



LAB REPORT OES 30

Q6 NEWTON

Analysis of Iron & Steel Alloys

The analysis of elemental composition in iron and steel is essential for quality control and process optimization in production. Bruker's Q6 NEWTON is a pioneering instrument that offers exceptional accuracy and precision in determining the concentrations of a wide range of elements, including carbon, sulfur, phosphorus, silicon, manganese, nitrogen, and much more. With improved sensitivity and resolution, the Q6 NEWTON represents a significant advancement over conventional systems.

The Q6 NEWTON is the superior OES solution for metallurgists and technicians to analyze alloy composition of iron and steel alloys. HighSense™ detection technology, SmartSpark™ source, and RockSteady™, the active thermal stability control, are the key elements to achieve ultimate precision, speed, and reliability in metals analysis.

One push of a button unleashes the power of the Q6 NEWTON, which provides lightning-fast measurements, excellent precision and accuracy, and extremely low detection limits at 24/7 operation.

Sampling and Sample Preparation

The chemical composition of different stages of the steel refining process and casting are monitored by determining the composition of the steel or iron samples taken from the molten bath.

The samples are prepared by grinding or milling to have a flat and homogenous surface.

All samples in this lab report were prepared following the sample preparation procedure with a grinding or milling machine.



Figure 1 Cast Iron Production

Certified Reference Material (CRM)

Certified Reference Materials (CRM) are reference materials characterized by a metrologically valid procedure for one or more specified properties, accompanied by a certificate that provides the value of the specified property, its associated uncertainty, and a statement of metrological traceability.

CRMs are certified by a recognized certifying organization using approved certification procedures, as instructed in the most recent ISO Guide 35. The organization is usually a function of a federal government or an accreditation entity.

A CRM is the highest level to which an analytical reference material can be elevated because it is directly traceable to SI units and because of the confidence attributed to the company or organization that produced the material.

Statistics

Population: the entire group that you want to draw conclusions about.

Sample: a specific group that you will collect data from.

Average ($\bar{X}$): a number expressing the central or typical value in a set of data, in particular the mode, median, or (most commonly) the mean, which is calculated by dividing the sum of the values in the set by their number.

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i$$

Standard Deviation (σ): a measure of the amount of variation or dispersion of a set of values.

$$\sigma(r) = \sqrt{\frac{1}{N-1} \sum_{i=1}^n (X_i - r)^2}$$

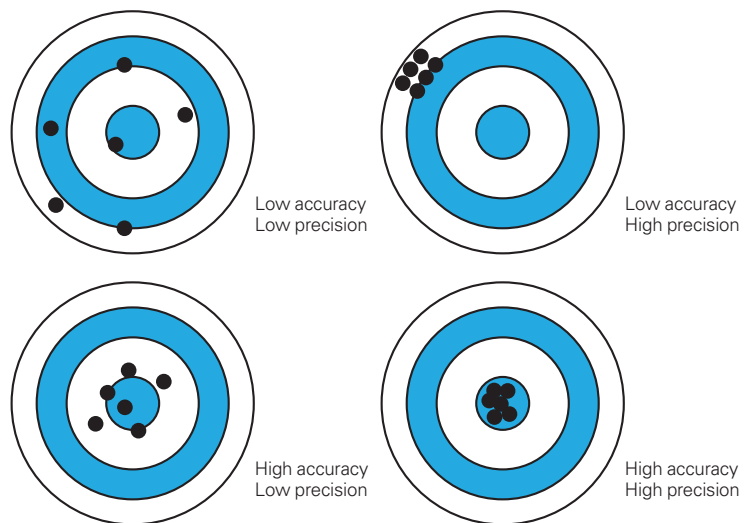
Precision and Accuracy

The International Organization for Standardization (ISO) defines precision as the closeness of agreement between independent test results obtained under stipulated conditions.

Precision depends only on the distribution of random errors and does not relate to the true value or the specified value, while accuracy is defined as the closeness of agreement between a test result and the accepted reference value.

Figure 2

Precision and accuracy



Q6 NEWTON – Certified Reference Material and Reference Materials

Table 1

Calibration ranges and detection limits (3 sigma) for iron base

Element	Fe-base		Detection Limit (ppm)
	Calibration Range		
	min %	max %	
Al	0.0003	9.5	3
As	0.0003	0.10	3
B	0.0001	2.2	1
Bi	0.0004	0.13	4
C	0.0007	4.7	7
Ca	0.00005	0.016	0.5
Ce	0.0008	0.25	8
Co	0.0003	19	3
Cr	0.0002	42	2
Cu	0.0001	8.2	1
La	0.0004	0.25	4
Mg	0.00005	0.20	0.5
Mn	0.0004	31	4
Mo	0.0004	11	4
N	0.0010	1.2	10
Nb	0.0003	3	3
Ni	0.0004	52	4
O	0.0060	0.03	60
P	0.0003	2.4	3
Pb	0.0002	0.25	2
S	0.0002	1.35	2
Sb	0.0016	0.22	16
Se	0.0002	0.4	2
Si	0.0005	6	5
Sn	0.0002	0.45	2
Ta	0.004	0.55	40
Te	0.001	0.09	10
Ti	0.0001	2.5	1
V	0.0003	11	3
W	0.0028	19.5	28
Zn	0.0001	0.03	1
Zr	0.0001	0.22	1



Table 2

CRM - Low Alloy Steel – ULC - Ultra Low Carbon Steels

Element %	C	Si	Mn	P	S	Cr	Mo	Ni	Cu	Al	Ti	Co	As	B	N
MEAN ¹⁾	0.0023	0.0053	0.018	0.012	0.0027	0.023	0.0053	0.011	0.0035	0.0077	0.0002	0.0015	0.0034	0.0004	0.0016
STD ²⁾	0.0001	0.0001	0.0003	0.0003	0.0001	0.0002	0.0002	0.0002	0.00006	0.0002	0.00002	0.00009	0.00009	0.00001	0.0002
1	0.0025	0.0051	0.018	0.012	0.0027	0.023	0.0053	0.011	0.0036	0.0073	0.0002	0.0016	0.0034	0.0004	0.0018
2	0.0023	0.0052	0.018	0.012	0.0027	0.023	0.0054	0.011	0.0036	0.0079	0.0002	0.0014	0.0034	0.0004	0.0015
3	0.0022	0.0054	0.018	0.012	0.0025	0.023	0.0056	0.011	0.0035	0.0077	0.0002	0.0017	0.0034	0.0004	0.0016
4	0.0023	0.0052	0.018	0.012	0.0028	0.023	0.005	0.011	0.0036	0.0076	0.0002	0.0015	0.0035	0.0004	0.0013
5	0.0024	0.0054	0.018	0.011	0.0026	0.023	0.0052	0.011	0.0034	0.0078	0.0002	0.0015	0.0033	0.0004	0.0017
<i>Certified Values</i>															
Value	0.0023	0.0054	0.018	0.012	0.0027	0.023	0.0053	0.011	0.0036	0.0078	0.0002	0.0015	0.0034	0.0004	0.0016
Error ³⁾	0.0002	0.0002	0.001	0.001	0.0002	0.001	0.0002	0.001	0.0002	0.0004	0.0001	0.0002	0.0002	0.0001	0.0001

Table 3

CRM - Low Alloy Steel – Medium Carbon Steels

Element %	C	Si	Mn	P	S	Cr	Mo	Ni	Cu
MEAN ¹⁾	0.385	0.436	1.476	0.038	0.030	0.406	0.071	0.206	0.166
STD ²⁾	0.0023	0.0029	0.0070	0.0009	0.0005	0.0058	0.0008	0.0015	0.0025
1	0.386	0.436	1.483	0.038	0.031	0.407	0.071	0.205	0.168
2	0.385	0.431	1.465	0.036	0.030	0.403	0.070	0.204	0.162
3	0.388	0.438	1.476	0.038	0.031	0.403	0.072	0.208	0.167
4	0.387	0.436	1.481	0.038	0.030	0.416	0.071	0.206	0.168
5	0.382	0.438	1.474	0.038	0.030	0.402	0.070	0.205	0.167
<i>Certified Values</i>									
Value	0.387	0.436	1.47	0.038	0.030	0.409	0.071	0.206	0.167
Error ³⁾	0.004	0.003	0.01	0.002	0.001	0.004	0.002	0.003	0.003

Element %	Al	Ti	V	Co	Nb	Sn	As	B	N
MEAN ¹⁾	0.051	0.123	0.207	0.248	0.112	0.152	0.043	0.0052	0.0051
STD ²⁾	0.0004	0.0014	0.0012	0.0030	0.0023	0.0018	0.0015	0.00015	0.0002
1	0.050	0.122	0.208	0.244	0.112	0.150	0.045	0.0052	0.0053
2	0.051	0.122	0.207	0.249	0.111	0.152	0.043	0.0054	0.0049
3	0.051	0.125	0.208	0.247	0.111	0.155	0.041	0.0051	0.0053
4	0.051	0.124	0.205	0.251	0.110	0.152	0.044	0.0051	0.0051
5	0.051	0.122	0.207	0.251	0.116	0.152	0.043	0.0054	0.0050
<i>Certified Values</i>									
Value	0.050	0.124	0.201	0.248	0.106	0.151	0.045	0.005	0.005
Error ³⁾	0.001	0.002	0.004	0.003	0.003	0.004	0.002	0.0003	0.0002

¹⁾ MEAN = arithmetic average²⁾ STD = absolute standard deviation (1σ)³⁾ Error = short for the absolute uncertainty of the certified value at the specified confidence level

Table 4
CRM - Low Alloy Steel – High Carbon Steels

Element %	C	Si	Mn	P	S	Cr	Mo	Ni	Cu	Al	As
MEAN ¹⁾	1.013	0.350	2.241	0.027	0.021	2.338	0.016	0.271	0.088	0.023	0.0065
STD ²⁾	0.0046	0.0011	0.0051	0.0003	0.0021	0.0098	0.0003	0.0012	0.0004	0.0006	0.00005
1	1.011	0.349	2.237	0.027	0.024	2.327	0.016	0.271	0.088	0.024	0.0065
2	1.010	0.350	2.242	0.027	0.022	2.329	0.016	0.272	0.089	0.023	0.0064
3	1.021	0.351	2.248	0.028	0.019	2.345	0.016	0.271	0.088	0.022	0.0065
4	1.013	0.350	2.241	0.027	0.022	2.349	0.015	0.269	0.089	0.022	0.0065
5	1.012	0.352	2.234	0.027	0.020	2.341	0.016	0.273	0.089	0.022	0.0065
<i>Certified Values</i>											
Value	1.013	0.348	2.23	0.028	-	2.33	0.016	0.250	0.089	0.022	0.006
Error ³⁾	0.012	0.008	0.03	0.002	-	0.02	0.004	0.008	0.002	0.002	0.001

Element %	B	Ce	Co	Mg	Nb	Pb	Sb	Sn	Ta	La	Ti
MEAN ¹⁾	0.0005	<0.0008	0.0070	0.0002	0.013	0.0007	0.0022	0.0071	<0.0040	0.0012	0.011
STD ²⁾	0.00002		0.0002	-	0.0006	0.00007	0.0005	0.00007	-	0.00009	0.0009
1	0.0004	<0.0008	0.0071	0.0002	0.013	0.0007	0.0018	0.0072	<0.0040	0.0012	0.010
2	0.0005	<0.0008	0.0067	0.0002	0.013	0.0006	0.0028	0.0071	<0.0040	0.0012	0.011
3	0.0005	<0.0008	0.0071	0.0002	0.014	0.0006	0.0026	0.0070	<0.0040	0.0012	0.012
4	0.0004	<0.0008	0.0069	0.0002	0.013	0.0007	0.0022	0.0071	<0.0040	0.0011	0.011
5	0.0004	<0.0008	0.0072	0.0002	0.013	0.0008	0.0017	0.0071	<0.0040	0.0014	0.012
<i>Certified Values</i>											
Value	0.0005	-	0.007	-	0.013	-	0.002	0.008	-	-	0.010
Error ³⁾	0.0002	-	0.002	-	0.001	-	0.0007	0.001	-	-	0.002

Element %	V	W	Zn	Zr	Se	Ca	Te	Bi	N	O	Fe
MEAN ¹⁾	0.018	0.0044	0.0005	0.0007	<0.0002	<0.00005	0.0022	0.0014	0.0106	<0.0060	93.52
STD ²⁾	0.00007	0.0014	0.00006	0.00005	-	-	0.0008	0.00006	0.0003	-	0.017
1	0.018	0.0031	0.0005	0.0008	0.0023	<0.00005	0.0028	0.0014	0.0105	<0.0060	93.54
2	0.018	0.0028	0.0006	0.0007	0.0004	<0.00005	0.0012	0.0013	0.0103	<0.0060	93.54
3	0.018	0.0062	0.0006	0.0007	<0.0002	<0.00005	0.0030	0.0014	0.0107	<0.0060	93.50
4	0.018	0.0052	0.0005	0.0007	<0.0002	<0.00005	0.0024	0.0014	0.0107	<0.0060	93.51
5	0.018	0.0049	0.0005	0.0007	<0.0002	<0.00005	0.0015	0.0014	0.0110	<0.0060	93.53
<i>Certified Values</i>											
Value	0.017	-	-	-	-	-	-	-	0.104	-	-
Error ³⁾	0.003	-	-	-	-	-	-	-	0.0005	-	-

¹⁾ MEAN = arithmetic average

²⁾ STD = absolute standard deviation (1σ)

³⁾ Error = short for the absolute uncertainty of the certified value at the specified confidence level

Table 5

CRM - Cast Iron

Element %	C	Si	Mn	P	S	Cr	Mo	Ni	Cu	Al
MEAN ¹⁾	4.064	0.494	0.098	0.272	0.0075	0.147	0.011	1.217	0.488	0.032
STD ²⁾	0.0078	0.0036	0.0009	0.0058	0.0005	0.0018	0.00005	0.0038	0.0048	0.0004
1	4.065	0.496	0.099	0.264	0.0070	0.145	0.011	1.215	0.484	0.032
2	4.065	0.490	0.099	0.270	0.0073	0.149	0.011	1.211	0.497	0.032
3	4.068	0.493	0.099	0.280	0.0084	0.147	0.011	1.217	0.487	0.032
4	4.071	0.490	0.097	0.274	0.0077	0.145	0.011	1.219	0.488	0.031
5	4.049	0.493	0.098	0.275	0.0074	0.149	0.011	1.219	0.484	0.032
6	4.059	0.496	0.099	0.275	0.0072	0.149	0.011	1.223	0.492	0.031
7	4.071	0.500	0.098	0.266	0.0071	0.148	0.011	1.215	0.485	0.032
Certified Values										
Value	4.06	0.49	0.099	0.27	0.0075	0.148	0.011	1.21	0.486	0.032
Error ³⁾	0.03	0.01	0.002	0.01	0.0007	0.002	0.001	0.02	0.005	0.002

Element %	As	B	Ce	Co	Mg	Nb	Pb	Sb	Sn	La
MEAN ¹⁾	0.016	0.017	0.019	0.014	0.042	0.011	0.0090	0.0048	0.0019	0.0045
STD ²⁾	0.0004	0.0002	0.0045	0.0003	0.0009	0.0002	0.0003	0.0010	0.00005	0.0003
1	0.015	0.017	0.029	0.014	0.043	0.011	0.0087	0.0039	0.0018	0.0040
2	0.015	0.017	0.017	0.015	0.042	0.011	0.0091	0.0054	0.0020	0.0049
3	0.017	0.017	0.018	0.014	0.043	0.011	0.0086	0.0042	0.0020	0.0048
4	0.016	0.017	0.017	0.014	0.041	0.011	0.0094	0.0051	0.0019	0.0041
5	0.016	0.018	0.018	0.014	0.041	0.011	0.0089	0.0060	0.0020	0.0043
6	0.016	0.017	0.017	0.013	0.042	0.011	0.0090	0.0059	0.0020	0.0043
7	0.016	0.017	0.018	0.014	0.043	0.011	0.0095	0.0034	0.0019	0.0047
Certified Values										
Value	0.016	0.017	0.017	0.014	0.042	0.011	0.009	0.005	0.002	0.004
Error ³⁾	0.001	0.001	0.002	0.001	0.002	0.001	0.001	0.001	0.001	0.001

Element %	Ti	V	W	Zn	Zr	Se	Te	Bi	N	Fe
MEAN ¹⁾	0.026	0.026	0.0079	0.0065	0.026	0.0027	0.0047	0.0040	0.011	92.91
STD ²⁾	0.0002	0.0003	0.0015	0.0002	0.0002	0.0002	0.0005	0.0004	0.0003	0.011
1	0.026	0.026	0.0098	0.0064	0.026	0.0025	0.0046	0.0034	0.011	92.92
2	0.026	0.026	0.0097	0.0067	0.026	0.0027	0.0054	0.0037	0.011	92.91
3	0.026	0.026	0.0084	0.0064	0.026	0.0031	0.0048	0.0041	0.011	92.90
4	0.026	0.026	0.0062	0.0063	0.026	0.0025	0.0046	0.0037	0.011	92.92
5	0.026	0.026	0.0068	0.0067	0.026	0.0027	0.0040	0.0046	0.010	92.93
6	0.026	0.026	0.0083	0.0067	0.026	0.0027	0.0043	0.0042	0.011	92.90
7	0.026	0.026	0.0064	0.0062	0.026	0.0027	0.0052	0.0043	0.011	92.92
Certified Values										
Value	0.026	0.026	0.009	0.006	0.027	-	-	0.004	-	92.9
Error ³⁾	0.002	0.002	0.001	0.001	0.001	-	-	0.001	-	-

Table 6

CRM – Austenitic Stainless Steel

Element %	C	Si	Mn	P	S	Cr	Mo	Ni	Cu	B	Co	Ti	N
MEAN ¹⁾	0.019	0.272	1.406	0.025	0.019	18.46	0.265	10.22	0.276	0.0022	0.116	0.0024	0.063
STD ²⁾	0.0001	0.0016	0.0030	0.0004	0.0006	0.020	0.0053	0.017	0.0016	0.00004	0.001	0.00006	0.0007
1	0.019	0.273	1.411	0.025	0.02	18.46	0.271	10.23	0.278	0.0022	0.117	0.0025	0.063
2	0.019	0.272	1.406	0.025	0.018	18.48	0.262	10.19	0.274	0.0022	0.115	0.0024	0.063
3	0.019	0.275	1.408	0.025	0.019	18.42	0.266	10.21	0.275	0.0022	0.118	0.0024	0.062
4	0.019	0.270	1.405	0.025	0.019	18.47	0.256	10.22	0.278	0.0023	0.116	0.0024	0.064
5	0.019	0.273	1.402	0.026	0.019	18.46	0.269	10.24	0.276	0.0023	0.116	0.0023	0.064
<i>Certified Values</i>													
Value	0.019	0.270	1.400	0.025	0.019	18.46	0.265	10.20	0.276	0.0022	0.116	0.002	0.063
Error ³⁾	0.002	0.008	0.011	0.002	0.002	0.05	0.008	0.06	0.005	0.0003	0.005	-	0.002

Table 7

CRM – High Speed Tool Steel

Element %	C	Si	Mn	P	S	Cr	Mo	Al	Co	V	W
MEAN ¹⁾	1.023	0.183	0.269	0.022	0.029	3.918	9.447	0.0068	7.943	1.145	1.810
STD ²⁾	0.0026	0.0029	0.0022	0.0001	0.0003	0.0054	0.036	0.0014	0.054	0.0074	0.020
1	1.020	0.185	0.270	0.022	0.029	3.918	9.415	0.0063	7.992	1.148	1.830
2	1.022	0.183	0.269	0.022	0.029	3.918	9.445	0.0082	7.980	1.150	1.823
3	1.024	0.185	0.272	0.022	0.028	3.920	9.408	0.0084	7.942	1.134	1.822
4	1.024	0.182	0.266	0.022	0.029	3.910	9.476	0.0060	7.951	1.153	1.789
5	1.027	0.178	0.268	0.022	0.029	3.925	9.491	0.0053	7.855	1.143	1.787
<i>Certified Values</i>											
Value	1.02	0.18	0.26	0.022	0.029	3.91	9.41	0.006	7.95	1.14	1.80
Error ³⁾	0.01	0.02	0.02	0.002	0.002	0.03	0.17	0.002	0.12	0.03	0.07

Table 8

CRM - Manganese Steel

Element %	C	Si	Mn	P	S	Cr	Mo	Ni	Cu
MEAN ¹⁾	0.876	0.788	11.78	0.096	0.0121	0.172	0.956	3.017	0.0141
STD ²⁾	0.0041	0.0052	0.027	0.0016	0.00014	0.0011	0.0092	0.0061	0.0002
1	0.882	0.788	11.79	0.096	0.0121	0.171	0.962	3.007	0.0140
2	0.874	0.786	11.76	0.095	0.0123	0.171	0.953	3.022	0.0141
3	0.879	0.787	11.77	0.099	0.0122	0.171	0.966	3.022	0.0140
4	0.873	0.798	11.78	0.095	0.0120	0.172	0.957	3.016	0.0145
5	0.873	0.785	11.83	0.096	0.0120	0.173	0.942	3.018	0.0140
<i>Certified Values</i>									
Value	0.873	0.782	11.74	0.098	0.0118	0.178	0.955	3.010	-
Error ³⁾	0.009	0.015	0.06	0.003	0.0008	0.006	0.018	0.029	-

¹⁾ MEAN = arithmetic average²⁾ STD = absolute standard deviation (1 σ)³⁾ Error = short for the absolute uncertainty of the certified value at the specified confidence level

Table 8 (cont.)
CRM - Manganese Steel

Element %	Al	Co	Nb	Sn	Ti	V	N	Fe
MEAN ¹⁾	0.037	0.0095	0.0047	0.0046	0.0027	0.0168	0.026	82.18
STD ²⁾	0.0021	0.00017	0.00007	0.00008	0.00001	0.0004	0.00055	0.075
1	0.036	0.0094	0.0048	0.0045	0.0027	0.017	0.026	82.17
2	0.035	0.0098	0.0047	0.0046	0.0027	0.016	0.026	82.21
3	0.039	0.0094	0.0047	0.0045	0.0027	0.017	0.027	82.18
4	0.040	0.0094	0.0046	0.0046	0.0027	0.017	0.026	82.18
5	0.037	0.0095	0.0047	0.0047	0.0027	0.017	0.027	82.15
Certified Values								
Value	0.0375	-	-	-	-	-	-	-
Error ³⁾	0.0017	-	-	-	-	-	-	-



Summary

The Q6 NEWTON is designed to revolutionize alloy composition analysis in the metals industry. With its cutting-edge features and unparalleled performance, the Q6 NEWTON empowers metallurgists and technicians to achieve precision, speed, and reliability like never before.

ELEMENTAL.SUITE

ELEMENTAL.SUITE software assists you in your daily work. Automated average and limit checks ensure safe operation. Saving, printing, and reporting your analyses can be done with one click.

Designed for maximum usability, the plug-in based architecture of **ELEMENTAL.SUITE** provides maximum flexibility for your analytical requirements now and in the future.



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