Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

A) Equations 1 and 2: related to the chemical composition of each sample matrix and for calculate the amount of oxygen required for sample combustion;

B) Equations 3: real gas equation, used to calculate the O_2 amount loaded in the digestion vessel;

C) Equation 4: Ideal gas equations, used to check the accuracy of Equation 3 in the working temperature and pressure.

$$C_qH_rN_sS_tO_u + \left(q + \frac{r}{4} + 0.3s + t - \frac{u}{2}\right)O_2 \rightarrow qCO_2 + \frac{r}{2}H_2O + \frac{s}{5}N_2 + 0.6sNO + tSO_2 \qquad \textbf{Eq. 1}$$

$$n_s = \sum_{i=1}^{N} f_i \cdot \frac{m_s}{M_i} \cdot \left(q_i + \frac{r_i}{4} + 0.3s_i + t_i - \frac{u_i}{2}\right) \qquad \textbf{Eq. 2}$$

$$P = \frac{nRT}{V} \qquad \textbf{Eq. 3}$$

$$P = \frac{nRT}{V - nb} - a\left(\frac{n}{V}\right)^2 \qquad \textbf{Eq. 4}$$

Where:

m_s is the sample mass;

f_i is mass fraction and $\dot{M}_i$ is the molar mass of an *i* component in the sample matrix;

P is the O_2 pressure in the vessel;

V is the headspace volume of the vessel;

n is the number of O_2 moles present in the combustion vessel;

R is the universal gas constant (0.082 atm L mol^{-1} K^{-1});

T is the temperature before combustion;

n_S is the number of O_2 moles required to obtain a complete combustion;

a is the van der Waals constant that provides a correction for the intermolecular forces; and

b is the van der Waals constant that provides a correction for finite molecular size related to the volume of one mole of the atoms or molecules.

D) Instructions of how to fill the left side of data sheet (system conditions) used for predicting combustion

1º) Complete only the yellow cells presented in the related data sheet;

2º) Follow the instructions, as presented below as dialog boxes;

3º) Final data will be presented at the right side of the data sheet.

Stoichiometric combustion application using microwave-induced combustion

$$C_qH_rN_sS_tO_u + \left(q + \frac{r}{4} + 0.3s + t - \frac{u}{2}\right)O_2 \rightarrow qCO_2 + \frac{r}{2}H_2O + \frac{s}{5}N_2 + 0.6sNO + tSO_2 \quad (1)$$

$$n_s = \sum_{i=1}^{N}\left(f_i \cdot \frac{m_s}{\overline{M}_i}\right) \cdot \left(q_i + \frac{r_i}{4} + 0.3s_i + t_i - \frac{u_i}{2}\right) \quad (2)$$

$$PV = nRT \quad (3)$$

Only fill the yellow cells

System condition	
Sample mass, g:	0.45
O_2 pressure in the vessel, atm:	20
R, (atm·L)/(mol·K):	0.082
Temperature before combustion, K:	298
Headspace volume of vessel, L:	0.068
Mass of igniter for combustion, g:	0.018

Compound:	Mass fraction:	Molar weight:	Elemental ratio C	H	N	S	O
A	1.0	84.18	6	12			
B	0.0	0					
C	0.0	0					
D	0.0	0					
Igniter (i.g. cellulose paper)			6	10			5

Data obtained by equation of ideal gas	
48.8	mmol of O_2 necessary to complete sample combustion
55.7	mmol of O_2 present in combustion vessel
14	% of O_2 excess considering stoichiometric combustion
0.6	mmol of O from sample
32.7	mmol of CO_2
32.6	mmol of H_2O
0.0	mmol of N_2 from 50% of total N present in sample
0.0	mmol of NO from 50% of total N present in sample
0.0	mmol of SO_2
15	atm* (final pressure) at 314 K

*Only for sample matrix as $C_qH_rO_u$ (without S and N).

In this cell, fill the sample mass, in grams.

In this cell, fill the oxygen pressure used in the vessel, in atmosphere.

In this cell, fill the room temperature, in Kelvin.

In this cell, fill the vessel headspace volume (total volume of vessel minus the volume of absorption solution minus quartz holder volume), in liter.

In this cell, fill the mass of igniter (cellulose paper) used, in grams

E) Instructions of how to fill the central part of data sheet used for predicting combustion

Stoichiometric combustion application using microwave-induced combustion

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$$n_x = \sum_{i=1}^{N}\left(f_i \cdot \frac{m_x}{M_i}\right) \cdot \left(q_i + \frac{r_i}{4} + 0.3s_i + t_i - \frac{u_i}{2}\right) \quad (2)$$

$$PV = nRT \quad (3)$$

Only fill the yellow cells

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0.0	mmol of SO_2
15	atm* (final pressure) at 314 K

*Only for sample matrix as $C_qH_rO_u$ (without S and N).

In these lines, fill each cell according to the elemental ratio presented in sample composition.

In these lines, fill each cell according to the elemental ratio of igniter (example already filled for cellulose paper).

The stoichiometric amount of oxygen, available for combustion, will be presented in this cell (in percentage). It is important to notice that a minimum excess oxygen must be used to ensure complete sample combustion