

Table of Amino Acids and Mass Accuracies

Moving Science Forward with Life Science Solutions.

AMINO ACIDS

Single Letter Code	Three Letter Code	Amino Acid	Average Mass	Accurate Monoisotopic Mass	Accurate Monoisotopic Mass of Immonium Ion
A	Ala	Alanine	71.07870	71.03712	44.04948
C	Cys	Cysteine	103.14500	103.00919	76.02155
D	Asp	Aspartic Acid	115.08850	115.02695	88.0393
E	Glu	Glutamic Acid	129.11560	129.04260	102.05495
F	Phe	Phenylalanine	147.17720	147.06842	120.08078
G	Gly	Glycine	57.05170	57.02147	30.03383
H	His	Histidine	137.14140	137.05891	110.07127
I	Ile	Isoleucine	113.15980	113.08407	86.09643
K	Lys	Lysine	128.17450	128.09497	101.10732
L	Leu	Leucine	113.15980	113.08407	86.09643
M	Met	Methionine	131.19940	131.04050	104.05285
N	Asn	Asparagine	114.10390	114.04293	87.05529
P	Pro	Proline	97.11680	97.05277	70.06513
Q	Gln	Glutamine	128.13091	128.05858	101.07094
R	Arg	Arginine	156.18800	156.10112	129.11347
S	Ser	Serine	87.07800	87.03203	60.04439
T	Thr	Threonine	101.10510	101.04768	74.06004
V	Val	Valine	99.13280	99.06842	72.08078
W	Trp	Tryptophan	186.21410	186.07932	159.09167
Y	Tyr	Tyrosine	163.17661	163.06332	136.07569
Cysteine, carbamidomethylated					133.04301
Cysteine, carboxymethylated					134.02703
PhosphoTyrosine					216.04202

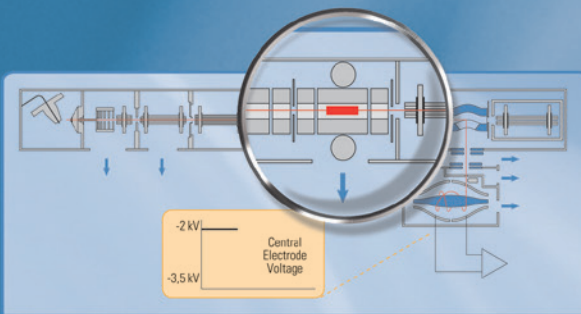
MASS ACCURACIES

Element	Accurate Mass	Rel. Abundance	DB
H	1.00782503	99.9885	-0.5
H	2.01410178	0.0115	-0.5
H	3.01604927	0	-0.5
D	2.01410178	100	-0.5
T	3.01604927	100	-0.5
Li	6.0151223	7.59	-0.5
Li	7.016004	92.41	-0.5
C	12.0	98.93	1
C	13.0033548	1.07	1
C	14.003242	0	1
N	14.003074	99.632	0.5
N	15.0001089	0.368	0.5
O	15.9949146	99.757	0
O	16.9991315	0.038	0
O	17.9991604	0.205	0
F	18.9984032	100	-0.5
Na	22.9897697	100	-0.5
Si	27.9769265	92.2297	1
Si	28.9764947	4.6832	1
Si	29.9737702	3.0872	1
P	30.9737615	100	0.5
P	31.9739072	0	0.5
S	31.9720707	94.93	0
S	32.9714585	0.76	0
S	33.9678668	4.29	0
S	35.9670809	0.02	0
Cl	34.9688527	75.78	-0.5
Cl	36.9659026	24.22	-0.5
K	38.9637069	93.2581	-0.5
K	39.9639987	0.0117	-0.5
K	40.961826	6.7302	-0.5
Br	78.9183376	50.69	-0.5
Br	80.916291	49.31	-0.5
I	126.904468	100	-0.5
I	124.904624	0	-0.5

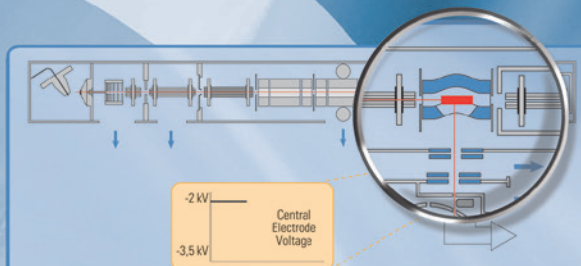
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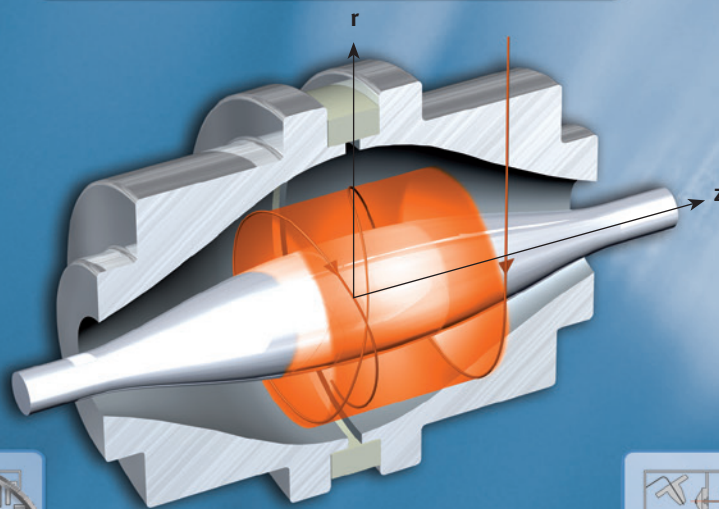
Thermo Scientific Orbitrap Technology – Principle of Operation



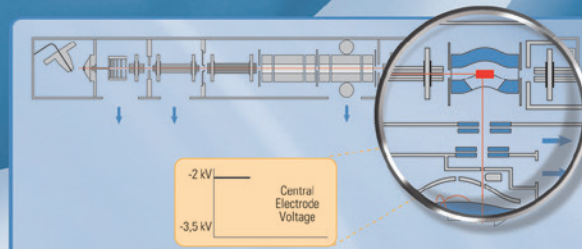
1. Ions are injected from the ion source and trapped in the linear ion trap. Ions of interest can be isolated and fragmented in the linear ion trap, and even scanned out and detected by an independent set of detectors.



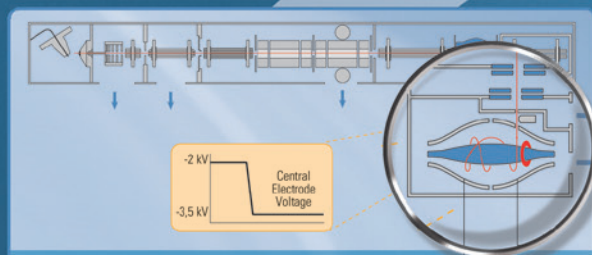
2. To obtain high accuracy measurements, the ions are axially ejected from the linear trap into the C-Trap where they are captured again and 'cooled' by collisions with nitrogen gas.



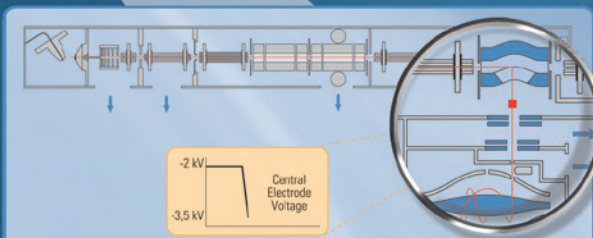
Measured mass is proportional to the frequency of axial oscillations: $\omega_z = \sqrt{\frac{k}{m/q}}$



3. The ions are squeezed into a smaller cloud within the C-Trap ready for injection into the Orbitrap™ mass analyzer.



5. The ions entered the Orbitrap slightly off axis, and keep oscillating along the central electrode (left-right). The image current is recorded on the outer split electrodes. The signals are amplified and transformed into a frequency spectrum by fast Fourier Transformation which is finally converted into a mass spectrum.



4. As the ions are entering the Orbitrap mass analyzer, the voltage on the central electrode increases and forces the ion packets into circling around the electrode. The Orbitrap, and voltages on the Orbitrap start to change.