TopSpec

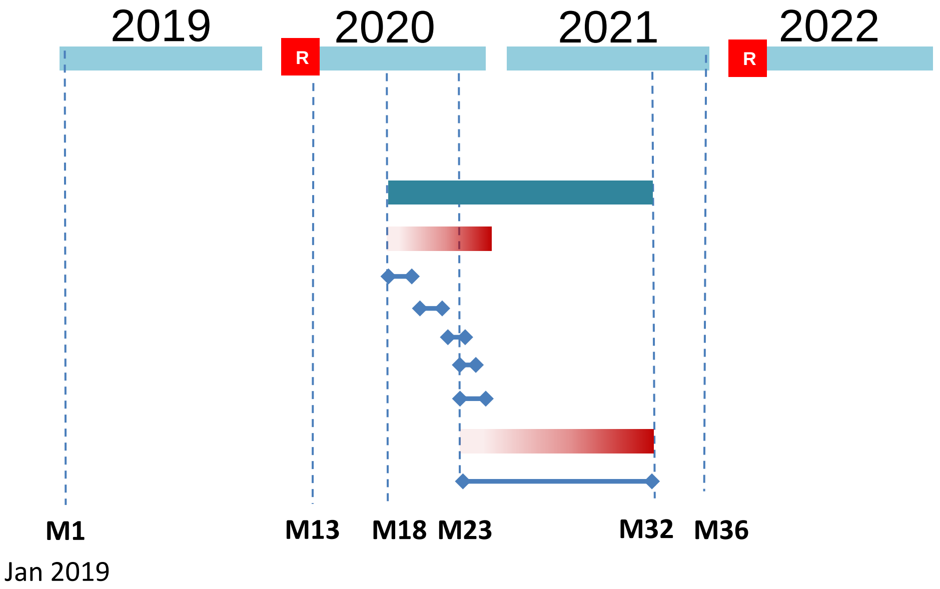
WP4 – Development & Application of CE

D4.1 – Prototype CED gun at KI

T4.1 – design 1KeV pulsed e source
T4.2 – construction
T4.3 – interfacing CED gun with omni
T4.4 – testing CED
T4.5 – optimizing software & hardware

D4.2 –Optimized CE guns at KI/IP

T4.6 – analysis of mAbs



NIST Atomic Spectra Database - Ionization Energies Data

At. Num.	Sp. Name.	Ion Charge	El. name	Isoel. Seq.	Ground Shells	Ground Level	Ionized Level	Ionization Energy (eV)	Uncertainty (eV)	References
6	C I	0	Carbon	C	$1s^2 2s^2 2p^2$	$^3P_0$	$2s^2 2p\ ^2P^\circ_{1/2}$	11.2602880	0.0000011	L20057
6	C II	+1	Carbon	B	$1s^2 2s^2 2p$	$^2P^\circ_{1/2}$	$2s^2\ ^1S_0$	24.383154	0.000016	c190
6	C III	+2	Carbon	Be	$1s^2 2s^2$	$^1S_0$	$2s\ ^2S_{1/2}$	47.88778	0.00025	L876c191
6	C IV	+3	Carbon	Li	$1s^2 2s$	$^2S_{1/2}$	$1s^2\ ^1S_0$	64.49352	0.00019	L11667
6	C V	+4	Carbon	He	$1s^2$	$^1S_0$	$1s\ ^2S_{1/2}$	[392.090515]	0.000025	L10054
6	C VI	+5	Carbon	H	$1s$	$^2S_{1/2}$		(489.993194)	0.000007	L7188

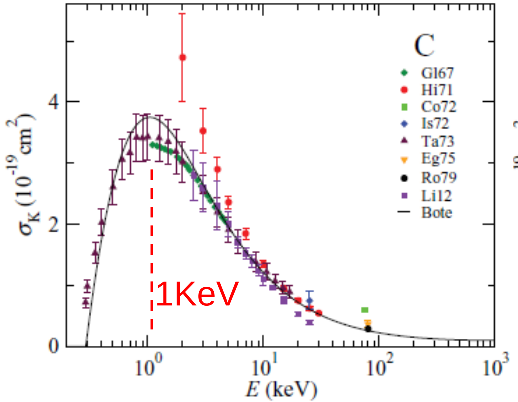
At. Num.	Sp. Name.	Ion Charge	El. name	Isoel. Seq.	Ground Shells	Ground Level	Ionized Level	Ionization Energy (eV)	Uncertainty (eV)	References
7	N I	0	Nitrogen	N	$1s^2 2s^2 2p^3$	$^4S^\circ_{3/2}$	$2p^2\ ^3P_0$	14.53413	0.00004	L1411
7	N II	+1	Nitrogen	C	$1s^2 2s^2 2p^2$	$^3P_0$	$2p\ ^2P^\circ_{1/2}$	[29.60125]	0.00009	L11770
7	N III	+2	Nitrogen	B	$1s^2 2s^2 2p$	$^2P^\circ_{1/2}$	$2s^2\ ^1S_0$	[47.4453]	0.0025	L11770
7	N IV	+3	Nitrogen	Be	$1s^2 2s^2$	$^1S_0$	$2s\ ^2S_{1/2}$	77.4735	0.0004	L7288,L876
7	N V	+4	Nitrogen	Li	$1s^2 2s$	$^2S_{1/2}$	$1s^2\ ^1S_0$	97.8901	0.0004	L4829
7	N VI	+5	Nitrogen	He	$1s^2$	$^1S_0$	$1s\ ^2S_{1/2}$	[552.06732]	0.00004	L10054
7	N VII	+6	Nitrogen	H	$1s$	$^2S_{1/2}$		(667.046116)	0.000013	L7188

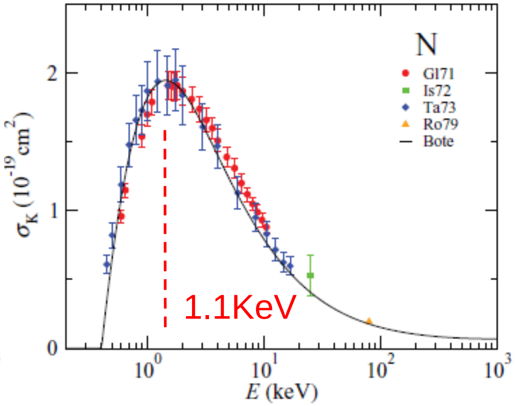
At. Num.	Sp. Name.	Ion Charge	El. name	Isoel. Seq.	Ground Shells	Ground Level	Ionized Level	Ionization Energy (eV)	Uncertainty (eV)	References
8	O I	0	Oxygen	O	$1s^2 2s^2 2p^4$	$^3P_2$	$2p^3\ ^4S^\circ_{3/2}$	13.618055	0.000007	L74,L3760
8	O II	+1	Oxygen	N	$1s^2 2s^2 2p^3$	$^4S^\circ_{3/2}$	$2p^2\ ^3P_0$	35.12112	0.00006	L11267,L10621
8	O III	+2	Oxygen	C	$1s^2 2s^2 2p^2$	$^3P_0$	$2p\ ^2P^\circ_{1/2}$	[54.93554]	0.00012	L11770
8	O IV	+3	Oxygen	B	$1s^2 2s^2 2p$	$^2P^\circ_{1/2}$	$2s^2\ ^1S_0$	77.41350	0.00025	L648
8	O V	+4	Oxygen	Be	$1s^2 2s^2$	$^1S_0$	$2s\ ^2S_{1/2}$	113.8990	0.0005	L7288
8	O VI	+5	Oxygen	Li	$1s^2 2s$	$^2S_{1/2}$	$1s^2\ ^1S_0$	[138.1189]	0.0021	L4713
8	O VII	+6	Oxygen	He	$1s^2$	$^1S_0$	$1s\ ^2S_{1/2}$	[739.32682]	0.00006	L10054
8	O VIII	+7	Oxygen	H	$1s$	$^2S_{1/2}$		(871.40988)	0.00003	L7188

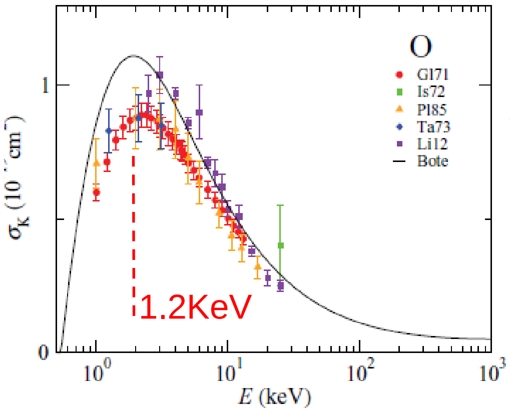
NIST Energy Levels and Wavelengths Bibliographic Reference # 10054
Theoretical Energies for the n=1 and 2 States of the Helium Isoelectronic Sequence up to Z=100,
G. W. F. Drake, Can. J. Phys. 66, 586–611 (1988) DOI:10.1139/p88-100

WP4 – Development & Application of CE

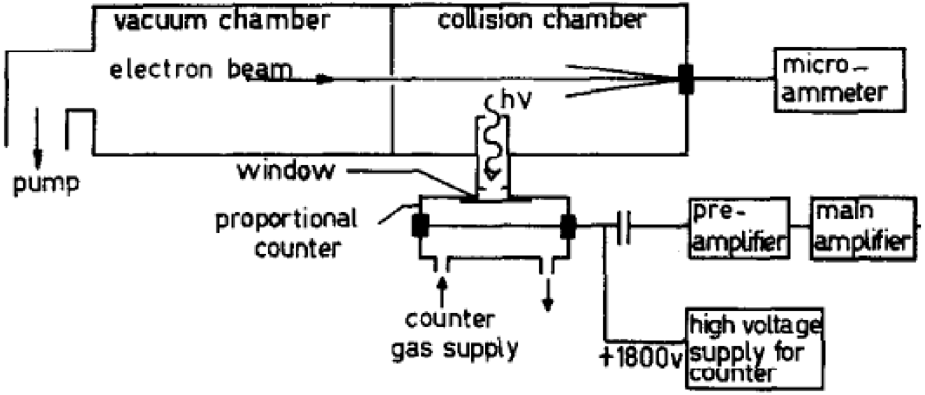
Prior Art







Absolute K-shell ionization cross sections *vs* incident electron energy. Calculations and measurements



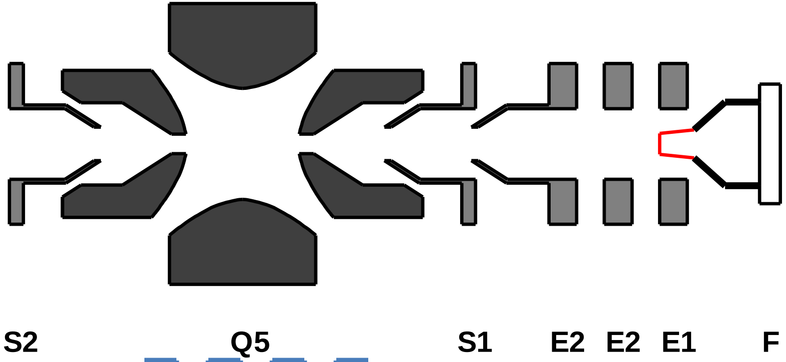
Electron beam 200-18KeV
Gas targets at variable pressure
X-rays measured normally to incident e-beam

X-ray emission cross sections and fluorescence yields for light atoms and molecules by electron impact, Tawara H *et al*, Physica 63 (1973) 351-367

Cross Sections for Inner-Shell Ionization by Electron Impact, Llovet X et al J Phys Chem Ref Data 43, 013102 (2014); doi: 10.1063/1.4832851

WP4 – Development & Application of CE

T4.1 Design 1KeV pulsed electron source

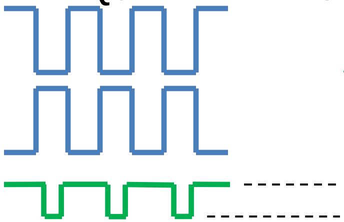


RF phase A

RF phase B

e^- beam

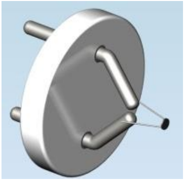
modulation pulse E2



E2 split electrode supplied with deflection pulse to inject at correct RF phase

------- deflection voltage level

---------- transmission windows



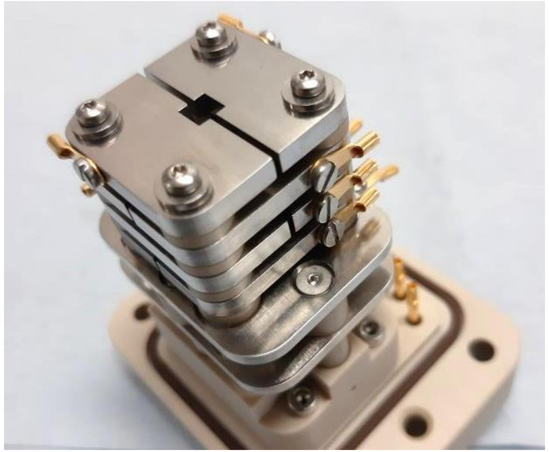
Ta disc

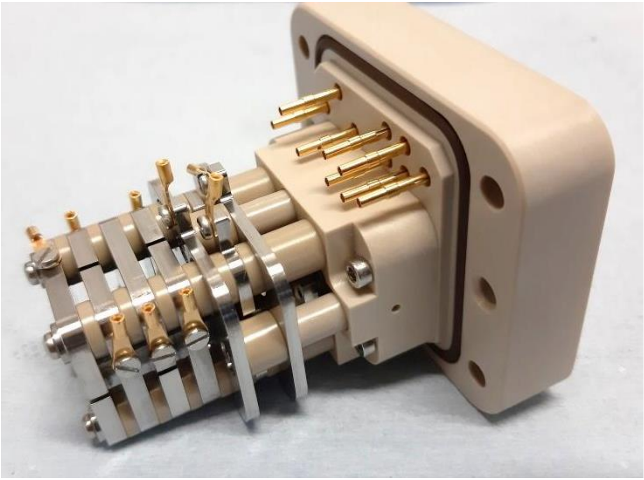
1.6mm diam / 0.1mm thick

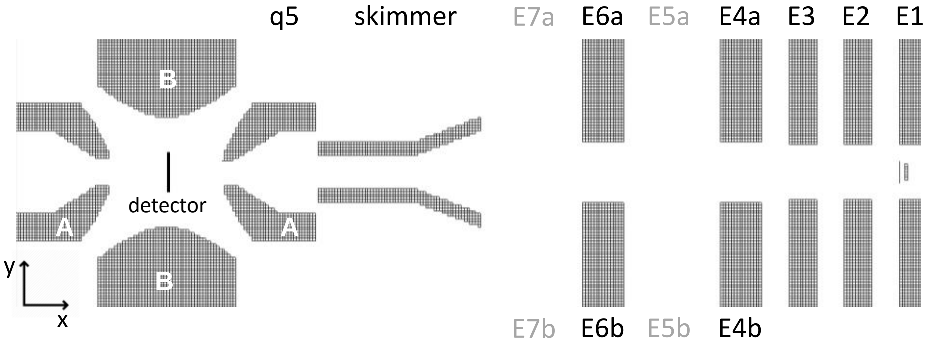
heating current 6A

WP4 – Development & Application of CE

T4.2 Construction 1KeV pulsed electron source



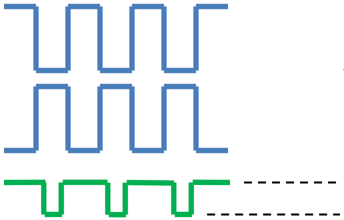




RF phase A

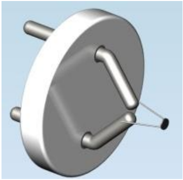
RF phase B

e^- beam
modulation pulse E2



deflection voltage level
transmission windows

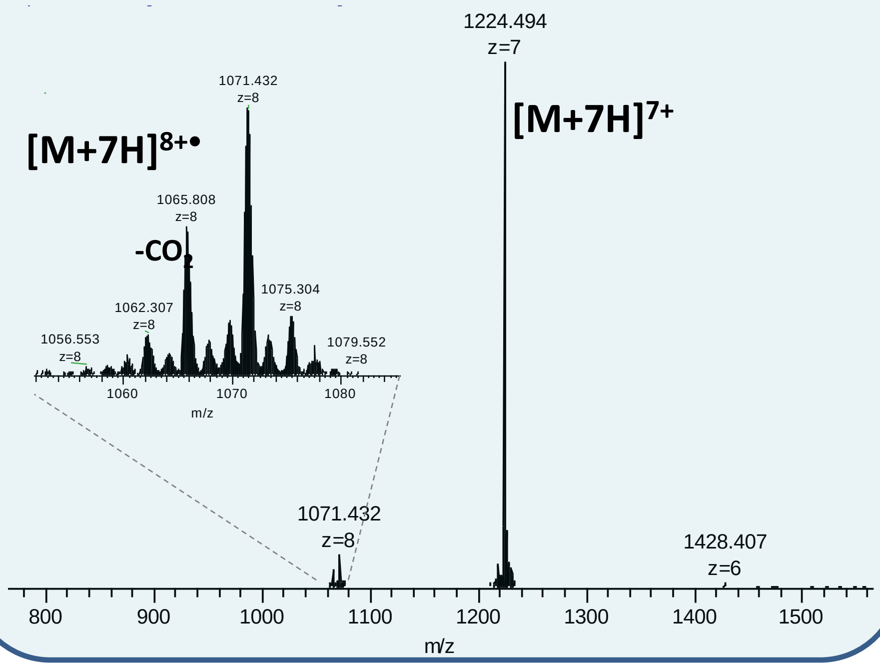
E2 split electrode supplied with deflection pulse to inject at correct RF phase



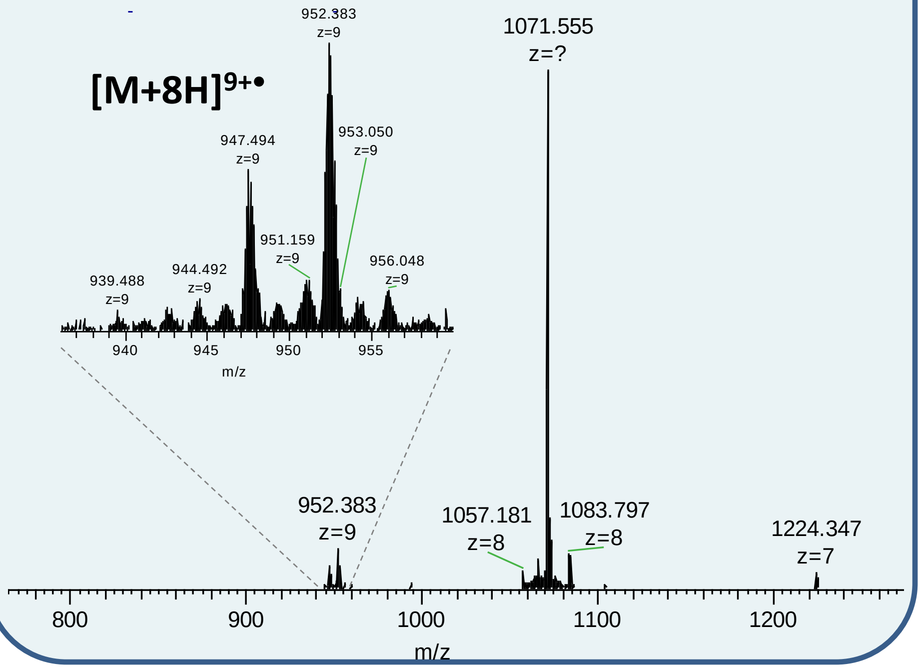
Ta disc
1.6mm diam / 0.1mm thick
heating current 6A

Ubiquitin Electron *meta*-Ionization

$$[M+7H]^{7+} + e^- \longrightarrow [M+7H]^{8+\bullet} + 2e^-$$



$$[M+8H]^{8+} + e^- \longrightarrow [M+8H]^{9+\bullet} + 2e^-$$



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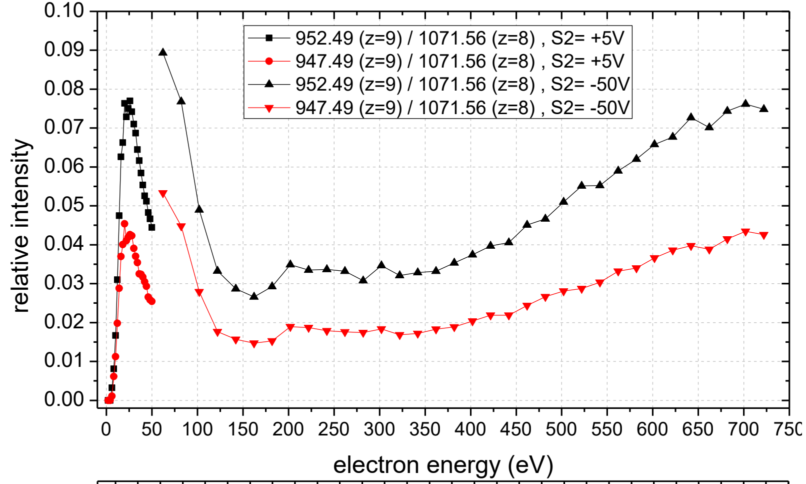
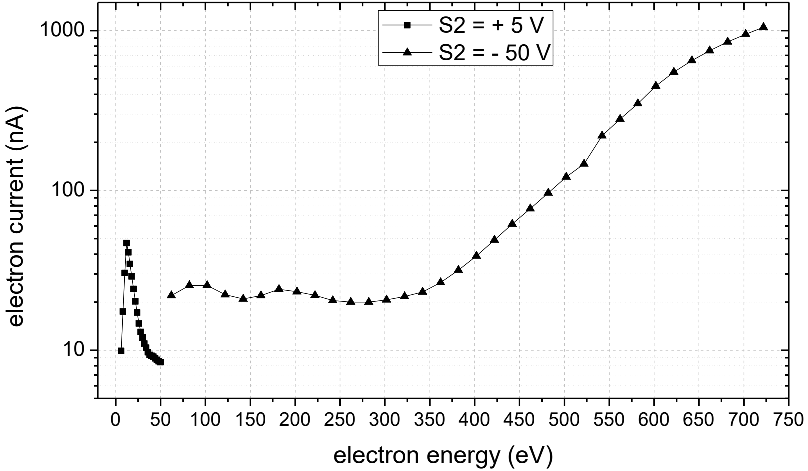
T4.4 Testing CE gun with Omni



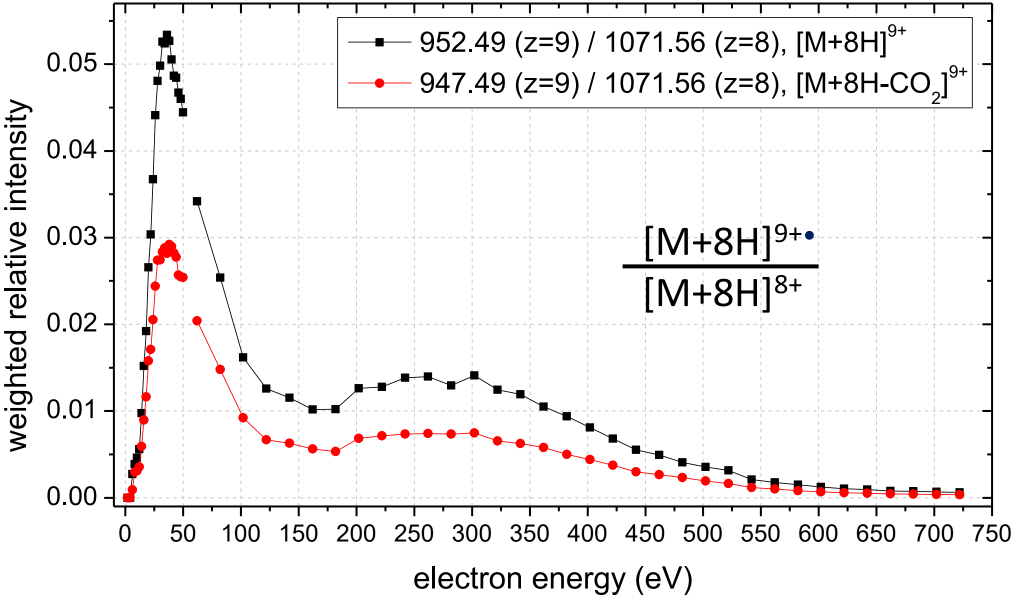


Single ionization of $[M+8H]^{8+}$

$$[M+8H]^{8+} + e_f^- \longrightarrow [M+8H]^{9+\bullet} + e_f^- + e_s^-$$

$$[M+8H]^{8+} + e_f^- \longrightarrow [M+8H\text{-}CO_2]^{9+\bullet} + e_f^- + e_s^-$$

weighted relative intensity = relative intensity × correction factor



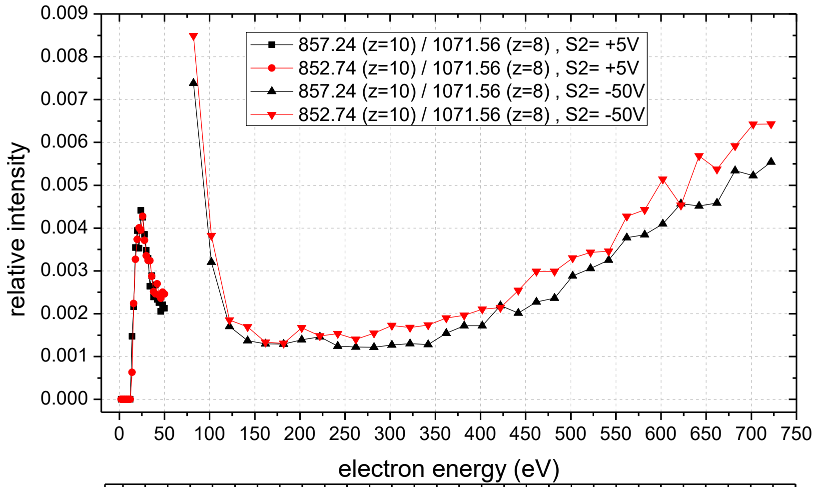
WP4 – Development & Application of CE

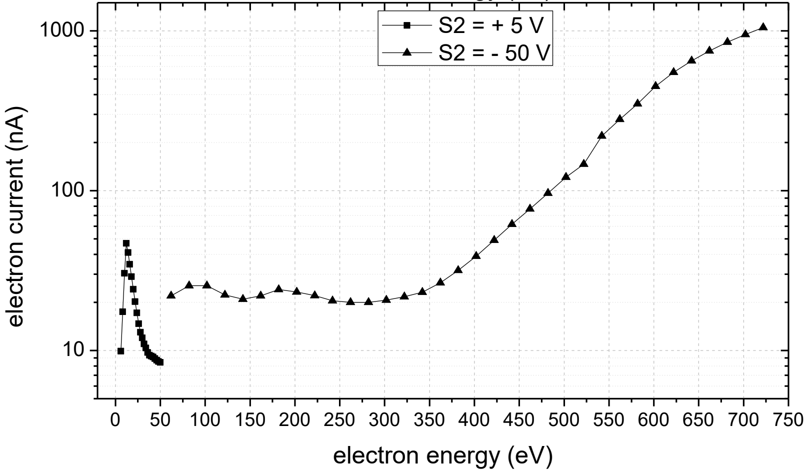
T4.4 Testing CE gun with Omni

Double ionization of $[M+8H]^{8+}$

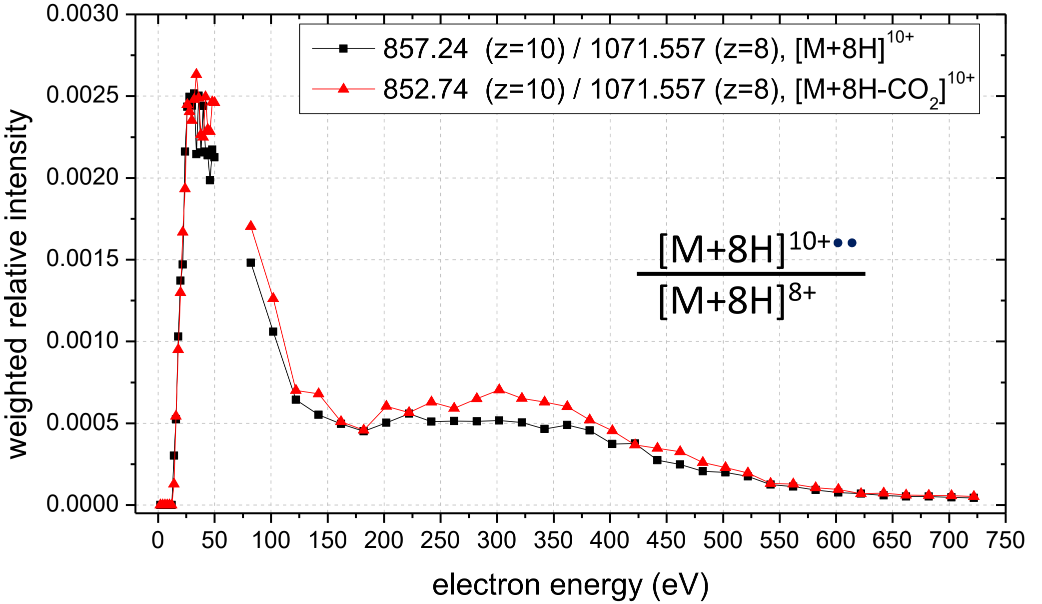
$$[M+8H]^{9+\bullet} + e_f^- \longrightarrow [M+8H]^{10+\bullet\bullet} + e_f^- + e_s^-$$

$$[M+8H]^{9+\bullet} + e_f^- \longrightarrow [M+8H-CO_2]^{10+\bullet\bullet} + e_f^- + e_s^-$$



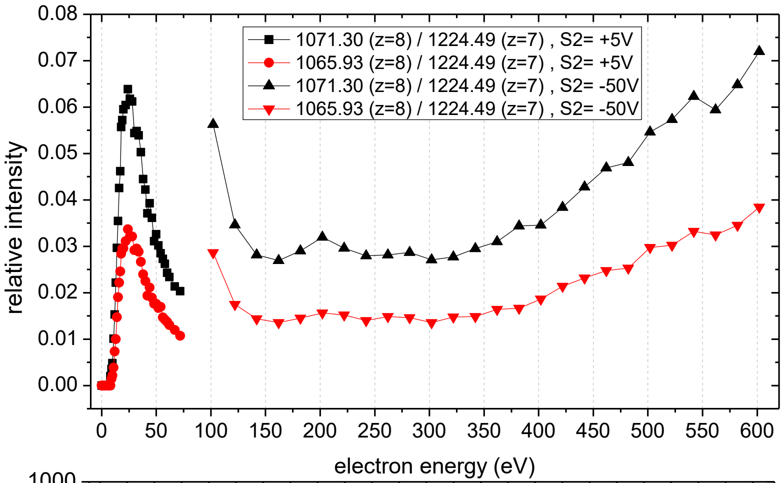


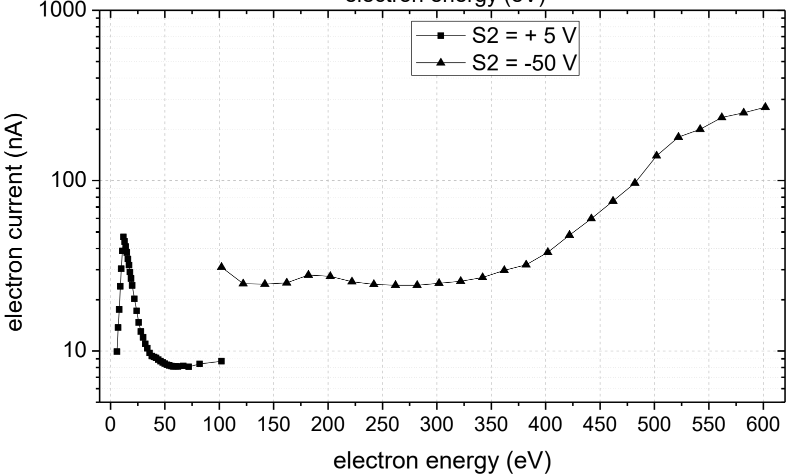
weighted relative intensity = relative intensity × correction factor



WP4 – Development & Application of CE

T4.4 Testing CE gun with Omni



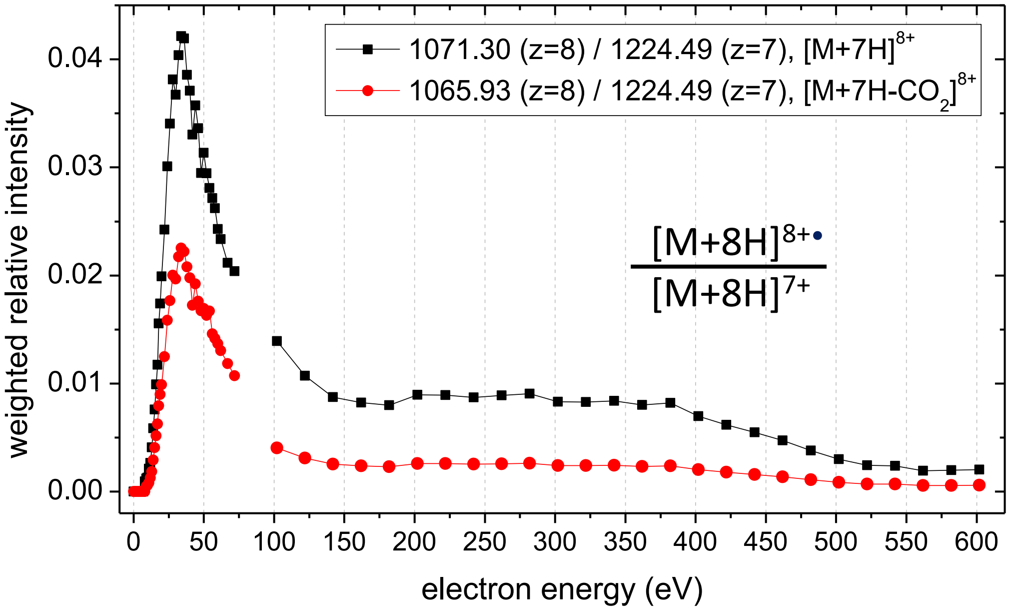


Single ionization of $[M+7H]^{7+}$

$$[M+7H]^{7+} + e_f^- \longrightarrow [M+7H]^{8+\bullet} + e_f^- + e_s^-$$

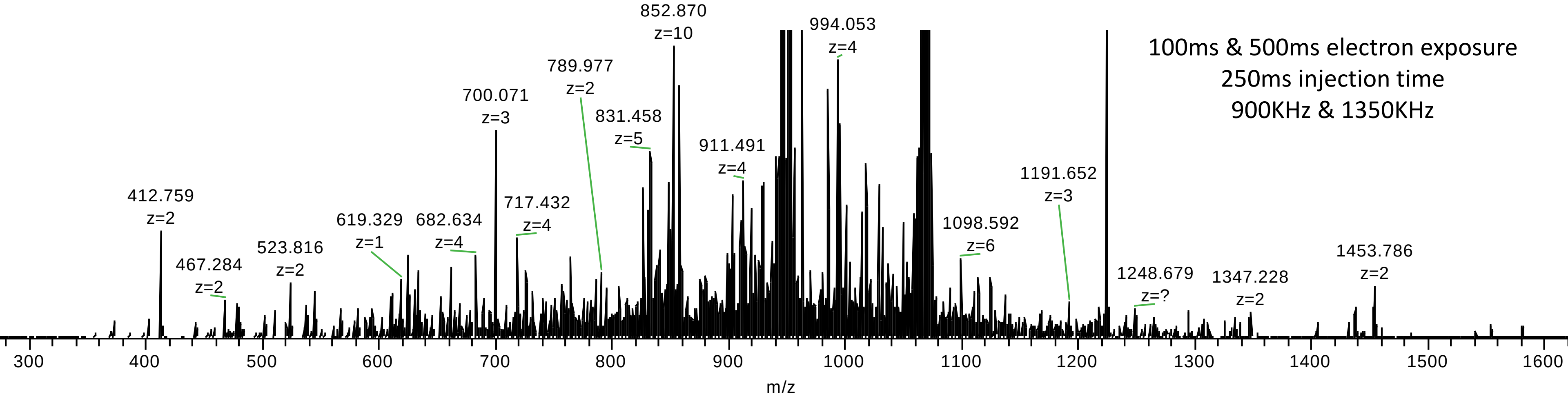
$$[M+7H]^{7+} + e_f^- \longrightarrow [M+7H\text{-}CO_2]^{8+\bullet} + e_f^- + e_s^-$$

weighted relative intensity = relative intensity × correction factor



Electron Induced Dissociation of ubiquitin has been performed at the two maxima observed in the ionization efficiency curves and at higher e energy (35eV, 350eV & 800eV)

Differences in EID performed at different energies are observed !



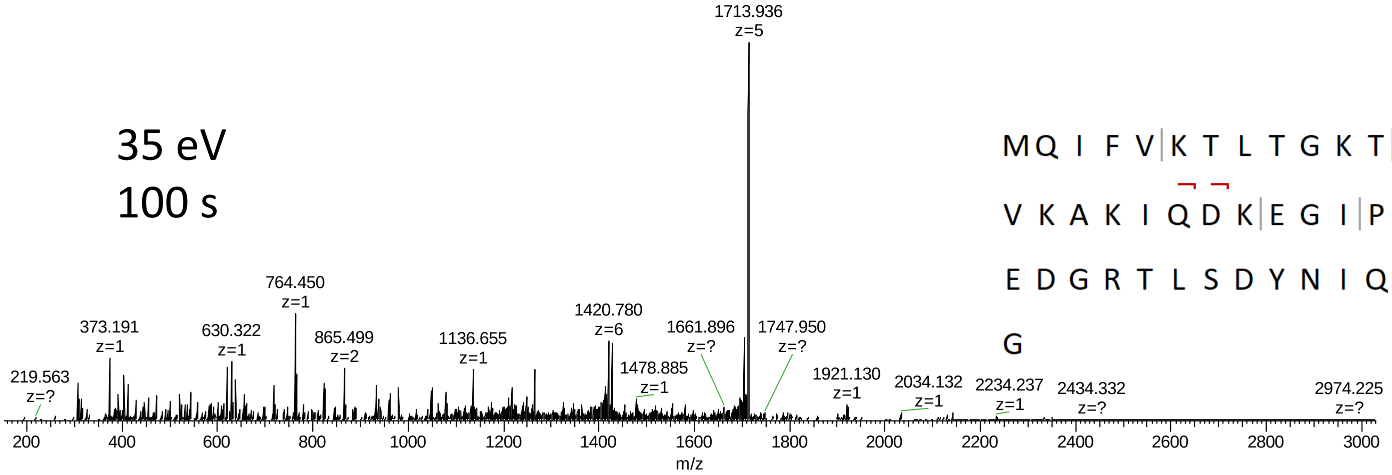
100ms & 500ms electron exposure
250ms injection time
900KHz & 1350KHz

$$[M+8H]^{8+} + e_f^- \longrightarrow [M+8H]^{9+\bullet} + e_f^- + e_s^- \longrightarrow \text{fragments}$$

WP4 – Development & Application of CE

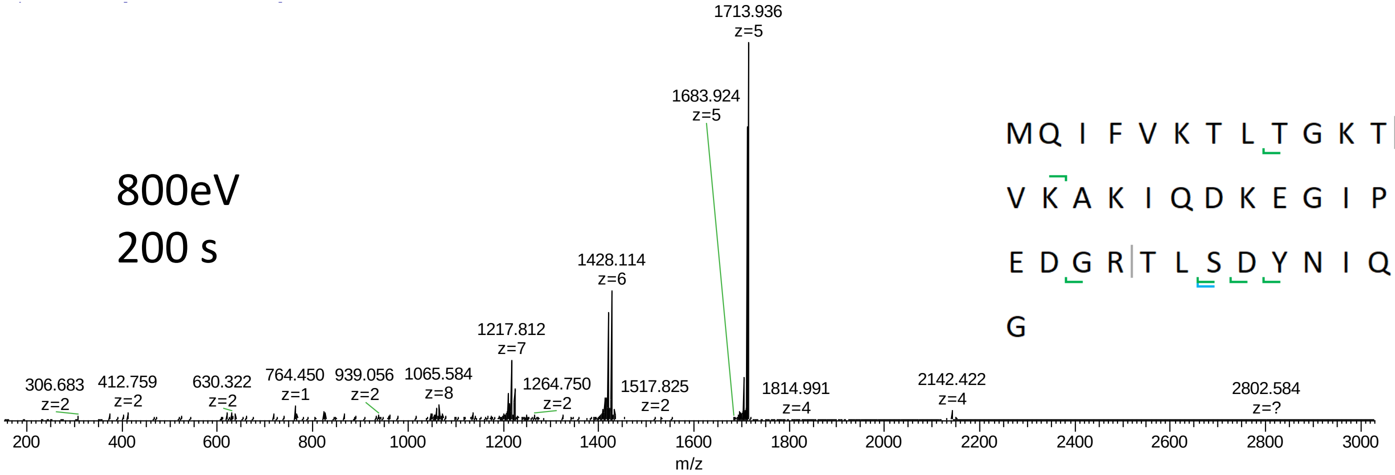
T4.4 Testing CE gun with Omni

35 eV
100 s



MQ I F V K T L T G K T I T L E V E P S D T I E N
V K A K I Q D K E G I P P D Q Q R L I F A G K Q L
E D G R T L S D Y N I Q K E S T L H L V L R L R G
G

800eV
200 s



MQ I F V K T L T G K T I T L E V E P S D T I E N
V K A K I Q D K E G I P P D Q Q R L I F A G K Q L
E D G R T L S D Y N I Q K E S T L H L V L R L R G
G