

Conductivity

offset, ISE5

PLS Cond. (mS/cm) - CALIBRATION R2 = 0.89 CC = 0.94 - CROSSVALIDATION R2 = 0.81 CC = 0.91
OLS Cond. (mS/cm) - CALIBRATION R2 = 0.88 CC = 0.94 - CROSSVALIDATION R2 = 0.77 CC = 0.89

OLS Regression Results

```
=====
Dep. Variable:          y      R-squared:          0.885
Model:                  OLS    Adj. R-squared:      0.882
Method:                 Least Squares  F-statistic:    413.9
Date:                  Thu, 06 Jul 2023  Prob (F-statistic): 5.50e-27
Time:                  07:53:57  Log-Likelihood:   -51.356
No. Observations:      56      AIC:             106.7
Df Residuals:          54      BIC:             110.8
Df Model:              1
Covariance Type:       nonrobust
=====
```

	coef	std err	t	P> t	[0.025	0.975]
const	-0.5848	0.178	-3.292	0.002	-0.941	-0.229
x1	118.2750	5.814	20.344	0.000	106.619	129.931

```
=====
Omnibus:                5.251  Durbin-Watson:      0.812
Prob(Omnibus):          0.072  Jarque-Bera (JB):    4.327
Skew:                   -0.516  Prob(JB):            0.115
Kurtosis:               3.889  Cond. No.            70.6
=====
```

Notes:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

C1- ISE1, ISE5

PLS [C1-] (ppm) - CALIBRATION R2 = 0.86 CC = 0.93 - CROSSVALIDATION R2 = 0.77 CC = 0.88
OLS [C1-] (ppm) - CALIBRATION R2 = 0.85 CC = 0.92 - CROSSVALIDATION R2 = 0.73 CC = 0.86

OLS Regression Results

```
=====
Dep. Variable:          y      R-squared (uncentered):          0.927
Model:                  OLS    Adj. R-squared (uncentered):      0.924
Method:                 Least Squares    F-statistic:          341.1
Date:                  Thu, 06 Jul 2023    Prob (F-statistic):    2.32e-31
Time:                  07:53:57    Log-Likelihood:       -375.12
No. Observations:      56    AIC:                  754.2
Df Residuals:          54    BIC:                  758.3
Df Model:              2
Covariance Type:       nonrobust
=====
```

```
=====
              coef      std err          t      P>|t|      [0.025      0.975]
-----
x1          -2.45e+04    3211.215     -7.630     0.000    -3.09e+04    -1.81e+04
x2           3.368e+04    1781.655     18.904     0.000     3.01e+04     3.73e+04
=====
```

```
=====
Omnibus:                  1.401    Durbin-Watson:          0.933
Prob(Omnibus):            0.496    Jarque-Bera (JB):        0.686
Skew:                    -0.166    Prob(JB):                0.710
Kurtosis:                 3.428    Cond. No.                4.59
=====
```

Notes:

- [1] R² is computed without centering (uncentered) since the model does not contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly specified.

NO3- offset, ISE2, ISE6

PLS [NO3-] (ppm) - CALIBRATION R2 = 0.69 CC = 0.83 - CROSSVALIDATION R2 = 0.28 CC = 0.63
OLS [NO3-] (ppm) - CALIBRATION R2 = 0.67 CC = 0.82 - CROSSVALIDATION R2 = 0.33 CC = 0.66

OLS Regression Results

=====

Dep. Variable:	y	R-squared:	0.674
Model:	OLS	Adj. R-squared:	0.662
Method:	Least Squares	F-statistic:	54.91
Date:	Thu, 06 Jul 2023	Prob (F-statistic):	1.21e-13
Time:	07:53:57	Log-Likelihood:	-268.13
No. Observations:	56	AIC:	542.3
Df Residuals:	53	BIC:	548.3
Df Model:	2		
Covariance Type:	nonrobust		

=====

	coef	std err	t	P> t	[0.025	0.975]
const	-23.6725	7.903	-2.995	0.004	-39.524	-7.821
x1	-1610.2816	696.117	-2.313	0.025	-3006.516	-214.047
x2	-2284.9903	944.133	-2.420	0.019	-4178.682	-391.299

=====

Omnibus:	4.249	Durbin-Watson:	0.806
Prob(Omnibus):	0.120	Jarque-Bera (JB):	4.251
Skew:	0.217	Prob(JB):	0.119
Kurtosis:	4.278	Cond. No.	287.

=====

Notes:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

SO42- offset, ISE1, ISE3, ISE5

PLS [SO42-] (ppm) - CALIBRATION R2 = 0.70 CC = 0.83 - CROSSVALIDATION R2 = 0.22 CC = 0.57
OLS [SO42-] (ppm) - CALIBRATION R2 = 0.71 CC = 0.84 - CROSSVALIDATION R2 = 0.34 CC = 0.64

OLS Regression Results

```
=====
Dep. Variable:          y      R-squared:          0.711
Model:                  OLS    Adj. R-squared:      0.694
Method:                 Least Squares  F-statistic:    42.60
Date:                  Thu, 06 Jul 2023  Prob (F-statistic): 4.86e-14
Time:                  07:53:57  Log-Likelihood:   -395.39
No. Observations:      56      AIC:              798.8
Df Residuals:          52      BIC:              806.9
Df Model:              3
Covariance Type:       nonrobust
=====
```

	coef	std err	t	P> t	[0.025	0.975]
const	-462.5752	123.452	-3.747	0.000	-710.300	-214.851
x1	2.231e+04	6463.228	3.452	0.001	9341.029	3.53e+04
x2	-2.855e+04	1.02e+04	-2.791	0.007	-4.91e+04	-8022.004
x3	5.272e+04	9996.868	5.273	0.000	3.27e+04	7.28e+04

```
=====
Omnibus:                0.580    Durbin-Watson:          0.889
Prob(Omnibus):          0.748    Jarque-Bera (JB):        0.563
Skew:                   0.227    Prob(JB):                0.755
Kurtosis:               2.812    Cond. No.:               362.
=====
```

Notes:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

HCO3- ISE1

PLS [HCO3-] (ppm) - CALIBRATION R2 = 0.15 CC = 0.38 - CROSSVALIDATION R2 =-0.27 CC =-0.03
OLS [HCO3-] (ppm) - CALIBRATION R2 =-0.15 CC = 0.14 - CROSSVALIDATION R2 =-0.32 CC = 0.01

OLS Regression Results

=====

Dep. Variable:	y	R-squared (uncentered):	0.636
Model:	OLS	Adj. R-squared (uncentered):	0.629
Method:	Least Squares	F-statistic:	95.90
Date:	Thu, 06 Jul 2023	Prob (F-statistic):	1.17e-13
Time:	07:53:57	Log-Likelihood:	-386.82
No. Observations:	56	AIC:	775.6
Df Residuals:	55	BIC:	777.7
Df Model:	1		
Covariance Type:	nonrobust		

=====

	coef	std err	t	P> t	[0.025	0.975]
x1	1.884e+04	1923.597	9.793	0.000	1.5e+04	2.27e+04

=====

Omnibus:	1.161	Durbin-Watson:	0.603
Prob(Omnibus):	0.560	Jarque-Bera (JB):	0.484
Skew:	0.059	Prob(JB):	0.785
Kurtosis:	3.440	Cond. No.	1.00

=====

Notes:

- [1] R² is computed without centering (uncentered) since the model does not contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Ca2+ offset, ISE1, ISE3, ISE5

PLS [Ca2+] (ppm) - CALIBRATION R2 = 0.74 CC = 0.86 - CROSSVALIDATION R2 = 0.24 CC = 0.58
OLS [Ca2+] (ppm) - CALIBRATION R2 = 0.77 CC = 0.88 - CROSSVALIDATION R2 = 0.51 CC = 0.73

OLS Regression Results

=====

Dep. Variable:	y	R-squared:	0.771
Model:	OLS	Adj. R-squared:	0.758
Method:	Least Squares	F-statistic:	58.44
Date:	Thu, 06 Jul 2023	Prob (F-statistic):	1.14e-16
Time:	07:53:57	Log-Likelihood:	-320.43
No. Observations:	56	AIC:	648.9
Df Residuals:	52	BIC:	657.0
Df Model:	3		
Covariance Type:	nonrobust		

=====

	coef	std err	t	P> t	[0.025	0.975]
const	-156.8045	32.373	-4.844	0.000	-221.765	-91.844
x1	8436.1321	1694.851	4.978	0.000	5035.165	1.18e+04
x2	-1.427e+04	2682.768	-5.318	0.000	-1.96e+04	-8882.416
x3	2.036e+04	2621.476	7.768	0.000	1.51e+04	2.56e+04

=====

Omnibus:	13.014	Durbin-Watson:	1.224
Prob(Omnibus):	0.001	Jarque-Bera (JB):	14.618
Skew:	0.963	Prob(JB):	0.000669
Kurtosis:	4.599	Cond. No.	362.

=====

Notes:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

K+ offset, ISE3

PLS [K+] (ppm) - CALIBRATION R2 = 0.70 CC = 0.83 - CROSSVALIDATION R2 = 0.49 CC = 0.72
OLS [K+] (ppm) - CALIBRATION R2 = 0.67 CC = 0.82 - CROSSVALIDATION R2 = 0.49 CC = 0.73

OLS Regression Results

=====

Dep. Variable:	y	R-squared:	0.674
Model:	OLS	Adj. R-squared:	0.668
Method:	Least Squares	F-statistic:	111.6
Date:	Thu, 06 Jul 2023	Prob (F-statistic):	9.40e-15
Time:	07:53:57	Log-Likelihood:	-146.72
No. Observations:	56	AIC:	297.4
Df Residuals:	54	BIC:	301.5
Df Model:	1		
Covariance Type:	nonrobust		

=====

	coef	std err	t	P> t	[0.025	0.975]
const	2.1330	0.835	2.554	0.014	0.459	3.808
x1	345.4761	32.698	10.566	0.000	279.921	411.031

=====

Omnibus:	6.632	Durbin-Watson:	0.615
Prob(Omnibus):	0.036	Jarque-Bera (JB):	6.001
Skew:	0.724	Prob(JB):	0.0498
Kurtosis:	2.309	Cond. No.	72.3

=====

Notes:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Mg2+ ISE5

PLS [Mg2+] (ppm) - CALIBRATION R2 = 0.77 CC = 0.88 - CROSSVALIDATION R2 = 0.64 CC = 0.81
OLS [Mg2+] (ppm) - CALIBRATION R2 = 0.76 CC = 0.87 - CROSSVALIDATION R2 = 0.63 CC = 0.80

OLS Regression Results

```
=====
Dep. Variable:          y      R-squared (uncentered):          0.928
Model:                  OLS    Adj. R-squared (uncentered):      0.927
Method:                 Least Squares    F-statistic:          707.6
Date:                  Thu, 06 Jul 2023    Prob (F-statistic):      4.39e-33
Time:                  07:53:57    Log-Likelihood:         -281.82
No. Observations:      56    AIC:                    565.6
Df Residuals:          55    BIC:                    567.7
Df Model:              1
Covariance Type:       nonrobust
=====
```

	coef	std err	t	P> t	[0.025	0.975]
x1	4354.0487	163.682	26.601	0.000	4026.022	4682.075

```
=====
Omnibus:                5.878    Durbin-Watson:          0.676
Prob(Omnibus):          0.053    Jarque-Bera (JB):        2.394
Skew:                   0.134    Prob(JB):                0.302
Kurtosis:               2.023    Cond. No.:               1.00
=====
```

Notes:

- [1] R² is computed without centering (uncentered) since the model does not contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly specified.

Na+ ISE1, ISE3

PLS [Na+] (ppm) - CALIBRATION R2 = 0.86 CC = 0.93 - CROSSVALIDATION R2 = 0.76 CC = 0.88
OLS [Na+] (ppm) - CALIBRATION R2 = 0.82 CC = 0.91 - CROSSVALIDATION R2 = 0.73 CC = 0.87

OLS Regression Results

```
=====
Dep. Variable:          y      R-squared (uncentered):          0.933
Model:                  OLS    Adj. R-squared (uncentered):      0.930
Method:                 Least Squares    F-statistic:          374.3
Date:                  Thu, 06 Jul 2023    Prob (F-statistic):      2.25e-32
Time:                  07:53:57    Log-Likelihood:         -338.05
No. Observations:      56    AIC:                    680.1
Df Residuals:          54    BIC:                    684.2
Df Model:              2
Covariance Type:       nonrobust
=====
              coef      std err          t      P>|t|      [0.025      0.975]
-----
x1          -3651.8894    1484.540      -2.460      0.017    -6628.213    -675.566
x2           1.673e+04     985.470     16.977      0.000     1.48e+04     1.87e+04
=====
Omnibus:                2.030    Durbin-Watson:          0.858
Prob(Omnibus):          0.362    Jarque-Bera (JB):        1.387
Skew:                   0.373    Prob(JB):                0.500
Kurtosis:               3.196    Cond. No.:               3.69
=====
```

Notes:

- [1] R² is computed without centering (uncentered) since the model does not contain a constant.
[2] Standard Errors assume that the covariance matrix of the errors is correctly specified.