

Isotope Ratio Mass spectrometry (IR-MS)

Extremely high accuracy of measuring ratios of isotope peak intensities

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The principle

- Ratios of isotope abundances of an element in a compound are measured with very high accuracy
- Gives information about the **origin of the element** in the sample
 - The most usual elements: H, C, N, O or S

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Element	Symbol	Atomic Weight	Relative Abundance (%)	Element	Symbol	Atomic Weight	Relative Abundance (%)
H	¹ H	1.007825	99.985	H	² H	2.014102	0.015
He	³ He	3.016029	0.000137	He	⁴ He	4.002603	99.999863
Li	⁶ Li	6.015122	7.59	Li	⁷ Li	7.016003	92.41
B	¹⁰ B	10.012937	19.9	B	¹¹ B	11.009305	80.1
C	¹² C	12.000000	98.93	C	¹³ C	13.003355	1.07
N	¹⁴ N	14.003074	99.63	N	¹⁵ N	15.003065	0.37
O	¹⁶ O	15.994915	99.76	O	¹⁷ O	16.999131	0.04
F	¹⁹ F	18.998403	100				
Ne	²⁰ Ne	19.992436	90.51	Ne	²¹ Ne	20.993847	0.27
Ne	²² Ne	21.991385	9.25				
Na	²³ Na	22.989769	100				
Mg	²⁴ Mg	23.985042	78.99	Mg	²⁵ Mg	24.985837	10.04
Mg	²⁶ Mg	25.982593	11.01				
Al	²⁷ Al	26.981538	100				
Si	²⁸ Si	27.976927	92.23	Si	²⁹ Si	28.976495	4.68
Si	³⁰ Si	29.973762	3.09				
P	³¹ P	30.973762	100				
S	³² S	31.972071	95.02	S	³³ S	32.971736	4.18
S	³⁴ S	33.973364	4.21				
S	³⁶ S	35.967081	0.02				
Cl	³⁵ Cl	34.968853	75.77	Cl	³⁷ Cl	36.965903	24.23
Ar	³⁶ Ar	35.967546	99.6	Ar	³⁸ Ar	37.962732	0.337
Ar	³⁹ Ar	38.964489	0.000119				
Ar	⁴⁰ Ar	39.962434	9.96				
K	³⁹ K	38.963707	93.26	K	⁴⁰ K	39.964037	6.73
K	⁴¹ K	40.961825	6.73				
Ca	⁴⁰ Ca	39.962494	96.94	Ca	⁴² Ca	41.958618	0.647
Ca	⁴³ Ca	42.958751	0.135				
Ca	⁴⁴ Ca	43.959467	2.08				
Ca	⁴⁶ Ca	45.952634	0.004				
Ca	⁴⁸ Ca	47.947152	0.187				
Sc	⁴⁵ Sc	44.955937	100				
Ti	⁴⁸ Ti	47.947152	72.8	Ti	⁴⁹ Ti	48.947867	5.41
Ti	⁵⁰ Ti	49.944789	5.11				
Ti	⁵² Ti	51.940769	3.61				
Ti	⁵⁴ Ti	53.937077	0.47				
V	⁵¹ V	50.943867	99.75	V	⁵⁰ V	49.944789	0.25
Cr	⁵² Cr	51.940769	73.73	Cr	⁵³ Cr	52.940651	2.62
Cr	⁵⁴ Cr	53.937077	2.36				
Cr	⁵⁶ Cr	55.934836	2.34				
Cr	⁵⁸ Cr	57.933279	0.15				
Mn	⁵⁵ Mn	54.938045	100				
Fe	⁵⁶ Fe	55.934836	91.75	Fe	⁵⁷ Fe	56.935297	2.12
Fe	⁵⁸ Fe	57.933279	0.28				
Fe	⁶⁰ Fe	59.930746	0.026				
Co	⁵⁹ Co	58.933195	100				

Example: carbon

- Natural elements are mostly **mixtures of isotopes**:
- In **standard** natural C:
 - Approximately 98.9 % is ¹²C
 - Approximately 1.1 % is ¹³C
- In reality, depending on origin ¹³C content can differ markedly: **isotopic fractionation**

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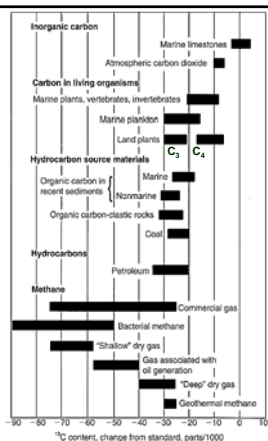
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¹³C content of carbon depending on origin

– $\delta^{13}\text{C}$ Scale:
 $\%^{13}\text{C} = 1.11\% \rightarrow \delta^{13}\text{C} = 0$
 $\%^{13}\text{C} = 1.06\% \rightarrow \delta^{13}\text{C} = -44$

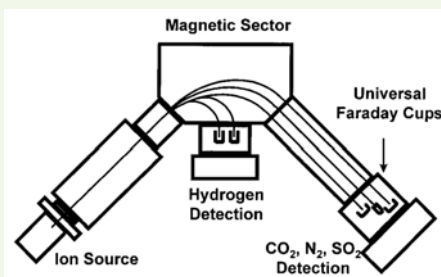
– Different photosynthesis pathways:
 • C₃ (wheat, rye, ...)
 • C₄ (sugar cane, tropical plants)

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IR-MS instrument

- Carbon is often converted to CO₂



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