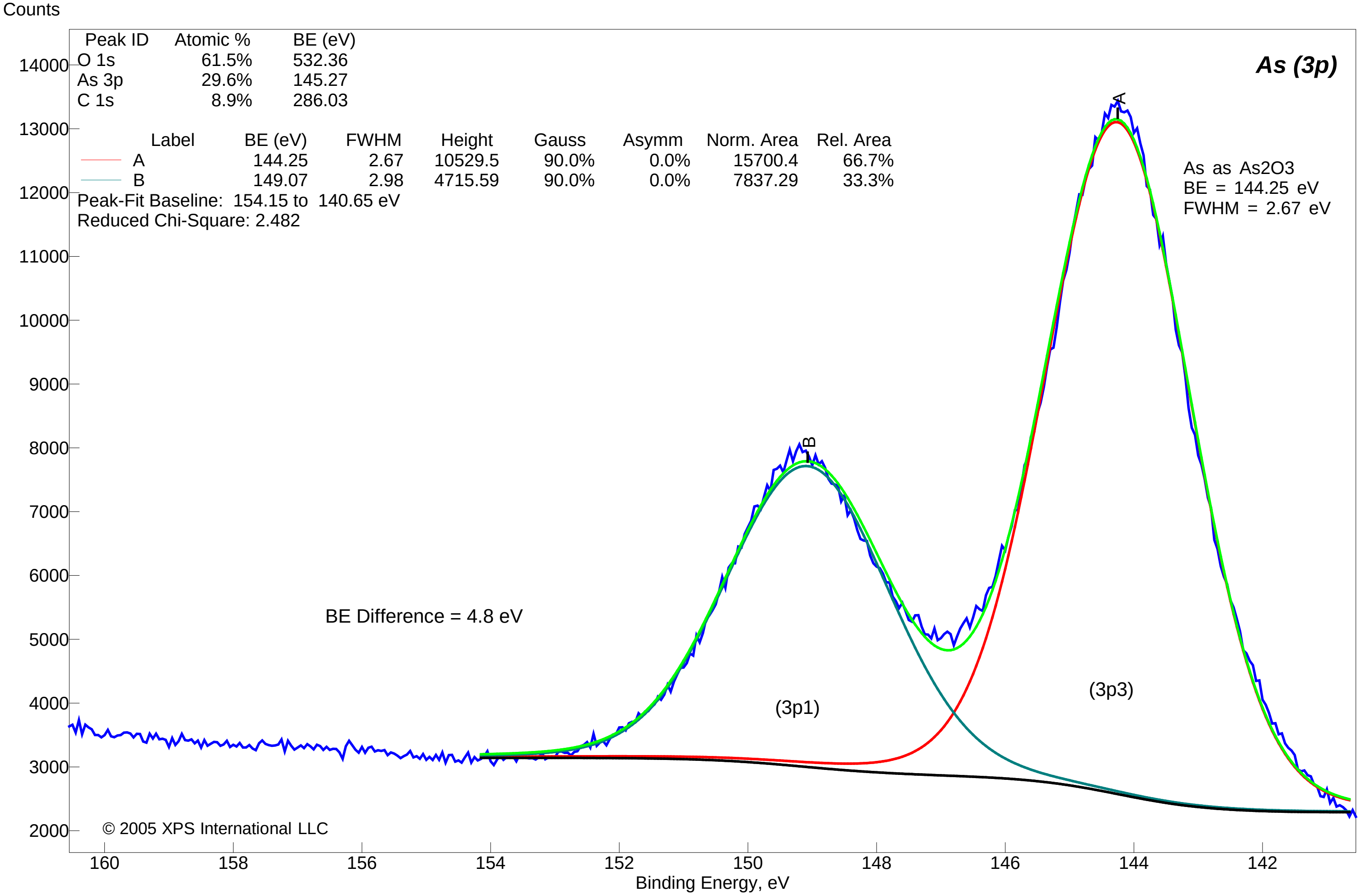
Peak-Fit Baseline: 1366.55 to 1356.85 eV
Reduced Chi-Square: 3.252

As in As2O3
BE = 1327.0 eV
FWHM = 2.12 eV

BE difference = 35.7 eV

Arsenic (III) Oxide (FW = 197.84)

Sample Description: As2O3 99.995% Aldr# 04445CW 3mm plt 90 TOA mesh



Peak ID	Atomic %	BE (eV)
O 1s	61.5%	532.36
As 3p	29.6%	145.27
C 1s	8.9%	286.03

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	144.25	2.67	10529.5	90.0%	0.0%	15700.4	66.7%
B	149.07	2.98	4715.59	90.0%	0.0%	7837.29	33.3%

Peak-Fit Baseline: 154.15 to 140.65 eV
Reduced Chi-Square: 2.482

As as As2O3
BE = 144.25 eV
FWHM = 2.67 eV

BE Difference = 4.8 eV

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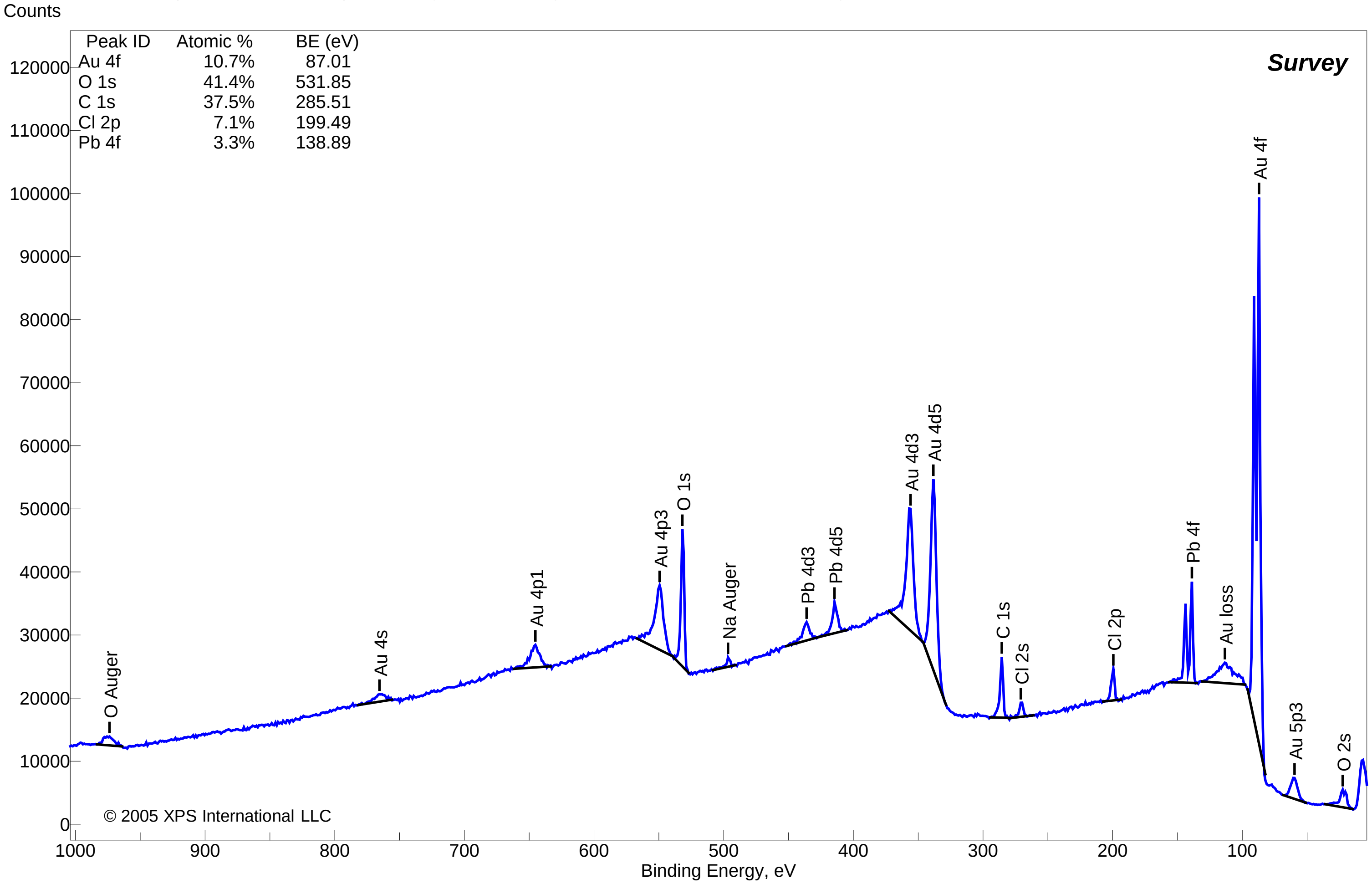
Gold (III) Oxide (FW = 441.93)
Surface Composition Table

Description: Au_2O_3 (Au 86%) from Aldrich Lot# 00306AW, analyzed at 90 deg TOA, mesh at 1mm, semi-conductive brown powder, pressed into 3 mm pellet, mp 150 C dec., sol in HCl, HNO_3

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
O 2s	22.6	22.6	0.14	1.5	15,712	
Au 5p3	59.7	59.7	1.10	1.5	17,360	
Au 4f	87.0	87.0	17.12	1.1	68,640	10.7%
Au loss	113.5	113.5	0.00	1.5	42,102	
Pb 4f	138.9	138.9	22.74	1.5	58,144	3.3%
Cl 2p	199.5	199.5	2.28	1.5	11,661	7.1%
Cl 2s	270.9	270.9	1.69	1.5	8,850	
C 1s	285.5	285.5	1.00	1.5	24,448	37.5%
Au 4d5	338.3	338.3	11.74	1.5	137,776	
Au 4d3	355.9	355.9	8.06	1.5	115,235	
Pb 4d5	414.5	414.5	13.02	1.5	20,249	
Pb 4d3	436.1	436.1	8.87	1.5	15,737	
Na Auger	496.7	496.7	0.00	1.5	5,574	
O 1s	531.8	531.8	2.93	1.5	56,013	41.4%
Au 4p3	549.4	549.4	5.89	1.5	72,433	
Au 4p1	645.2	645.2	2.14	1.5	25,057	
Au 4s	765.5	765.5	1.92	1.5	12,209	
O Auger	973.7	973.7	0.00	1.5	11,355	

Gold (III) Oxide (FW = 441.93)

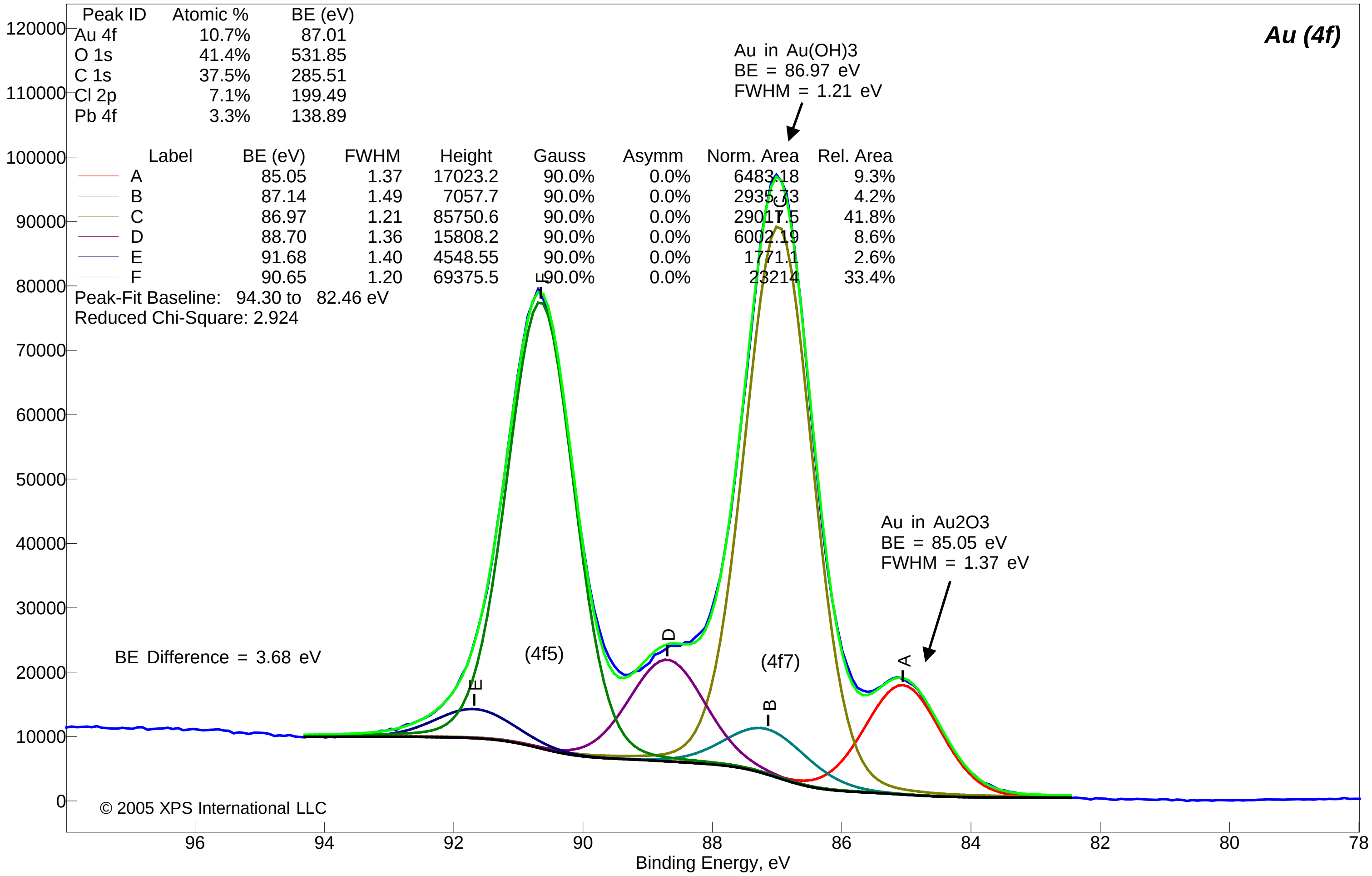
Sample Description: Au2O3 (Au 86%) from Aldrich Lot# 00306AW, Semi-Conductive
pressed into 3 mm pellet, analyzed at 90 deg TOA, mesh-screen at 1 mm height



Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

Gold (III) Oxide (FW = 441.93)

Sample Description: Au2O3 (Au 86%) Aldr 00306AW, 3 mm pellet, 90 TOA, Semi-Conductive



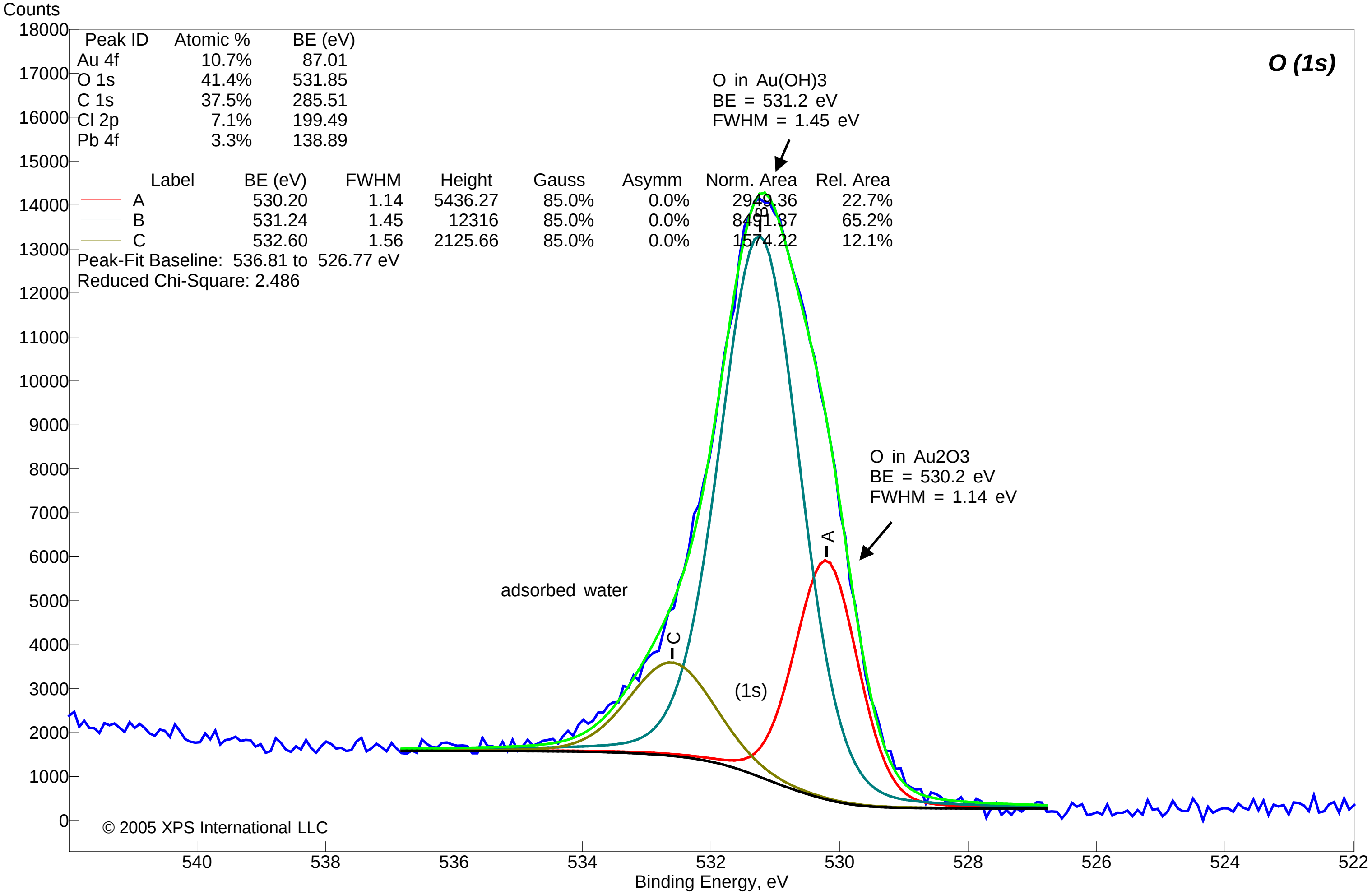
Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	85.05	1.37	17023.2	90.0%	0.0%	6483.18	9.3%
B	87.14	1.49	7057.7	90.0%	0.0%	2935.73	4.2%
C	86.97	1.21	85750.6	90.0%	0.0%	29017.5	41.8%
D	88.70	1.36	15808.2	90.0%	0.0%	6002.19	8.6%
E	91.68	1.40	4548.55	90.0%	0.0%	1771.1	2.6%
F	90.65	1.20	69375.5	90.0%	0.0%	23214	33.4%

Peak-Fit Baseline: 94.30 to 82.46 eV
Reduced Chi-Square: 2.924

Gold (III) Oxide (FW = 441.93)

Sample Description: Au2O3 (Au 86%) Aldr 00306AW, 3 mm pellet, 90 TOA, Semi-Conductive



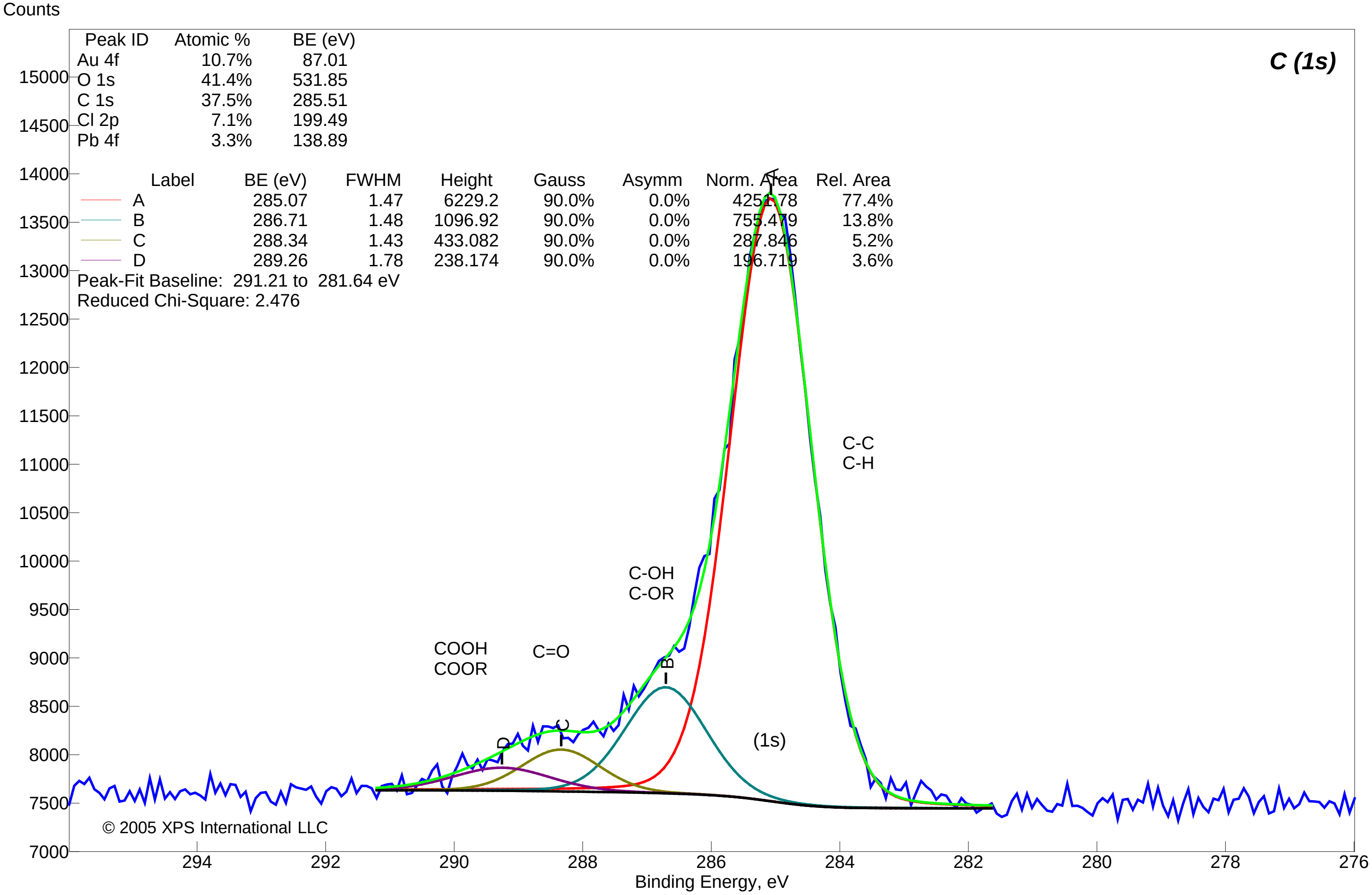
Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	530.20	1.14	5436.27	85.0%	0.0%	2949.36	22.7%
B	531.24	1.45	12316	85.0%	0.0%	8491.37	65.2%
C	532.60	1.56	2125.66	85.0%	0.0%	1574.22	12.1%

Peak-Fit Baseline: 536.81 to 526.77 eV
Reduced Chi-Square: 2.486

Gold (III) Oxide (FW = 441.93)

Sample Description: Au2O3 (Au 86%) Aldr 00306AW, 3 mm pellet, 90 TOA, Semi-Conductive



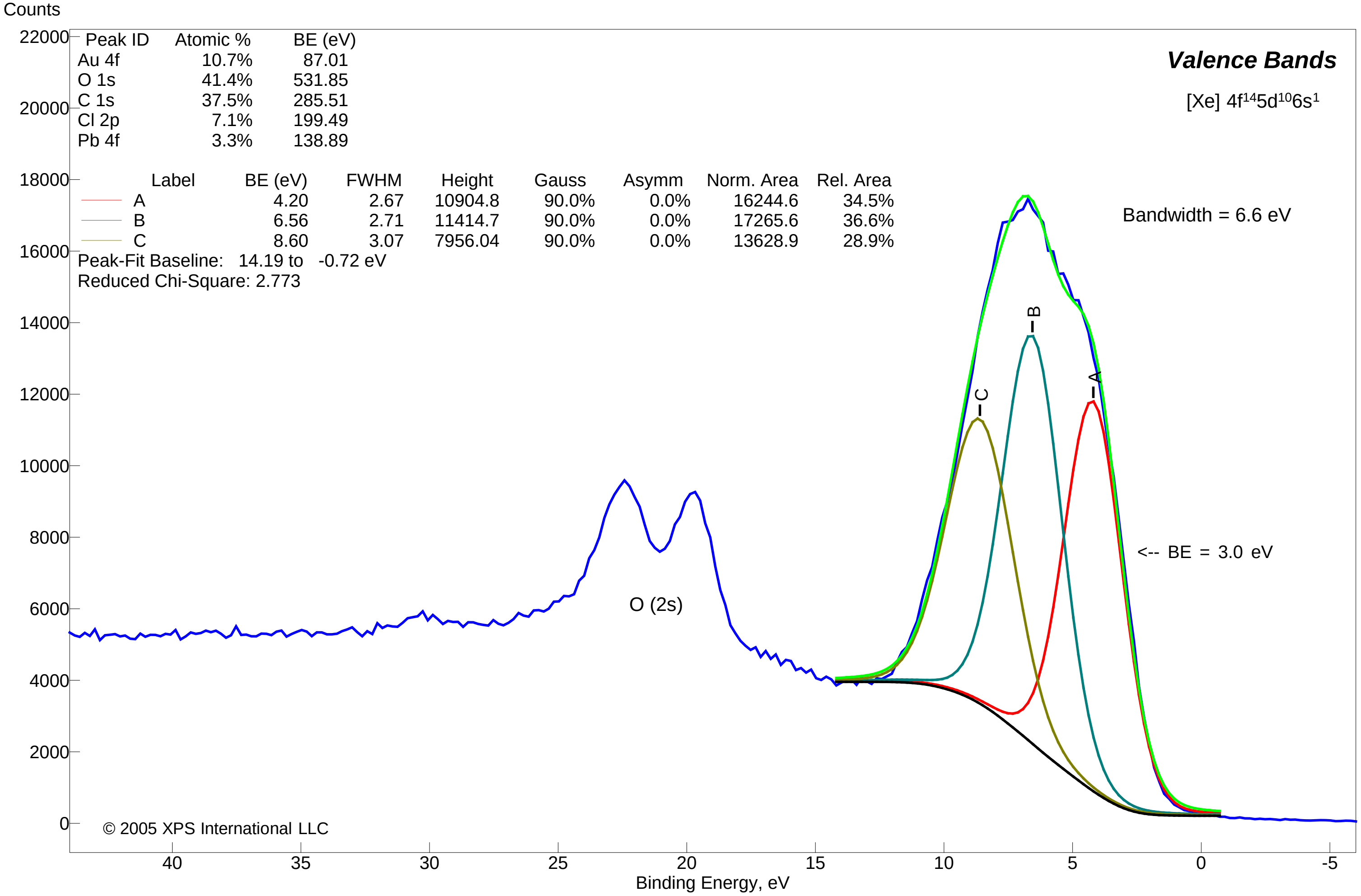
Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	285.07	1.47	6229.2	90.0%	0.0%	4251.78	77.4%
B	286.71	1.48	1096.92	90.0%	0.0%	755.479	13.8%
C	288.34	1.43	433.082	90.0%	0.0%	287.846	5.2%
D	289.26	1.78	238.174	90.0%	0.0%	196.719	3.6%

Peak-Fit Baseline: 291.21 to 281.64 eV
Reduced Chi-Square: 2.476

Gold (III) Oxide (FW = 441.93)

Sample Description: Au2O3 (Au 86%) Aldr 00306AW, 3 mm pellet, 90 TOA, Semi-Conductive



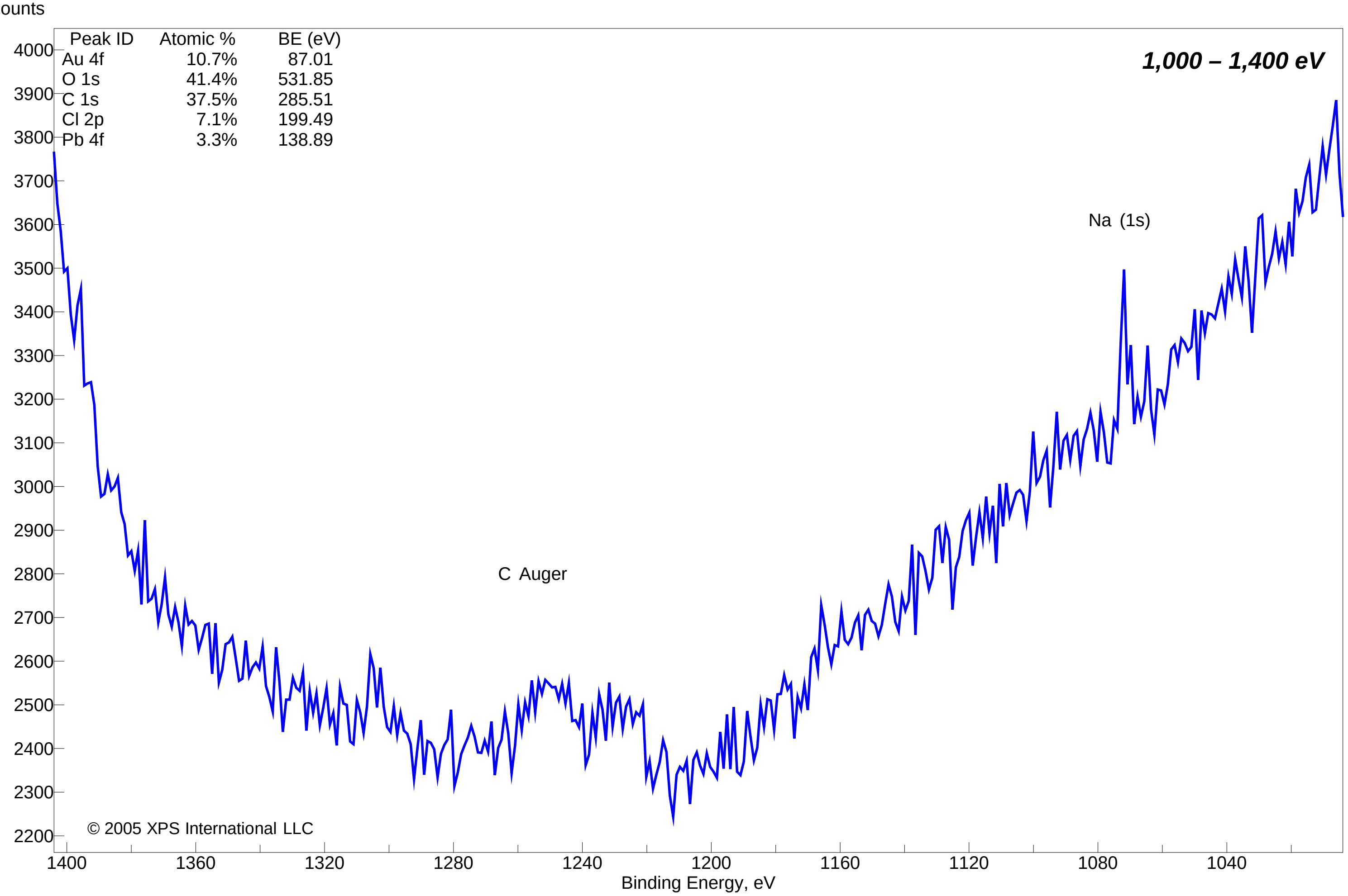
Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

	Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
—	A	4.20	2.67	10904.8	90.0%	0.0%	16244.6	34.5%
—	B	6.56	2.71	11414.7	90.0%	0.0%	17265.6	36.6%
—	C	8.60	3.07	7956.04	90.0%	0.0%	13628.9	28.9%

Peak-Fit Baseline: 14.19 to -0.72 eV
Reduced Chi-Square: 2.773

Gold (III) Oxide (FW = 441.93)

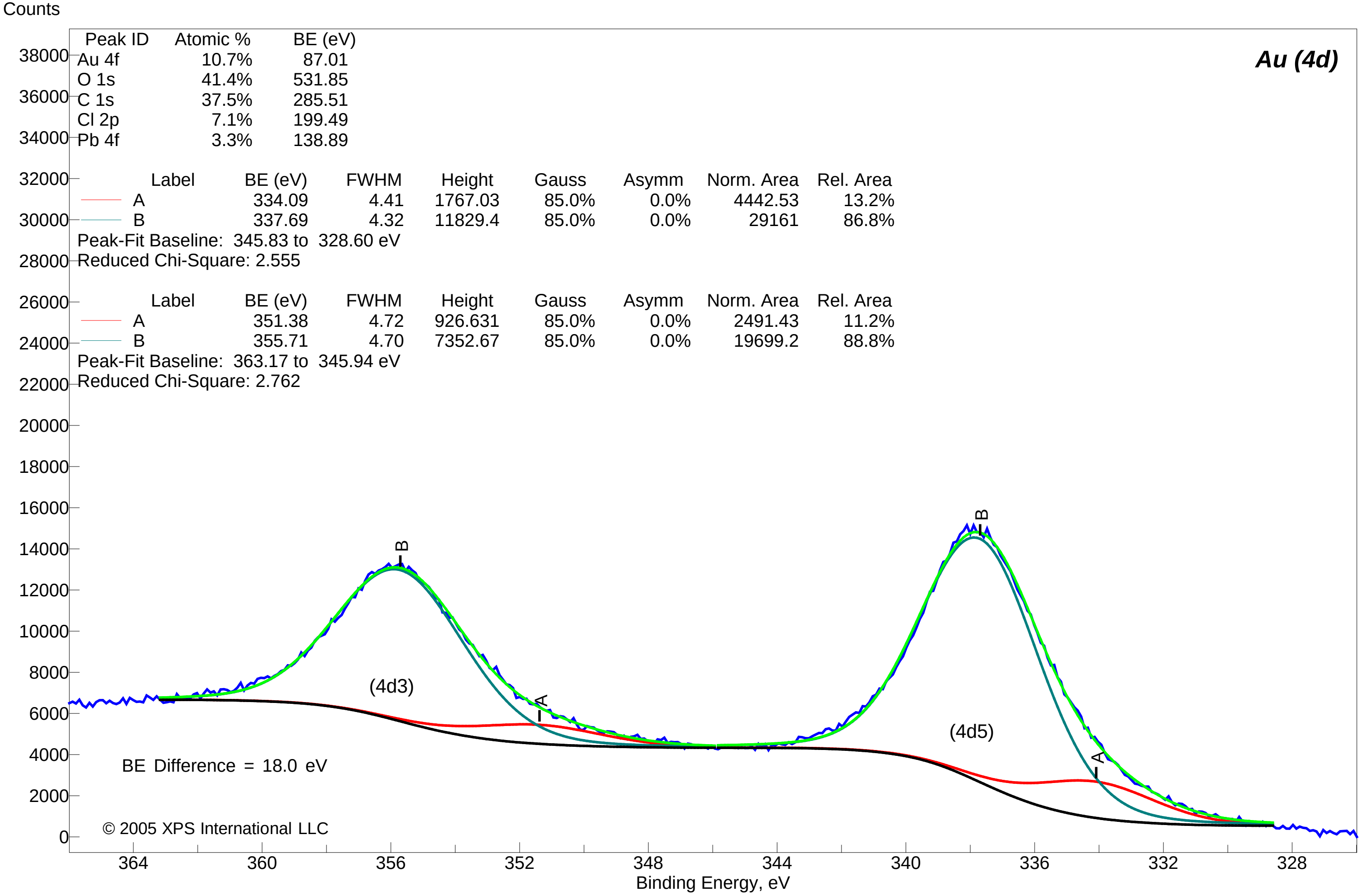
Sample Description: Au2O3 (Au 86%) Aldr 00306AW, 3 mm pellet, 90 TOA, Semi-Conductive



Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

Gold (III) Oxide (FW = 441.93)

Sample Description: Au2O3 (Au 86%) Aldr 00306AW, 3 mm pellet, 90 TOA, Semi-Conductive



Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	334.09	4.41	1767.03	85.0%	0.0%	4442.53	13.2%
B	337.69	4.32	11829.4	85.0%	0.0%	29161	86.8%

Peak-Fit Baseline: 345.83 to 328.60 eV
Reduced Chi-Square: 2.555

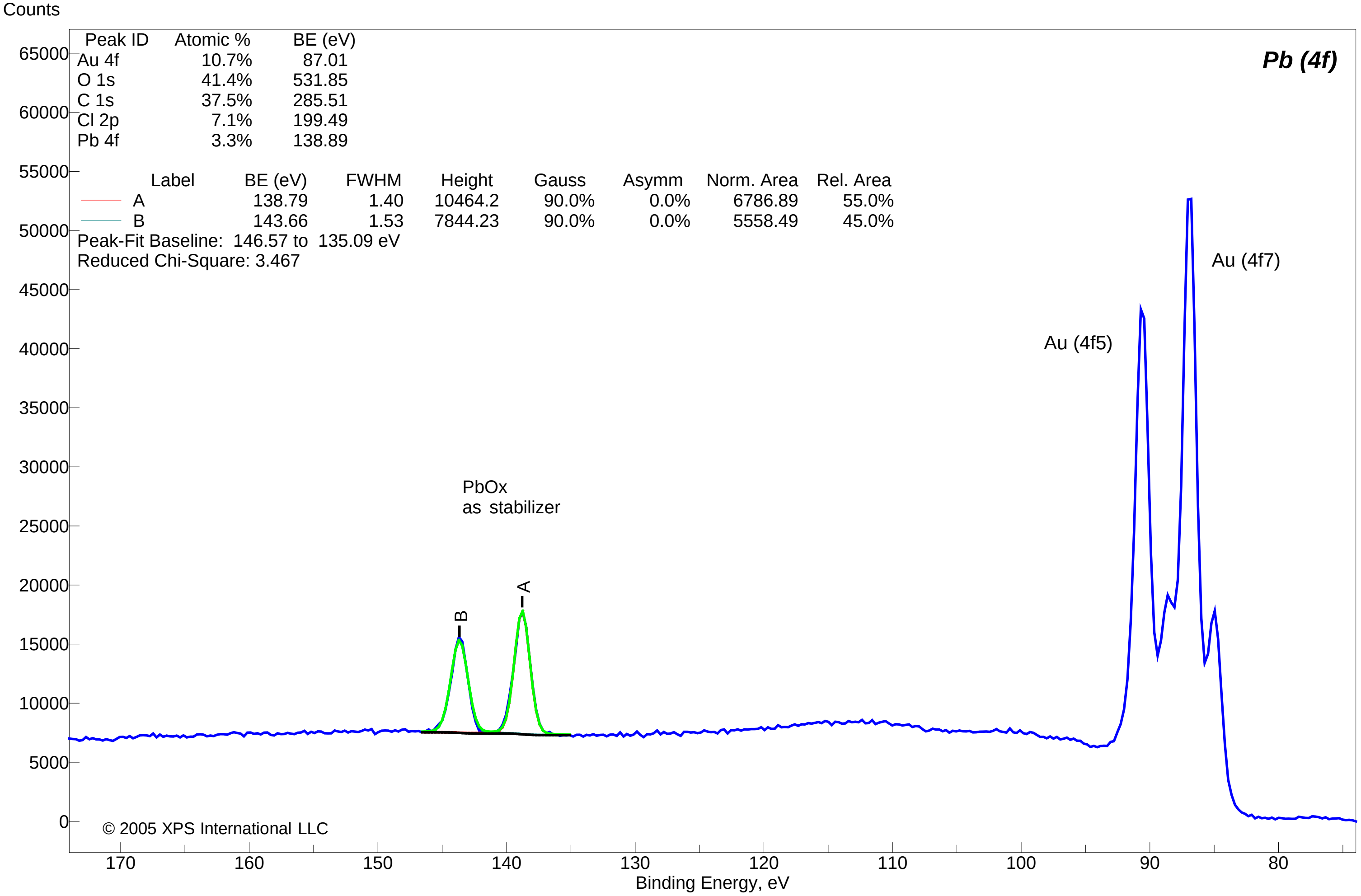
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	351.38	4.72	926.631	85.0%	0.0%	2491.43	11.2%
B	355.71	4.70	7352.67	85.0%	0.0%	19699.2	88.8%

Peak-Fit Baseline: 363.17 to 345.94 eV
Reduced Chi-Square: 2.762

BE Difference = 18.0 eV

Gold (III) Oxide (FW = 441.93)

Sample Description: Au2O3 (Au 86%) Aldr 00306AW, 3 mm pellet, 90 TOA, Semi-Conductive



Peak ID	Atomic %	BE (eV)
Au 4f	10.7%	87.01
O 1s	41.4%	531.85
C 1s	37.5%	285.51
Cl 2p	7.1%	199.49
Pb 4f	3.3%	138.89

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	138.79	1.40	10464.2	90.0%	0.0%	6786.89	55.0%
B	143.66	1.53	7844.23	90.0%	0.0%	5558.49	45.0%

Peak-Fit Baseline: 146.57 to 135.09 eV
Reduced Chi-Square: 3.467

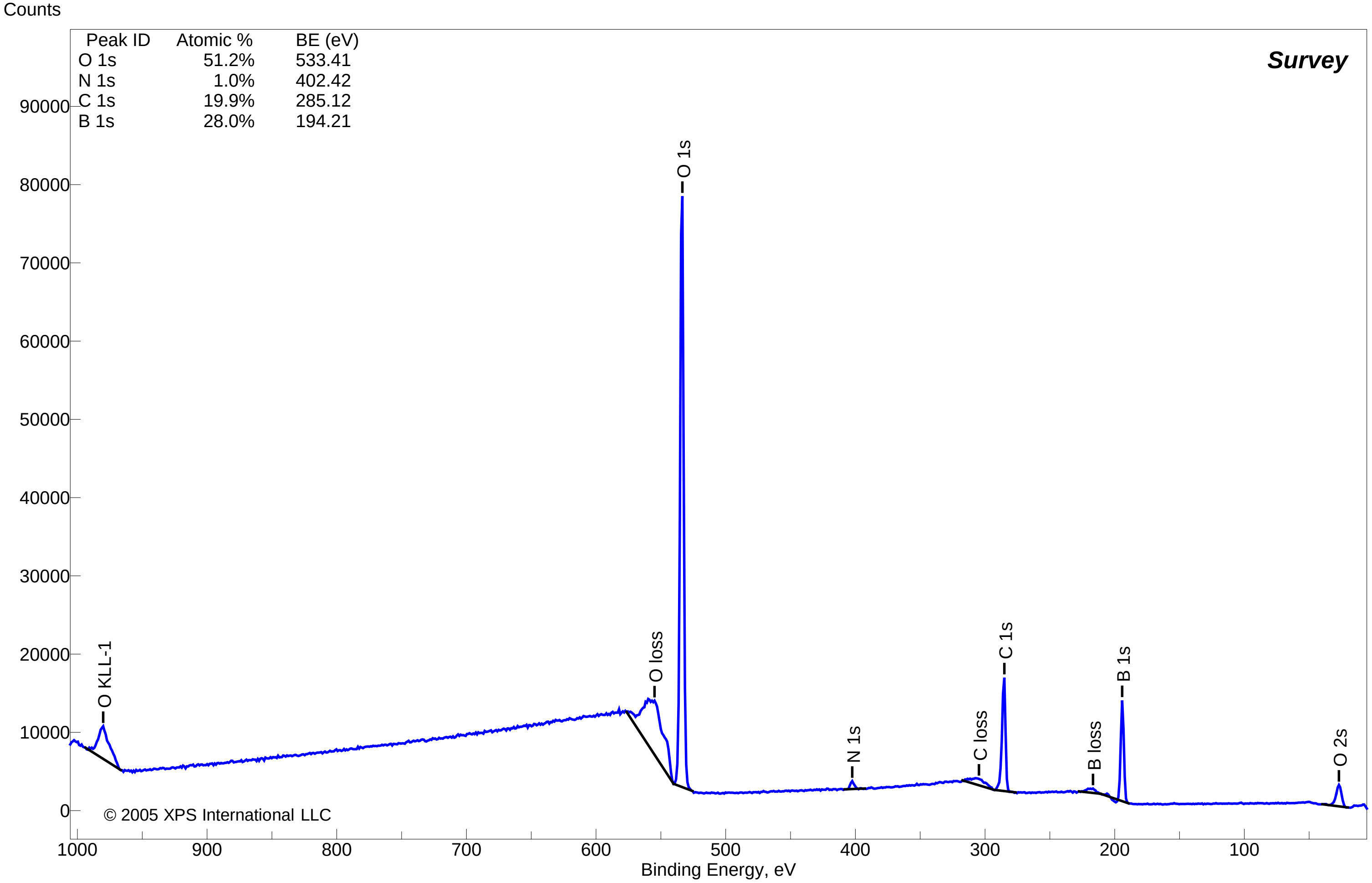
Boron (III) Oxide (FW = 69.62)
Surface Composition Table

Description: B_2O_3 (99.999%) from Aldrich Lot# 02829BV, analyzed at 90 deg TOA, mesh at 1mm, non-conductive white pieces, bulk freshly exposed, mp 450 C, d. 2.46, sol in boiling water

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
O 2s	27.1	23.6	0.14	1.5	8,540	
B 1s	194.2	190.7	0.49	1.5	22,156	28.0%
B loss	216.7	213.2	0.00	1.5	2,580	
C 1s	285.1	281.6	1.00	1.5	28,994	19.9%
C loss	304.7	301.2	0.00	1.5	7,042	
N 1s	402.4	398.9	1.80	1.5	2,184	1.0%
O 1s	533.4	529.9	2.93	1.5	154,657	51.2%
O loss	554.9	551.4	0.00	1.5	79,553	
O KLL-1	980.1	976.6	0.70	1.5	26,712	

Boron (III) Oxide (FW = 69.62)

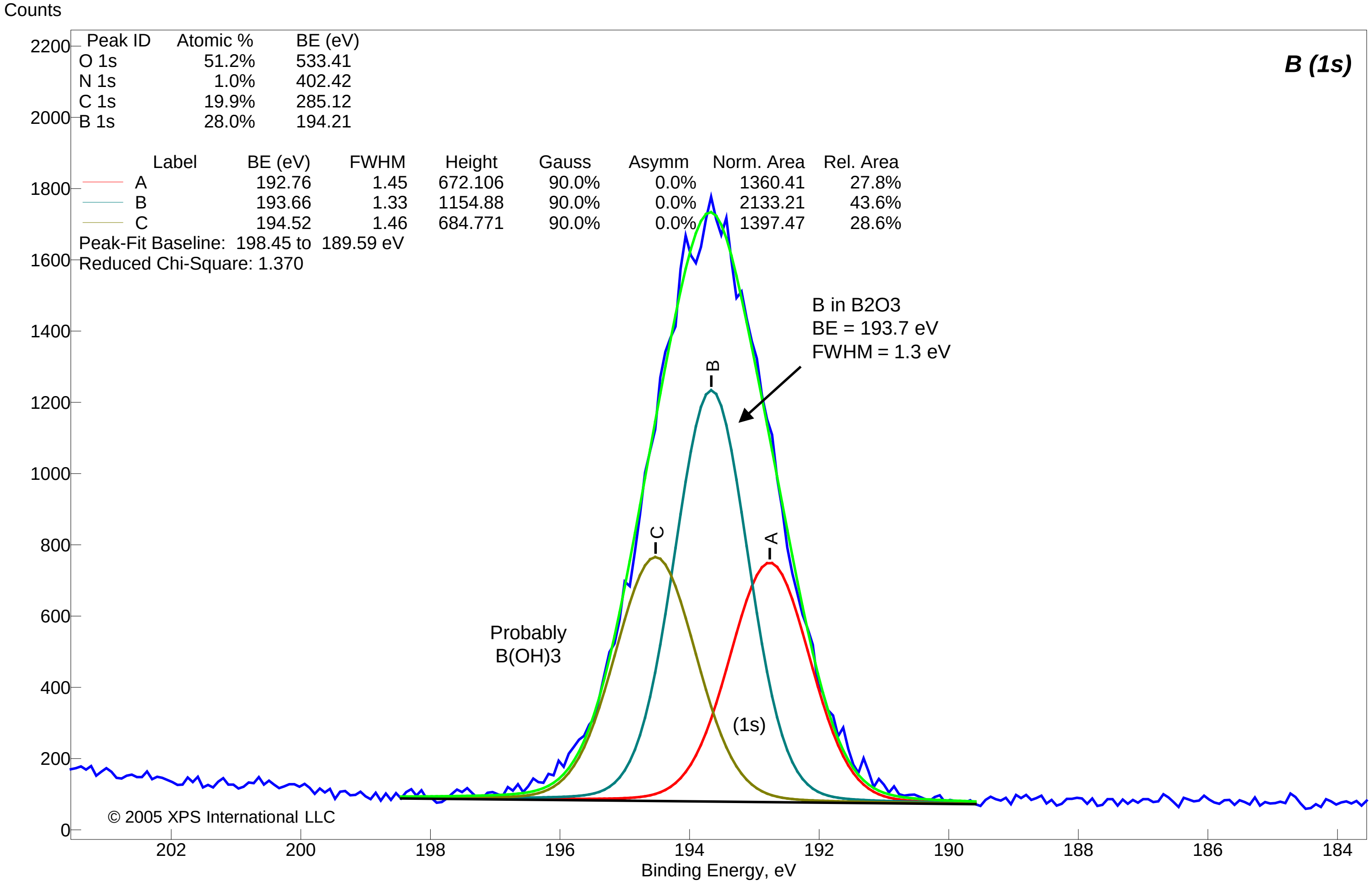
Sample Description: B2O3 (99.999%) crystal, from Aldrich Chem Co., Lot# 02829BV
freshly exposed bulk, analyzed at 90 deg TOA, mesh-screen at 1 mm height



Peak ID	Atomic %	BE (eV)
O 1s	51.2%	533.41
N 1s	1.0%	402.42
C 1s	19.9%	285.12
B 1s	28.0%	194.21

Boron (III) Oxide (FW = 69.62)

Sample Description: B2O3 (99.999%) crystal, Aldrich Chem Co., Lot# 02829BV
freshly exposed bulk, screen, 90 TOA



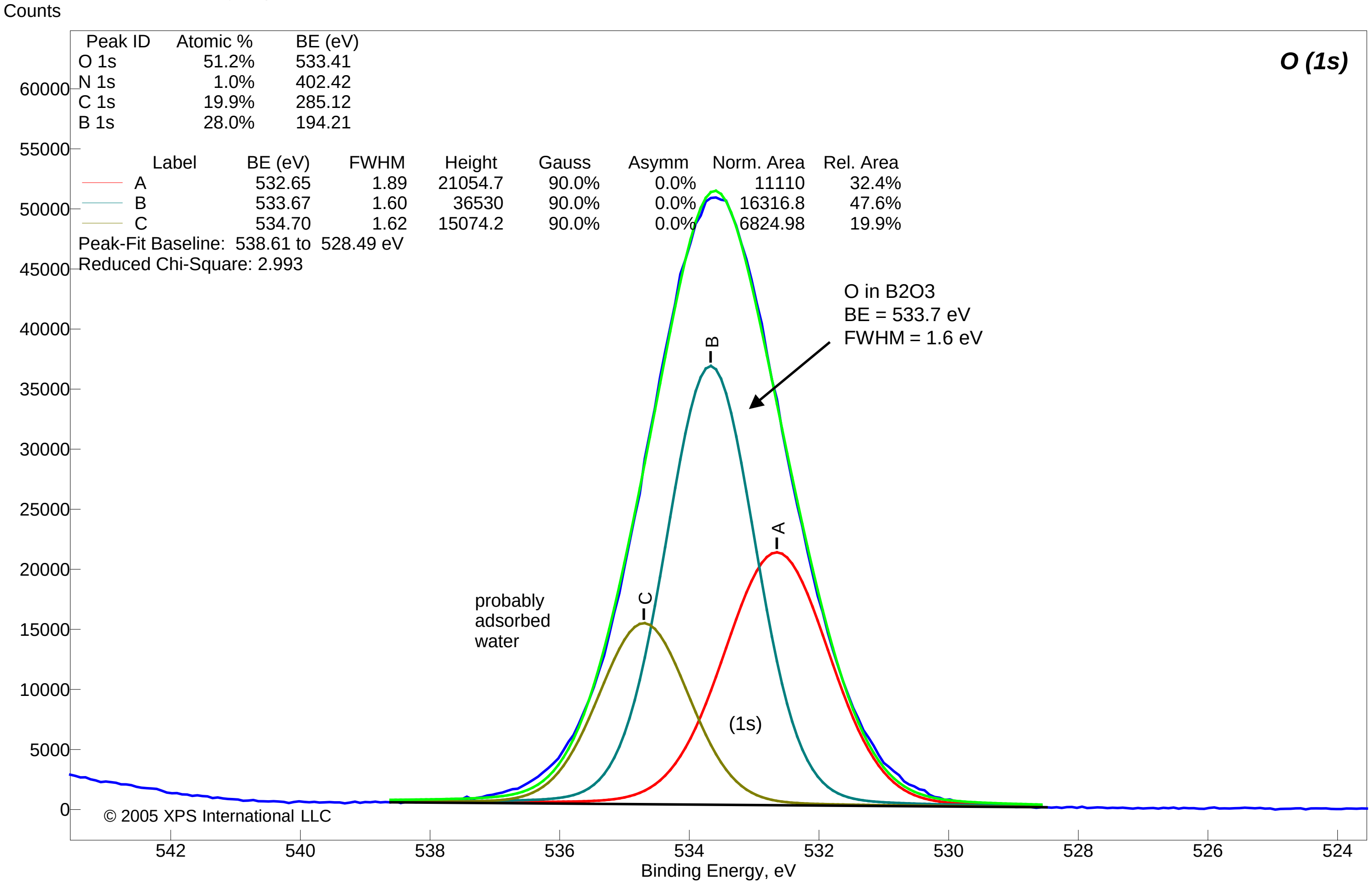
Peak ID	Atomic %	BE (eV)
O 1s	51.2%	533.41
N 1s	1.0%	402.42
C 1s	19.9%	285.12
B 1s	28.0%	194.21

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	192.76	1.45	672.106	90.0%	0.0%	1360.41	27.8%
B	193.66	1.33	1154.88	90.0%	0.0%	2133.21	43.6%
C	194.52	1.46	684.771	90.0%	0.0%	1397.47	28.6%

Peak-Fit Baseline: 198.45 to 189.59 eV
Reduced Chi-Square: 1.370

Boron (III) Oxide (FW = 69.62)

Sample Description: B2O3 (99.999%) crystal, Aldrich Chem Co., Lot# 02829BV
freshly exposed bulk, screen, 90 TOA



Peak ID	Atomic %	BE (eV)
O 1s	51.2%	533.41
N 1s	1.0%	402.42
C 1s	19.9%	285.12
B 1s	28.0%	194.21

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	532.65	1.89	21054.7	90.0%	0.0%	11110	32.4%
B	533.67	1.60	36530	90.0%	0.0%	16316.8	47.6%
C	534.70	1.62	15074.2	90.0%	0.0%	6824.98	19.9%

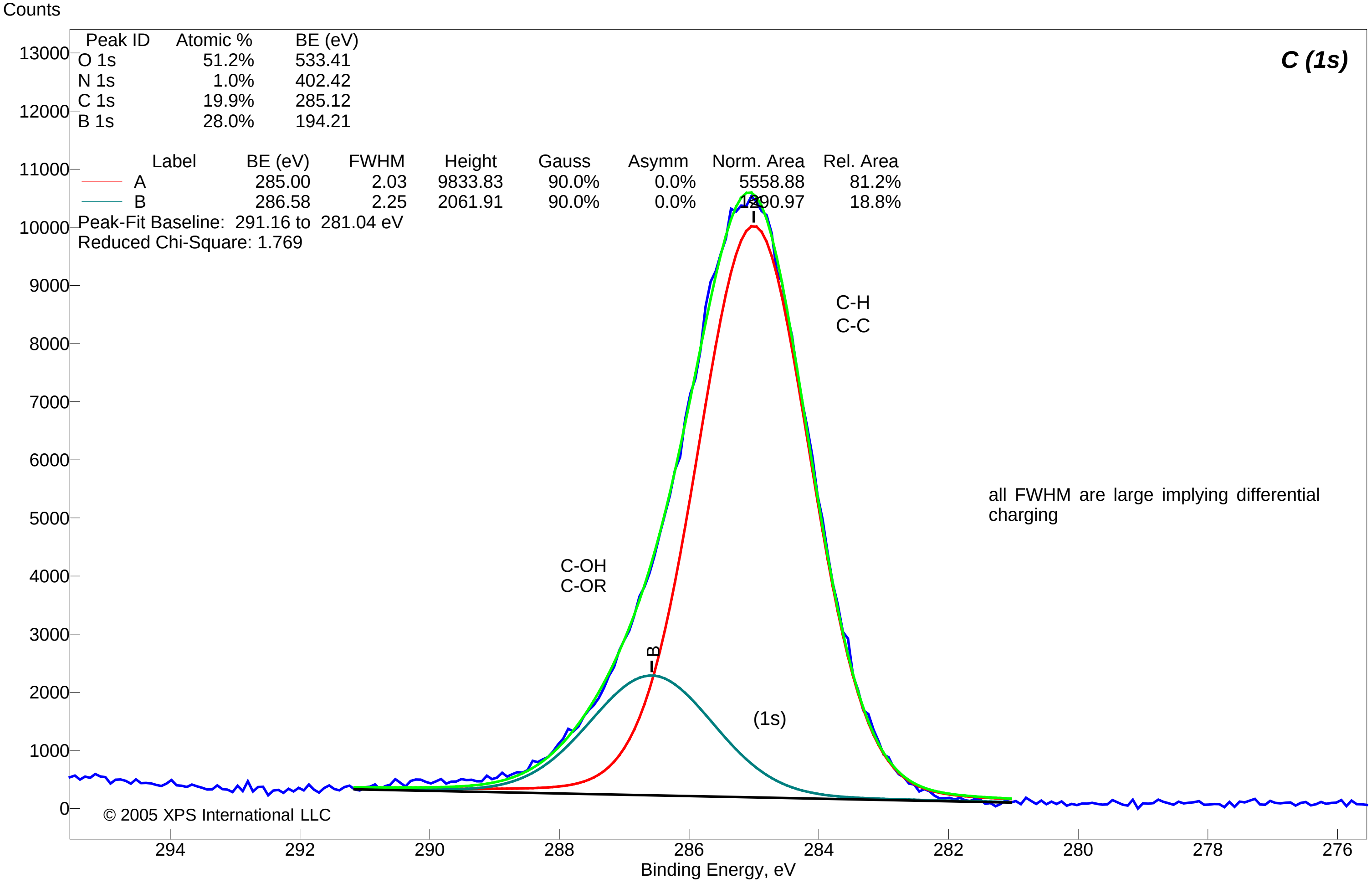
Peak-Fit Baseline: 538.61 to 528.49 eV
Reduced Chi-Square: 2.993

O in B2O3
BE = 533.7 eV
FWHM = 1.6 eV

probably adsorbed water

Boron (III) Oxide (FW = 69.62)

Sample Description: B2O3 (99.999%) crystal, Aldrich Chem Co., Lot# 02829BV
freshly exposed bulk, screen, 90 TOA



Peak ID	Atomic %	BE (eV)
O 1s	51.2%	533.41
N 1s	1.0%	402.42
C 1s	19.9%	285.12
B 1s	28.0%	194.21

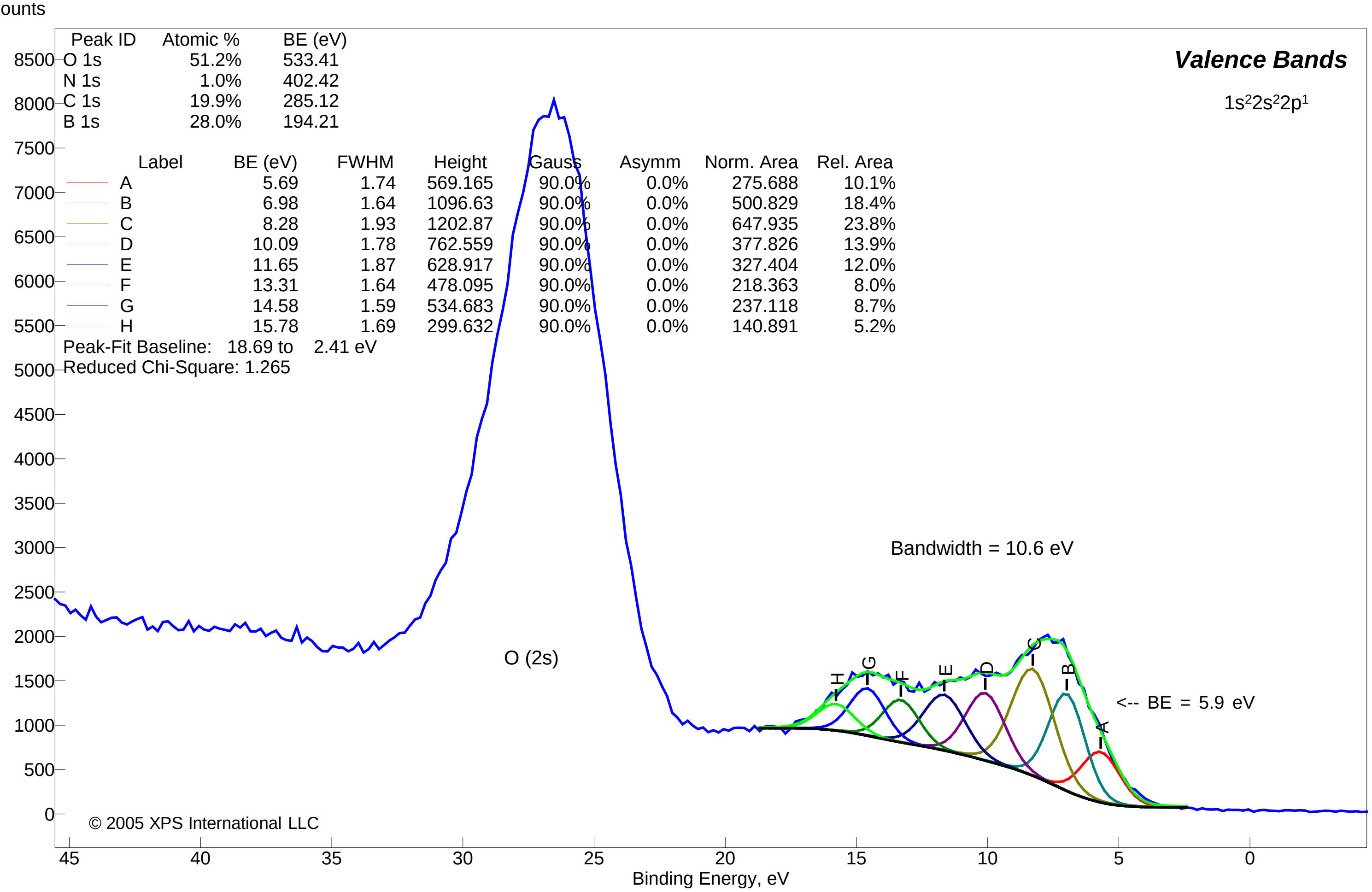
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	285.00	2.03	9833.83	90.0%	0.0%	5558.88	81.2%
B	286.58	2.25	2061.91	90.0%	0.0%	1290.97	18.8%

Peak-Fit Baseline: 291.16 to 281.04 eV
Reduced Chi-Square: 1.769

all FWHM are large implying differential charging

Boron (III) Oxide (FW = 69.62)

Sample Description: B2O3 (99.999%) crystal, Aldrich Chem Co., Lot# 02829BV
freshly exposed bulk, screen, 90 TOA



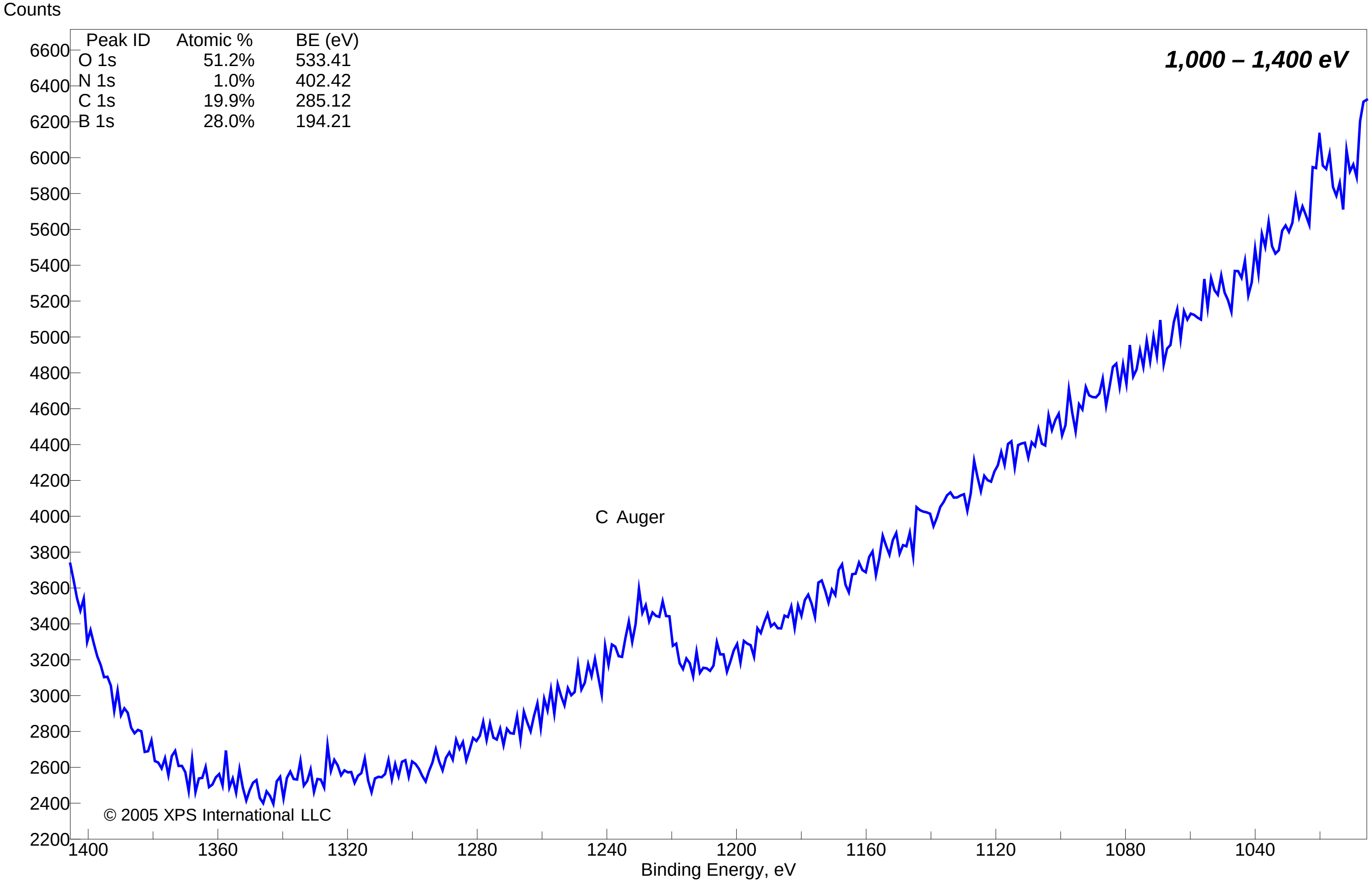
Peak ID	Atomic %	BE (eV)
O 1s	51.2%	533.41
N 1s	1.0%	402.42
C 1s	19.9%	285.12
B 1s	28.0%	194.21

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	5.69	1.74	569.165	90.0%	0.0%	275.688	10.1%
B	6.98	1.64	1096.63	90.0%	0.0%	500.829	18.4%
C	8.28	1.93	1202.87	90.0%	0.0%	647.935	23.8%
D	10.09	1.78	762.559	90.0%	0.0%	377.826	13.9%
E	11.65	1.87	628.917	90.0%	0.0%	327.404	12.0%
F	13.31	1.64	478.095	90.0%	0.0%	218.363	8.0%
G	14.58	1.59	534.683	90.0%	0.0%	237.118	8.7%
H	15.78	1.69	299.632	90.0%	0.0%	140.891	5.2%

Peak-Fit Baseline: 18.69 to 2.41 eV
Reduced Chi-Square: 1.265

Boron (III) Oxide (FW = 69.62)

Sample Description: B2O3 (99.999%) crystal, Aldrich Chem Co., Lot# 02829BV
freshly exposed bulk, screen, 90 TOA



Peak ID	Atomic %	BE (eV)
O 1s	51.2%	533.41
N 1s	1.0%	402.42
C 1s	19.9%	285.12
B 1s	28.0%	194.21

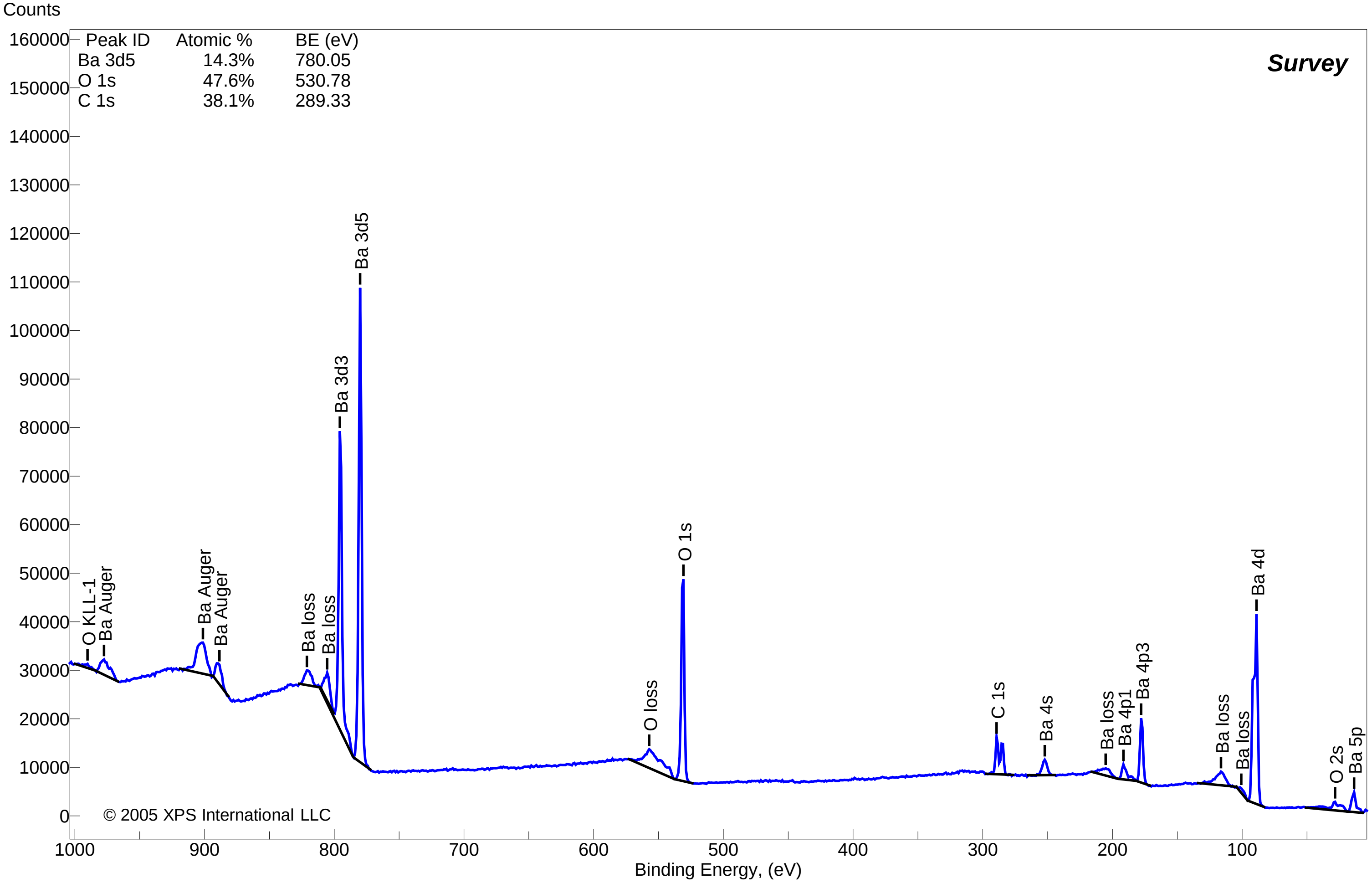
Barium (II) Carbonate (FW = 197.33)
Surface Composition Table

Description: $BaCO_3$ (99%) from Takeda Chem. Co., analyzed at 90 deg TOA, mesh at 1mm, non-conductive, ion-etched white powder pressed onto double sided tape, mp 811 C, d 4.43, sol in dilute HCl, acetic acid

Peak ID	Corrected BE (eV)	Measured BE (eV)	Scofield RSF	RSF Exponent	Normalized Peak Area	Atomic %
Ba 5p	9.7	13.7	0.60	0.6	14,087	
O 2s	24.3	28.3	0.14	0.6	16,029	
Ba 4d	84.9	88.9	5.86	0.6	126,404	
Ba loss	96.7	100.7	0.00	0.6	3,987	
Ba loss	112.3	116.3	0.00	0.6	21,001	
Ba 4p3	173.9	177.9	2.73	0.6	31,102	
Ba 4p1	187.6	191.6	2.73	0.6	12,297	
Ba loss	201.3	205.3	0.00	0.6	11,815	
Ba 4s	248.2	252.2	1.13	0.6	12,022	
C 1s	285.3	289.3	1.00	0.6	31,178	38.1%
O 1s	526.8	530.8	2.93	0.6	99,714	47.6%
O loss	553.2	557.2	0.00	0.6	52,032	
Ba 3d5	776.0	780.0	25.84	0.6	219,761	14.3%
Ba 3d3	791.7	795.7	17.92	0.6	191,859	
Ba loss	801.5	805.5	0.00	0.6	24,083	
Ba loss	817.1	821.1	0.00	0.6	16,753	
Ba Auger	884.6	888.6	0.00	0.6	18,109	
Ba Auger	897.3	901.3	0.00	0.6	49,697	
Ba Auger	973.5	977.5	0.00	0.6	22,408	
O KLL-1	986.2	990.2	0.70	0.6	4,185	

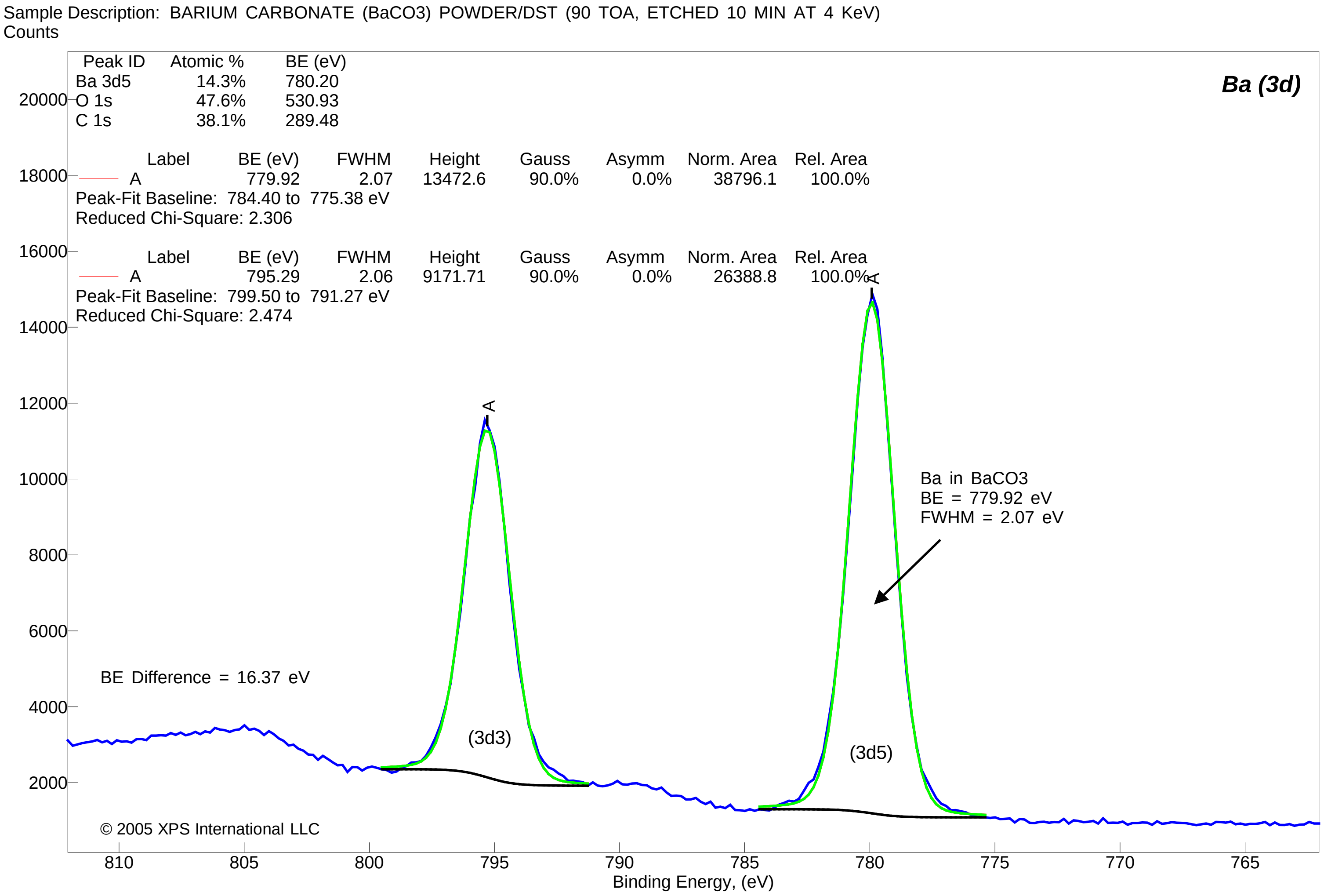
Barium (II) Carbonate (FW = 197.33)

Sample Description: BaCO3
ion etched 10 min. at 4 keV, pressed onto double sided tape, 90 deg TOA



Peak ID	Atomic %	BE (eV)
Ba 3d5	14.3%	780.05
O 1s	47.6%	530.78
C 1s	38.1%	289.33

Barium (II) Carbonate (FW = 197.33)



Sample Description: BARIUM CARBONATE (BaCO3) POWDER/DST (90 TOA, ETCHED 10 MIN AT 4 KeV)

Peak ID	Atomic %	BE (eV)
Ba 3d5	14.3%	780.20
O 1s	47.6%	530.93
C 1s	38.1%	289.48

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	779.92	2.07	13472.6	90.0%	0.0%	38796.1	100.0%

Peak-Fit Baseline: 784.40 to 775.38 eV
Reduced Chi-Square: 2.306

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	795.29	2.06	9171.71	90.0%	0.0%	26388.8	100.0%

Peak-Fit Baseline: 799.50 to 791.27 eV
Reduced Chi-Square: 2.474

Ba in BaCO3
BE = 779.92 eV
FWHM = 2.07 eV

BE Difference = 16.37 eV

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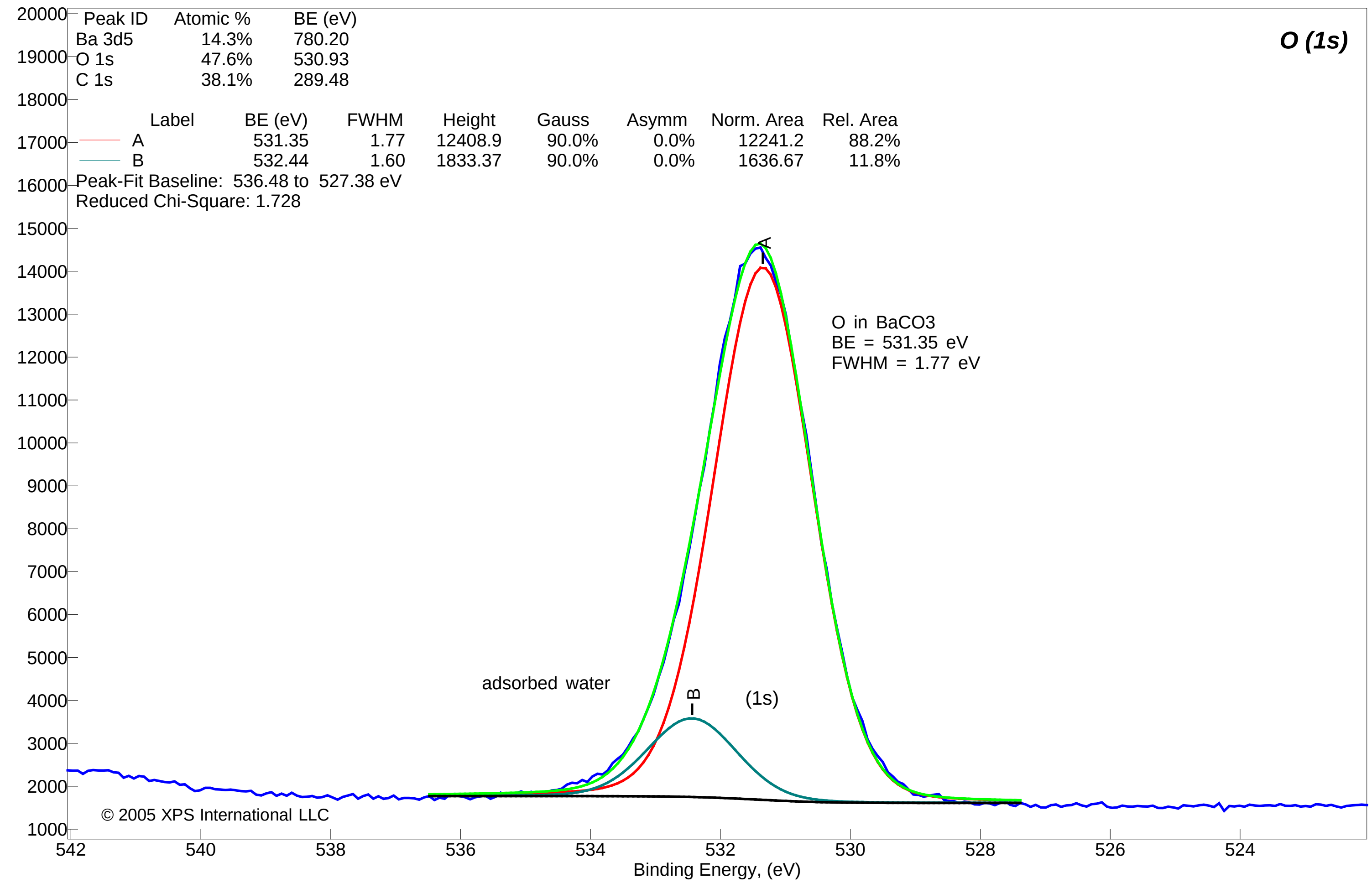
Barium (II) Carbonate (FW = 197.33)

Sample Description: BARIUM CARBONATE (BaCO3) POWDER/DST (90 TOA, ETCHED 10 MIN AT 4 KeV)



Peak ID	Atomic %	BE (eV)
Ba 3d5	14.3%	780.20
O 1s	47.6%	530.93
C 1s	38.1%	289.48

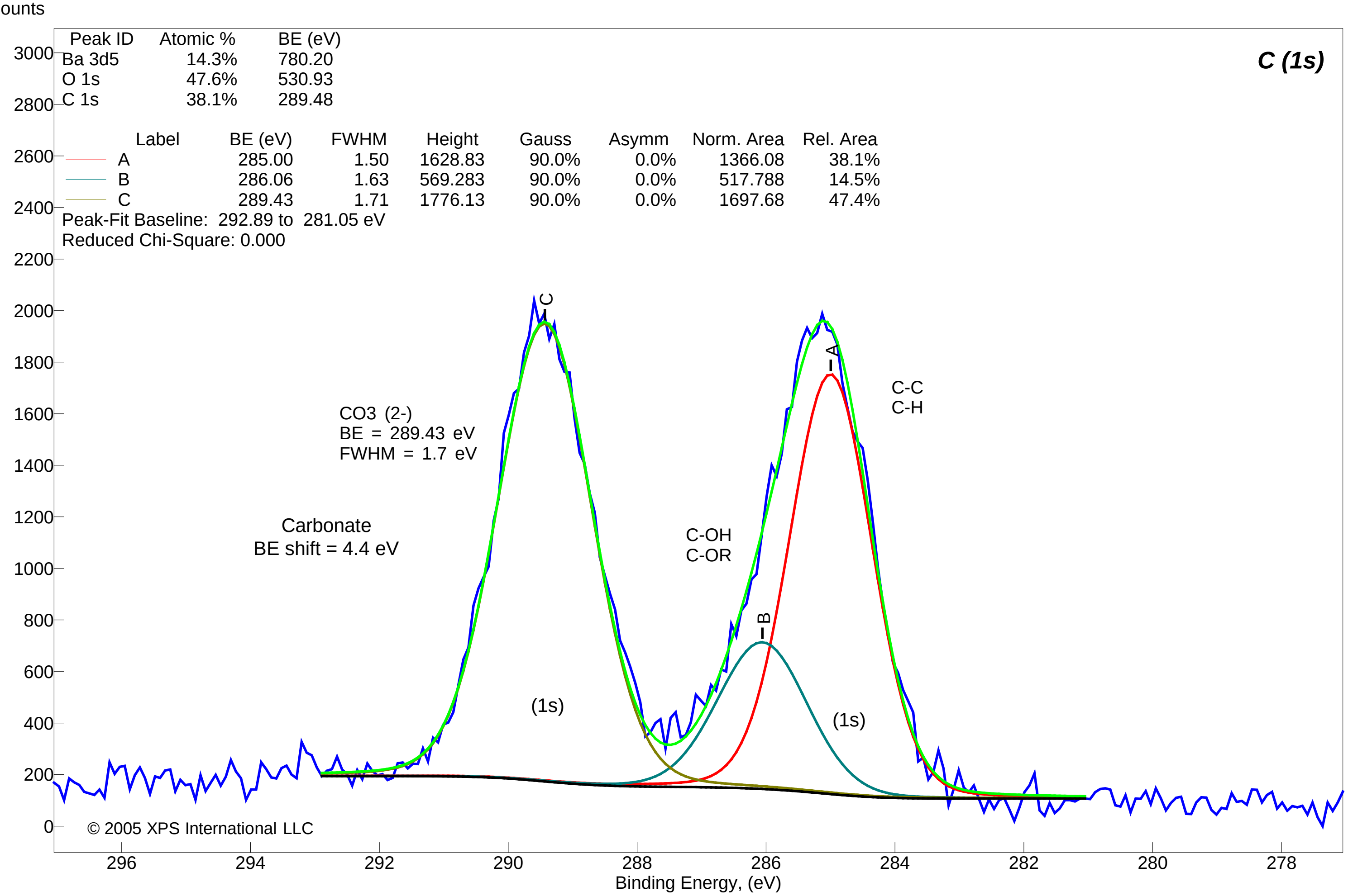
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	531.35	1.77	12408.9	90.0%	0.0%	12241.2	88.2%
B	532.44	1.60	1833.37	90.0%	0.0%	1636.67	11.8%

Peak-Fit Baseline: 536.48 to 527.38 eV
Reduced Chi-Square: 1.728

O in BaCO3
BE = 531.35 eV
FWHM = 1.77 eV

Barium (II) Carbonate (FW = 197.33)

Sample Description: BARIUM CARBONATE (BaCO3) POWDER/DST (90 TOA, ETCHED 10 MIN AT 4 KeV)



Peak ID	Atomic %	BE (eV)
Ba 3d5	14.3%	780.20
O 1s	47.6%	530.93
C 1s	38.1%	289.48

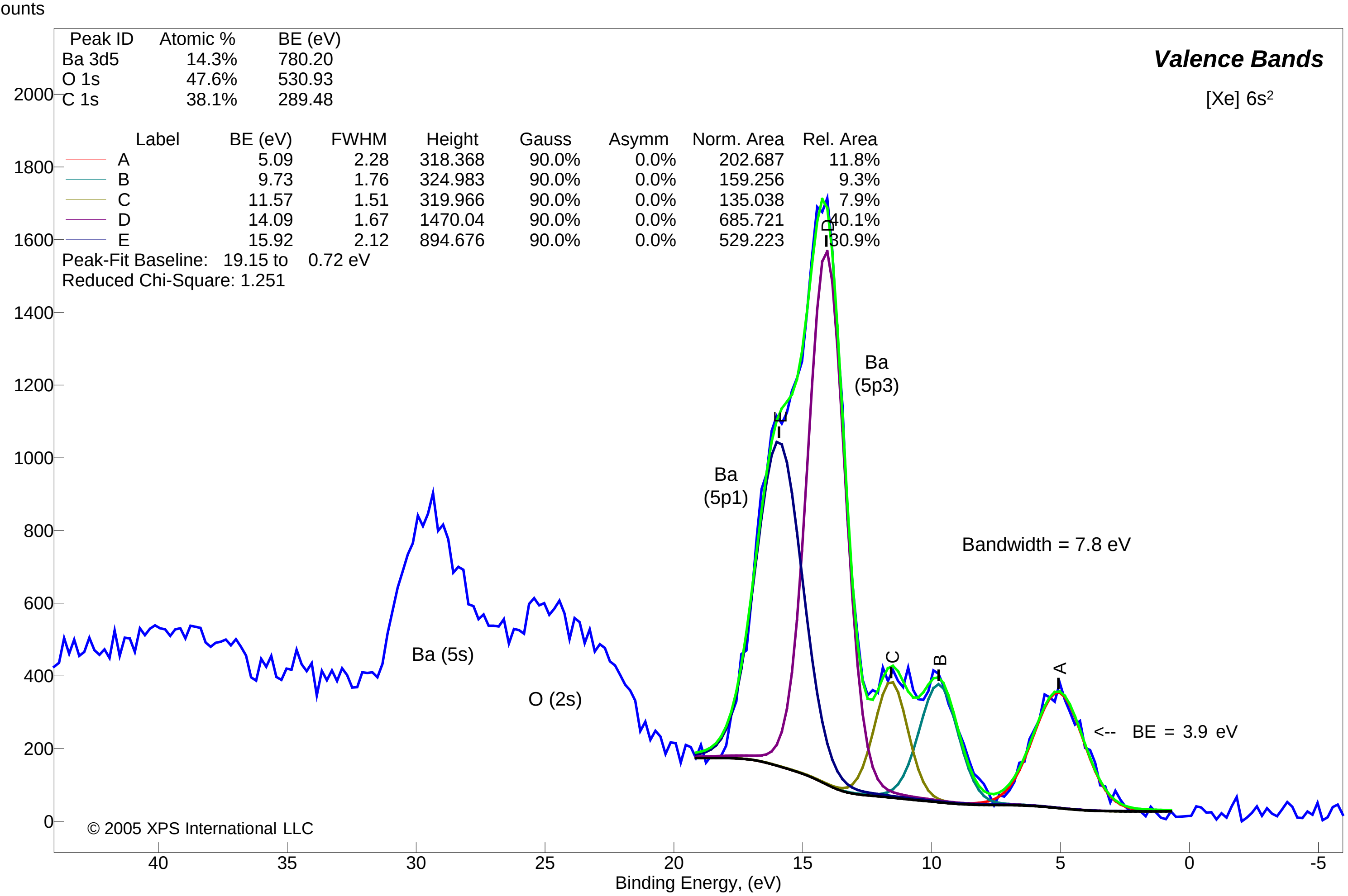
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	285.00	1.50	1628.83	90.0%	0.0%	1366.08	38.1%
B	286.06	1.63	569.283	90.0%	0.0%	517.788	14.5%
C	289.43	1.71	1776.13	90.0%	0.0%	1697.68	47.4%

Peak-Fit Baseline: 292.89 to 281.05 eV

Reduced Chi-Square: 0.000

Barium (II) Carbonate (FW = 197.33)

Sample Description: BARIUM CARBONATE ($BaCO_3$) POWDER/DST (90 TOA, ETCHED 10 MIN AT 4 KeV)



Peak ID	Atomic %	BE (eV)
Ba 3d5	14.3%	780.20
O 1s	47.6%	530.93
C 1s	38.1%	289.48

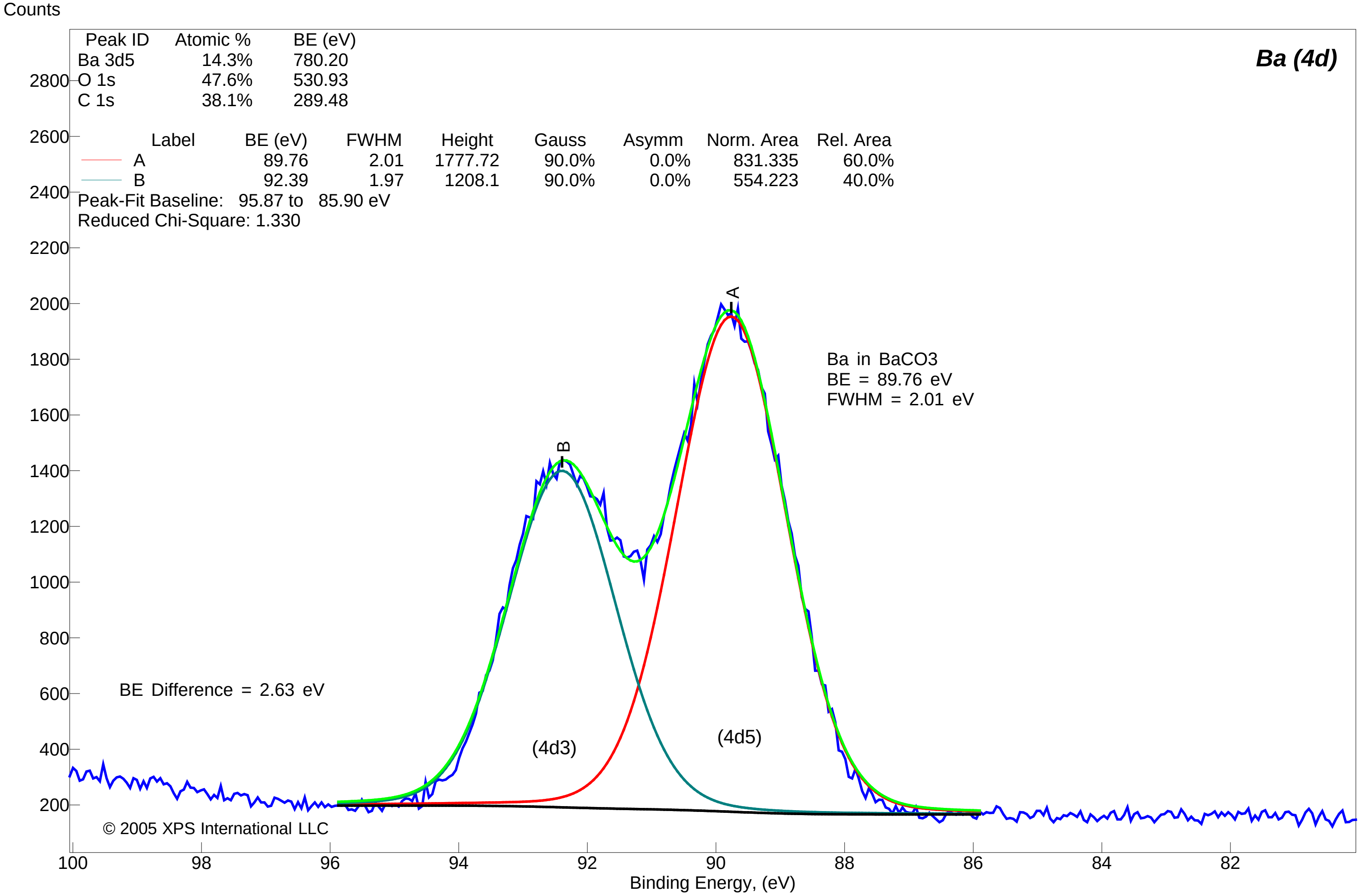
Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	5.09	2.28	318.368	90.0%	0.0%	202.687	11.8%
B	9.73	1.76	324.983	90.0%	0.0%	159.256	9.3%
C	11.57	1.51	319.966	90.0%	0.0%	135.038	7.9%
D	14.09	1.67	1470.04	90.0%	0.0%	685.721	40.1%
E	15.92	2.12	894.676	90.0%	0.0%	529.223	30.9%

Peak-Fit Baseline: 19.15 to 0.72 eV

Reduced Chi-Square: 1.251

Barium (II) Carbonate (FW = 197.33)

Sample Description: BARIUM CARBONATE (BaCO3) POWDER/DST (90 TOA, ETCHED 10 MIN AT 4 KeV)



Peak ID	Atomic %	BE (eV)
Ba 3d5	14.3%	780.20
O 1s	47.6%	530.93
C 1s	38.1%	289.48

Label	BE (eV)	FWHM	Height	Gauss	Asymm	Norm. Area	Rel. Area
A	89.76	2.01	1777.72	90.0%	0.0%	831.335	60.0%
B	92.39	1.97	1208.1	90.0%	0.0%	554.223	40.0%

Peak-Fit Baseline: 95.87 to 85.90 eV
Reduced Chi-Square: 1.330

Ba in BaCO3
BE = 89.76 eV
FWHM = 2.01 eV

BE Difference = 2.63 eV

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