



Supplementary Information

Use of an Automatic System in the Preparation of Gas Mixtures for Multivariate Calibration: A Case Study Involving NIR Analysis of Natural Gas

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Table S1. Concentrations of the components of the mixtures prepared by the automatic system

| Prepared mixture | Concentration / (% mol mol ⁻¹) | | | | Prepared mixture | Concentration / (% mol mol ⁻¹) | | | |
|------------------|--|--------|---------|----------|------------------|--|--------|---------|----------|
| | Methane | Ethane | Propane | Nitrogen | | Methane | Ethane | Propane | Nitrogen |
| 1 | 80.2 | 13.9 | 5.9 | 0.0 | 34 | 88.2 | 0.0 | 1.9 | 9.9 |
| 2 | 85.9 | 9.2 | 4.9 | 0.0 | 35 | 83.6 | 2.5 | 3.8 | 10.1 |
| 3 | 84.8 | 12.2 | 3.1 | 0.0 | 36 | 88.6 | 3.2 | 0.7 | 7.6 |
| 4 | 87.2 | 6.7 | 6.1 | 0.0 | 37 | 94.4 | 2.5 | 1.9 | 1.2 |
| 5 | 81.5 | 8.6 | 6.8 | 3.1 | 38 | 87.8 | 2.5 | 1.8 | 7.9 |
| 6 | 78.7 | 4.8 | 7.8 | 8.7 | 39 | 80.2 | 3.6 | 1.2 | 15.0 |
| 7 | 78.5 | 10.5 | 11.1 | 0.0 | 40 | 78.0 | 13.4 | 8.6 | 0.0 |
| 8 | 87.2 | 7.9 | 4.9 | 0.0 | 41 | 79.6 | 14.2 | 6.2 | 0.0 |
| 9 | 63.1 | 14.4 | 9.4 | 13.1 | 42 | 100.0 | 0.0 | 0.0 | 0.0 |
| 10 | 80.6 | 6.9 | 7.5 | 5.0 | 43 | 80.7 | 5.0 | 5.0 | 9.3 |
| 11 | 70.6 | 11.9 | 8.8 | 8.7 | 44 | 75.1 | 11.7 | 3.9 | 9.3 |
| 12 | 62.5 | 12.5 | 5.6 | 19.4 | 45 | 82.4 | 12.8 | 3.7 | 1.1 |
| 13 | 79.2 | 17.1 | 3.1 | 0.7 | 46 | 83.8 | 9.2 | 3.1 | 3.9 |
| 14 | 63.5 | 3.8 | 5.1 | 27.7 | 47 | 87.5 | 10.2 | 2.3 | 0.0 |
| 15 | 67.7 | 7.3 | 3.1 | 21.9 | 48 | 84.6 | 4.4 | 5.5 | 5.4 |
| 16 | 71.8 | 15.6 | 4.4 | 8.1 | 49 | 83.5 | 9.3 | 6.8 | 0.4 |
| 17 | 75.6 | 6.2 | 2.5 | 15.6 | 50 | 92.5 | 5.7 | 1.8 | 0.0 |
| 18 | 65.4 | 8.6 | 6.2 | 19.7 | 51 | 86.6 | 6.6 | 2.9 | 3.9 |
| 19 | 82.0 | 10.5 | 5.0 | 2.5 | 52 | 85.8 | 5.8 | 4.0 | 4.4 |
| 20 | 71.2 | 5.4 | 8.4 | 15.0 | 53 | 79.2 | 9.3 | 2.2 | 9.3 |
| 21 | 70.6 | 6.6 | 3.0 | 19.7 | 54 | 81.2 | 4.4 | 4.4 | 9.9 |
| 22 | 91.9 | 4.3 | 3.8 | 0.0 | 55 | 67.8 | 13.0 | 6.7 | 12.5 |
| 23 | 91.9 | 2.5 | 3.1 | 2.5 | 56 | 79.8 | 7.0 | 8.6 | 4.6 |
| 24 | 92.8 | 0.0 | 3.0 | 4.1 | 57 | 70.4 | 9.3 | 4.5 | 15.9 |
| 25 | 84.8 | 4.3 | 4.3 | 6.7 | 58 | 63.8 | 9.2 | 3.6 | 23.4 |
| 26 | 90.1 | 2.5 | 3.1 | 4.3 | 59 | 79.1 | 11.1 | 1.4 | 8.3 |
| 27 | 87.1 | 3.7 | 2.5 | 6.7 | 60 | 70.1 | 3.5 | 3.5 | 22.9 |
| 28 | 95.6 | 4.4 | 0.0 | 0.0 | 61 | 69.4 | 4.6 | 2.8 | 23.2 |
| 29 | 97.6 | 0.0 | 2.4 | 0.0 | 62 | 71.9 | 3.7 | 4.8 | 19.6 |
| 30 | 89.4 | 0.0 | 1.9 | 8.7 | 63 | 67.6 | 6.1 | 5.8 | 20.5 |
| 31 | 91.9 | 4.4 | 0.0 | 3.7 | 64 | 78.2 | 6.7 | 2.8 | 12.3 |
| 32 | 83.6 | 0.0 | 1.2 | 15.2 | 65 | 72.3 | 7.5 | 4.0 | 16.2 |
| 33 | 84.8 | 1.8 | 0.0 | 13.4 | 66 | 68.1 | 7.2 | 3.6 | 21.2 |
| | | | | | 67 | 75.0 | 8.1 | 2.0 | 15.0 |

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Table S2. Concentrations of the major components of the certified mixtures. Values observed in the certification label

| Certified mixture | Concentration / (% mol mol ⁻¹) | | | |
|-------------------|--|--------|---------|--------|
| | Methane | Ethane | Propane | Others |
| 1 | 70.0 | 11.0 | 2.5 | 16.5 |
| 2 | 90.0 | 0.8 | 0.8 | 8.4 |
| 3 | 81.0 | 6.0 | 1.5 | 11.5 |

Table S3. Concentrations of the major components of the comercial samples. Values obtained in the chromatographic analysis

| Real NG sample | Concentration / (% mol mol ⁻¹) | | | |
|----------------|--|--------|---------|--------|
| | Methane | Ethane | Propane | Others |
| 1 | 89.3 | 6.8 | 1.0 | 2.8 |
| 2 | 89.4 | 6.9 | 1.0 | 2.6 |
| 3 | 86.9 | 6.9 | 1.0 | 5.2 |
| 4 | 85.4 | 7.1 | 1.1 | 6.3 |
| 5 | 85.6 | 7.2 | 1.1 | 6.1 |
| 6 | 83.2 | 6.9 | 1.1 | 8.9 |
| 7 | 86.7 | 6.9 | 1.1 | 5.3 |
| 8 | 87.3 | 7.1 | 1.1 | 4.5 |