

User Manual: Calculation №86 «Chromos: Natural gas»

> «CHROMOS Engineering», LLC Dzerzhinsk, Russia

Release date: 2025-05-05 Latest software version: 1.0.6.37 Internet: <u>kb.has.ru</u>

Contents

1. Introduction	3
2. Installing the Software	4
3. Running the Plug-in	5
4. Program Overview	6
5. Measurement Procedure	7
6. Adding Data	8
7. Determining of C6, C7, C8 Pseudo-Components	9
8. Adding Calibration Mixtures	10
9. Calibrating	11
9.1. Methods A, B	11
9.2. Method C	11
10. Calculations	13
10.1. Calculation of Molar Concentrations of Components and Their Uncertainties	13
10.2. Calculation of Physical Indicators	14
10.3. Calculation of Methane Number	15
11. Reporting	16
12. Adding Additional Parameters to the Report	17
13. Exporting Data	18
14. Managing the Components	19
14.1. Name Alias	19
14.2. Conditionally Constant Components	19
15. Configuring the Program Settings	21
16. Hotkeys	26
17. Program Identification	27

1. Introduction

The «Chromos: Natural gas» program is designed for calculating calibration factors and mole fractions of components in accordance with GOST 31371.7-2020 «Natural gas. Determination of composition by gas chromatography with uncertainty assessment. Part 7. Methodology for measuring the mole fraction of components», calculation in accordance with GOST 31369-2021 «Natural gas. Calculation of the heat of combustion, density, relative density and Wobbe index based on the component composition» (ISO 6976:2016), as well as for calculating the methane number based on the known component composition according to GOST 34704-2020 «Natural gas. Determination of the methane number».

Before getting started, it is recommended to study the foregoing document.

This software works as an extension and can only be launched on a registered copy of «Chromos» software. To run the program you need a key.

The plug-in installation file and documentation are available on the Internet at: <u>kb.has.ru/soft:dop_raschjot_86</u>.

E-mail your suggestions and comments on the software to: soft@has.ru

2. Installing the Software

Before installing the program «Chromos: Natural Gas» on the PC, the software «Chromos 4» must be installed. You need 5 Mb of free space on your local drive. To install the software, do the following:

- 1. Run the installation file.
- 2. Choose your language.
- 3. In the installer (Fig. 1), specify the components to be installed and click **Install**.

🔘 Chromos: Natural gas 1.0.6.36 Setup	a r a		×
Choose Install Location Choose the folder in which to install Chromos: Natural gas 1.0.6.36.			
Setup will install Chromos: Natural gas 1.0.6.36 in the following folder. folder, dick Browse and select another folder. Click Install to start the in Destination Folder	To insta nstallatio	ll in a differ	rent
C:\Program Files (x86)\Chromos4\Plugins\ChromosNaturalGas	Bro	wse]
Space required: 2.4 MB Space available: 26.0 GB			
© 000 Chromos-Engineering 2024 Build version 1.0.6.36, 22.04.2025 12	:56:32 - tall	Cano	cel

Fig. 1: Installation

4. When installed, click **Finish**.

After the software is successfully installed you can run it from «Chromos» software.

3. Running the Plug-in

3. Running the Plug-in

This software works as an extension for «Chromos» software. To run the extension, do the following:

- 1. Connect the key to a USB port.
- 2. Run «Chromos» software.
- 3. In the *Data* menu, navigate to **Calculations** > **Chromos: Natural gas**. The main program window opens (Fig. 2).

Chromatogram Method Devices	Data Database Window Help	
i 🚅 🔲 🎒 I 😵	Volume/Mass Percentage	
	Extension Manager	
	Language 🕨 🕨	
	External Tools	
	Calculations	Natural Gas
	Verification	Shewhart Control Chart
		Statistics

Fig. 2: Running the plug-in

4. Program Overview

4. **Program Overview**

The main program window (Fig. 3) consists of a work area and a notification log. The work area contains the information tabs and operation buttons. The notification log displays errors that occurred during the calculation process.

LIOTEOOD				Contro	d Calibrat	ion Accou	Bomovo
Refresh				Contro	Calibrat	IOTI ASSAY	Remove
_ File		Sample	Mixture	Time	Туре	Method	Atm. pressur
egory	Description						

Fig. 3: Main program window

Work area tabs provides the following information:

- *Chromatograms* a list of chromatograms used for calculation, with data on identifier, sample, mixture, date and time of analysis, type of chromatogram (assay or calibration), method and atmospheric pressure at the start of recording;
- *Calibration* data for calculating calibration coefficients;
- *Components* data for calculating the mole fraction of components and their uncertainties;
- *Calculation* calculation data of physical properties of natural gas;
- *Methane number* methane number calculation data;
- *Report* printed form of the report on the component composition of gas;
- *Export* data export options;
- *Mixtures* list of calibration mixtures used in the calculation;
- *Aliases* names of components;
- *Conditionally constant* data on conditionally constant components;
- *Shewhart map* Shewhart control map;
- *Settings* program settings;
- *About...* program identifier.

5. Measurement Procedure

The «Chromos: Natural gas» software performs the calculation in accordance with GOST 31371.7-2020, GOST 31369-2021 (ISO 6976:2016), and GOST 34704-2020 in the following order:

- 1. Checking the compliance of a certified reference material (CRM) to GOST 31371.7-2020;
- 2. Calculation of calibration coefficients;
- 3. Calculation of molar concentrations of components and their uncertainties;
- 4. Verification of the correspondence of the values of the molar fractions of the components being determined in the calibration mixture and in the analyzed gas;
- 5. Calculation of physical indicators;
- 6. Calculation of the methane number.

If an error occurs at one of the stages, the calculation stops and a warning is displayed on the screen (Fig. 4). The notification log displays messages describing errors.

🗘 Natural gas ·	version 1.0	.6.36												\times
Chromatograms	Calibration	Components	Calculation	Methane number	Report	Export	Mixtures	Aliases	Conditionally cons	Shewhart ma	PP Settings	About		
				Warning	n error h heck the	nas occu e errors	urred. Calci list below.	ulation is	> not possible.	K				
									ОК					
Category Calibration	Description Calibration m	nixture is not s	pecified.											
													(ОК

Fig. 4: Calculation error warning

6. Adding Data

To add chromatograms for calculation, on the *Chromatograms* tab, do the following:

- 1. Click **Calibration, Assay, or Control** depending on the type of a chromatogram you want to add. The *Select chromatograms* window opens.
- 2. In the *Select chromatograms* window, select the chromatograms and click **OK**.
- 3. To refresh the list, click **Refresh**.
- 4. To remove the selected chromatogram, click **Remove**.
- 5. (Optional) To show/hide chromatogram identifiers, check the *File* option.

Added chromatograms are displayed in the table with the following information:

- *UUID* unique chromatogram identifier;
- *File* chromatogram file name;
- *Sample* sample name from the chromatogram passport;
- *Mixture* mixture name from the chromatogram passport;
- *Time* assay date/time;
- *Type* chromatogram type (assay, calibration, control);
- *Method* method name;
- *Atm. pressure (kPa)* atmospheric pressure at the start of the analysis recording.

To eliminate the influence of atmospheric pressure changes during measurements, in the passport (Fig. 5) of each chromatogram for the parameter *Ambient pressure (kPa)* it is necessary to indicate a value equal to the atmospheric barometric pressure in kPa.

If atmospheric barometric pressure is not indicated for the chromatogram, then normal atmospheric pressure is used for calculations – 101.325 kPa.

To measure atmospheric barometric pressure, it is necessary to use verified measuring instruments.

Properties	Values	
	Values	
 Sample 		
Semela nomo		
	Netwolfer	
	NaturalGas	
Defect	INO	
Mixture		
Calibration	No	
Date and time of selection	on 25.04.2025 13:05:16	
Column		
Others		
Sample volume	1	
Dilution	1	
Norm (100%)	100	
Eluent		
Reagent		
Ambient pressure (kPa)	99.866	
Ambient pressure (kPa)		
· · · · · · · · · · · · · · · · · · ·		

Fig. 5: Passport > Ambient pressure

7. Determining of C6, C7, C8 Pseudo-Components

To use pseudo-components C6, C7, C8 in the calculation, it is necessary to mark all the peaks to be determined in the chromatograms and assign them names with the prefix C6, C7 or C8, in accordance with which pseudo-component they are part of. In the calculation for pseudo-components C6, C7 and C8, the sums of the areas of the peaks included in the component will be used.

When changing the name alias of components C6, C7 and C8, the prefixes for determining the pseudo-components also change.

8. Adding Calibration Mixtures

8. Adding Calibration Mixtures

To add calibration mixtures, in the *Mixtures* tab (Fig. 6), do the following::

- 1. Click Add. The Certified Reference Material (CRM) window opens.
- 2. In the *Compound* field, select the compound from the list. To select all the compounds, choose **All components**.
- 3. In the *CRM 1* field, select the mixture from the list and indicate its type:
 - CRM-NGS natural gas simulator CRM;
 - CRM-MNG main natural gas CRM;
 - CRM-Methane methane CRM.
- 4. (Optional) In the *CRM* 2 field, select the mixture from the list and indicate its type.
- 5. Click **Save**.
- 6. (Optional) To remove the selected compound, click **Remove**.

C	hromatograms	Calibration	Components	Calculation	Methane number	Report	Export	Mixtures	S Aliases	Conditionally constant	Shewhart map	Settings	About	
												[Add	Remove
	Component		CRM 1		CRM 1 type	CRM	check	Т	Type CRM o	heck				
							· ·	~ . /·	• ,	_				1

Fig. 6: Mixtures

9. Calibrating

To perform the calculation, you need to obtain a set of calibration chromatograms. Chromatograms are selected on the *Chromatograms* tab. The chromatograms must be calibration chromatograms, and the names of the mixtures must match the settings in the program. The software provides calibration by methods A, B, C1 and C2.

Method A is intended for measuring the molar fraction of all components.

Method B is intended for measuring the molar fraction of nitrogen, oxygen, helium, hydrogen, carbon dioxide, hydrocarbons from C1 to C5 individually, and all hydrocarbons heavier than N-pentane are considered as a single pseudo-component C6+.

Method C is designed for the analysis of natural gas of variable composition. Method C can be implemented in two versions:

- *C1* for measuring the values of the mole fraction of individual components: helium, hydrogen, nitrogen, oxygen, carbon dioxide, methane, ethane, propane, isobutane, N-butane, isopentane, neopentane, N-pentane, benzene, toluene, and the mole fraction of heavy hydrocarbon isomers in total in the form of pseudo-components C6, C7 and C8;
- *C*2 for measuring the mole fraction of nitrogen, oxygen, helium, hydrogen, carbon dioxide, hydrocarbons from C1 to C5 individually, and the mole fraction of all heavy hydrocarbons in the form of a single pseudo-component C6+ in total using the back-flushing method by the total area of the peaks of hydrocarbons heavier than N-pentane.

9.1. Methods A, B

To calibrate using methods A and B, three measurements for the mixture must be selected. The *Calibration* tab (Fig. 2) displays the following information:

- *Component* component name;
- *Concentration 1* molar fraction of a component in CRM 1;
- *C1* calibration factor for the chromatogram 1;
- *C2* calibration factor for the chromatogram 2;
- *C*3 calibration factor for the chromatogram 3;
- *K* arithmetic mean of calibration coefficients;
- *Area* 1 arithmetic mean value of the area of a component in the analysis of CRM 1;
- *Acceptability* 1 the value of the relative range of the obtained values of the calibration coefficients;
- *Acceptability standard* 1 limit of permissible values of the relative range of the obtained values of the calibration coefficients.

9.2. Method C

For calibration using method C, five measurements for each mixture must be selected. The *Calibration* tab (Fig. 3) displays the following information:

- *Component* component name;
- *Concentration 1* molar fraction of a component in CRM 1;
- *Concentration 2* concentration of the component from CRM 2;
- *Area* 1 arithmetic mean value of the area of a component in the analysis of CRM 1;
- *Area 2* arithmetic mean value of the area of the component in the analysis of CRM 2;
- *b* equation coefficient;

- *B* equation coefficient;
- *Acceptability* 1 the permissible value 1 of the relative standard deviation of the detector signal, multiplied by two;
- *Acceptability standard* 1 relative deviation of the obtained value of the mole fraction of a component from its value in CRM 1;
- *Acceptability 2* the permissible value 2 of the relative standard deviation of the detector signal, multiplied by two;
- *Acceptability standard 2* relative deviation of the obtained value of the mole fraction of a component from its value in CRM 2;
- *Check. relative range* relative range control;
- *Check. tolerance range* range tolerance control;
- *Control rate* control rate;
- *Control standard* control standard;
- *RSD 1 area* area of relative standard deviation 1;
- *RSD 1 tolerance* tolerance of area of relative standard deviation 1;
- *RSD 2 area* area of relative standard deviation 2;
- *RSD 2 tolerance* tolerance of area of relative standard deviation 2.

10. Calculations

10.1. Calculation of Molar Concentrations of Components and Their Uncertainties

The molar fraction of components is calculated using the previously performed calibration. The component composition is calculated using the chromatograms selected in the *Chromatograms* tab. A flow (process) chromatograph requires one chromatogram, while a laboratory chromatograph requires two. The calculation result is presented in the *Components* tab (Fig. 4). The following information is displayed:

- *Component* component name;
- *Time* component peak exit time;
- *Area* peak area;
- *Height* peak height;
- *Concentration (mol. %)* molar fraction, % of the measured component;
- *Expanded uncertainty* absolute expanded uncertainty;
- *CRM* molar fraction, % of the component in the state standard sample used to control the accuracy of measurement results according to GOST 31371.7-2020, clause 12.3;
- *Concentration (vol.%)* volumetric fraction, % of the measured component;
- *Concentration (mass.%)* mass fraction, % of the measured component;
- *Acceptability* the value of the discrepancy between two consecutive measurements, % (for a laboratory instrument);
- *Tolerance* permissible value of discrepancy between two consecutive measurements;
- *X1* non-normalized value (molar fraction, %) of the measured component in the first analyzed chromatogram;
- *X2* non-normalized value (molar fraction, %) of the measured component in the second analyzed chromatogram.

The software implements a check of the conformity of the values of the molar fraction of the components to be determined in the calibration mixture and in the analyzed gas. The check is carried out in accordance with clause 9.5.2.1 of GOST 31371.7-2020 «Natural gas. Determination of composition by gas chromatography with uncertainty assessment. Part 7. Methodology for measuring the molar fraction of components».

Components marked with (*) are not included in the calculation of physical indicator values according to GOST 31369-2021 (ISO 6976:2016), since their molar fraction is less than 0.00005 (0.005% molar fraction).

After the measurements are taken, the results are checked for accuracy in accordance with clause 12.3 of GOST 31371.7-2020. The results of measurements are checked for accuracy using a CRM of natural gas simulator (CRM-NGS) or a CRM of main natural gas (CRM-MNG) for components whose molar fraction exceeds 0.01%. The control result is considered satisfactory if the following condition is met:

$$|x_{meas} - x_{pass}| \leq U(x_{meas})$$
, where

 x_{meas} — result of measurements of the molar fraction of a component in CRM, %; x_{pass} — the value of the molar fraction of a component in CRM, by its passport, %;

10.1. Calculation of Molar Concentrations of Components and Their Uncertainties

 $U(x_{meas})$ — the value of the absolute expanded uncertainty of the measurement of the molar fraction of a component, calculated using the formulas given in Table 1, %.

10.2. Calculation of Physical Indicators

The calculation of the physical indicators of natural gas is carried out on the basis of previously obtained data on the component composition of the gas. The calculation result is presented in the *Calculation* tab (Fig. 7). The following information is displayed:

- *Name* name of the calculated value;
- *Value* value;
- *Expanded uncertainty* absolute expanded uncertainty.

Chromatograms	Calibration	Components	Calculation	Methane number	Report	Export	Mixtures	Aliases	Conditionally cons	tant	Shewhart map	Settings	About		
Name										Valu	e		Expande	ed uncertainty	·
Mixture molar	mass [kg/km	nol]								-	_			_	() ()
Compressibility	/ factor									-	_			-	
Higher molar h	leat of comb	ustion of a mix	ture of ideal a	and real gas [kJ/mo	ol]					-	_			_	÷
Lower molar h	eat of combu	ustion of a mixt	ure of ideal a	nd real gas [kJ/mo	0					-	_			_	
Higher mass h	eat of combu	stion of a mixt	ure of ideal a	nd real gas [MJ/kg]					-	_			-	
The lower mas	s heat of co	mbustion of a r	mixture of ide	al and real gas [M	l/kg]					-	_			_	
Higher volume	tric heat of c	ombustion of a	n ideal gas n	nixture [MJ/m³]						-	_			-	
Lower volumet	ric heat of o	ombustion of a	n ideal gas m	ixture [MJ/m³]						-	-			_	
Higher volume	tric heat of c	ombustion of a	n ideal gas n	nixture [kcal/m³]						-	_			_	
Lower volumet	ric heat of o	ombustion of a	n ideal gas m	ixture [kcal/m³]						-	-			-	
Higher volume	tric heat of c	ombustion of a	real gas mix	ture [MJ/m³]						-	_			_	
Lower volumet	ric heat of o	ombustion of a	real gas mix	ture [MJ/m³]						-	-			-	
Higher volume	tric heat of c	ombustion of a	real gas mix	ture [kcal/m³]						-	_			-	
Lower volumet	ric heat of c	ombustion of a	real gas mix	ture [kcal/m³]						-	-			_	
Ideal gas relat	ive density									-	_			-	
Ideal gas dens	ity [kg/m³]									-	-			_	

Fig. 7: Calculation

The following values are calculated:

- Mixture molar mass, (kg/kmol);
- Compressibility factor;
- Higher molar heat of combustion of a mixture of ideal and real gas (kJ/mol);
- Lower molar heat of combustion of a mixture of ideal and real gas (kJ/mol);
- Higher mass heat of combustion of a mixture of ideal and real gas (MJ/kg);
- Lower mass heat of combustion of a mixture of ideal and real gas (MJ/kg);
- Higher volumetric heat of combustion of an ideal gas mixture (MJ/m³);
- Lower volumetric heat of combustion of an ideal gas mixture (MJ/m³);
- Higher volumetric heat of combustion of a real gas mixture (MJ/m³);
- Lower volumetric heat of combustion of a real gas mixture (MJ/m³);
- Ideal gas relative density;
- Ideal gas density (kg/m³);
- Real gas relative density;
- Real gas density (kg/m³);
- Higher Wobbe index of ideal gas (MJ/m³ and kcal/m³);
- Lower Wobbe index of ideal gas (MJ/m³ and kcal/m³);
- Higher Wobbe index of real gas (MJ/m³ and kcal/m³);
- Lower Wobbe index of real gas (MJ/m³ and kcal/m³).

10.2. Calculation of Physical Indicators

In accordance with GOST 31369-2021 «Natural gas. Calculation of combustion heat, density, relative density and Wobbe index based on component composition» (ISO 6976:2016), calculations are reliable only for compressibility coefficient values > 0.9. In case of discrepancy, a warning is displayed in the software.

10.3. Calculation of Methane Number

The calculation of the methane number of natural gas is carried out on the basis of previously obtained data on the component composition of the gas. The calculation result is presented in the *Methane Number* tab (Fig. 8). The following information is displayed:

- *Value* calculated value;
- Absolute expanded uncertainty. absolute expanded uncertainty;

Champhannan Calibrative Constants Calibrative Mathana number Deart Kinter Aliana Cadificanth undertaine Cational Atout

- Vol.%, unnorm. non-normalized volumetric fraction of a component, %;
- *Vol.%*, *norm*. volumetric fraction of a component, %.

Informatograms	Calibration Com	ponents	Calculation	methane number	Report	Export	Mixtures	Allases	Conditionally constant	Snewnart map	Settings About
Methane numb	ber									Value	Absolute expanded uncertainty
Simplified mixt	ture methane num	ber								0	1
Gas motor fue	I methane number									0	1
Simplified mixt	ture								Vol. %	, unnorm.	Vol. %, norm
Methane											
Ethane											
Propane											
Butane											
Simplified mixt	ture								Vol. %	, unnorm.	Vol. %, norm
Methane											
Carbon dioxide	e										
Nitrogen											
Initial methane	e number values									Value	
Initial methane	e number values									Value	

Fig. 8: Methane number

11. Reporting

11. Reporting

The program can be used to prepare a printed report form with the obtained data on the component composition of the gas (Fig. 9).

Chromatograms	Calibration	Components	Calculation	Methane numb	er Repor	t Export	Mixtures	Aliases	Conditionally constant	Shewhart map	Settings	About		
Settings										F	Print	View	Save	
						R	leport							^
		Detern	ination of o	composition by	gas chr	Na omatogr	atural gas aphy with	uncerta	inty assessment. G	OST 31371.7-2	020			
	Natural ga	s — Calculat	ion of calor	ific values. m	ss volun	ie. relati	ive densit	v and W	obbe indices from t	e composition	GOST 3	1369-202	21	
		5 Calcula	ion of calor	,			ive delisit	, 				1007 101		
Chromatogr	ams	s carcula		,				,						
Chromatogr File	ams Samj	ple	Mixtur	e	Time	T	ype	Me	thod	Atm.	pressure (l	kPa)]	
Chromatogr File Calibration	ams Samj	ple	Mixtur	e	Time	T	ype	Me	thod	Atm.	pressure (l	kPa)		
Chromatogr File Calibration	ams Samj nent	ple Concer	Mixtur stration 1	e	Time	T K	ype Area 1	Me	thod Acceptability 1	Atm.	pressure (l Acceptabili	kPa) ty standard	1	~

Fig. 9: Report form

To fill in the report form, do the following:

- 1. Navigate to the *Report* tab.
- 2. Click **Save**. A dialog window opens.
- 3. In the dialog window, enter the file name and the folder, then click **Save**. The report is saved as an .html file.
- 4. To open the print preview, click **View.** To switch between pages, use buttons or enter the page number in the corresponding field.
- 5. To print the report, click **Print**. A dialog window opens.
- 6. In the dialog window, select the printing parameters, enter the number of copies, then click **Print**.

12. Adding Additional Parameters to the Report

To add additional parameters to a report, do the following:

- 1. Navigate to the *Report* tab.
- 2. Click Settings. The Report: Parameters window opens (Fig. 10).
- 3. To add a parameter, click **Add**. A dialog window opens.
- 4. In the dialog window, enter the name and the value of the parameter.
- 5. (Optional) To remove the selected parameter, click **Remove**.
- 6. Click **OK**.

Report: Parame	ters		×
		Add	Remove
Name	Value		
		ОК	Cancel

Fig. 10: Report parameters

13. Exporting Data

To export gas component composition data, on the *Export* tab (Fig. 11), do the following:

- 1. In the *Format* field, select the file format (TXT, JSON, XML).
- 2. To select data to add to the report, check the corresponding options:
 - *Chromatograms* list of chromatograms used in the calculation;
 - *Calibration* result of calculating the calibration coefficients;
 - *Components* result of calculation of component composition;
 - *Calculation* result of calculation of physical properties;
 - *Methane number* methane number calculation result;
 - *Mixtures* list of calibration mixtures used in the calculation and their component composition;
 - *Settings* program settings;
 - *Log* event log.
- 3. In the *Exporter path* field, enter the path to the application from the LIMS system, that loads the information to the system.
- 4. In the *Additional* field, enter additional parameters for the data transfer application. **Note:** Instead of the exported file name, enter **%F**. See examples below.
- 5. Click **Export**.

Example 1.

- «Exporter path» CMD
- «Additional» /C move /Y %F C:\out\data.xml

Example 2.

- «Exporter path» **notepad.exe**
- «Additional» **none**

Example 3 (to call the system dialog for saving a file).

- «Exporter path» **SaveAs**
- «Additional» **none**

Chromatogram	Calibration	Components	Calculation	Methane number	Report	Export	Mixtures	Aliases	Conditionally constant	Shewhart map	Settings	About	
Settings													Export
Format		XML		\sim									
Exported da	ta:												
Chromat	ograms	Methane r	number										
🗸 Calibrati	on	Mixtures											
Compon	ents	Settings											
🗸 Calculati	on	✓ Log											
Exporter pa	h												
CMD													
Additional													
/C move /\	%F C:\out\da	ata.xml											

Fig. 11: Export

14. Managing the Components

14.1. Name Alias

To compare components from the calculation and chromatograms, a table of aliases is used (Fig. 12). The table shows the designation of the component and its name (alias), by which the search is performed on the chromatogram.

To change the alias, do the following:

- 1. Navigate to the *Aliases* tab.
- 2. In the corresponding cell of the *Name alias* column, double-click and enter the needed value.

romatograms Calibration Compor	ents Calculation Methane number Report Export Mixtures Aliases Conditionally constant Shewhart map Settings About	
		Reset
Component	Name alias	
methane	Метан	
ethane	Этан	
propane	Пропан	
2_methylpropane	И-бутан	
n_butane	н-Бутан	
2_methylbutane	И-пентан	
n_pentane	н-Пентан	
2_2_dimethylpropane	Неопентан	
n_hexane	н-Гексан	
n_heptane	н-Гептан	
n_octane	н-Октан	
benzene	Бензол	
toluene	Толуол	
carbon_dioxide	Диоксид углерода	

Fig. 12: *Aliases*

14.2. Conditionally Constant Components

If the method used does not allow for the measurement of the molar fraction of individual components of natural gas (helium, hydrogen, oxygen, methanol, etc.), information on their content should be obtained from other sources and taken into account when calculating the component composition of the natural gas sample. It is also necessary to take into account the molar fraction of unmeasured components, which include sulfur-containing compounds, water vapor, etc.

Information on the content of the specified components must be checked at intervals established for a specific measurement unit in accordance with the enterprise quality system (if necessary, taking into account subsection 4.2 of GOST 31370-2007), but not less than once per quarter, and accepted over the established period as conditionally constant.

To include conditionally constant components in the calculation, in the *Conditionally constant* tab (Fig. 13), do the following:

- 1. Click Add. The Component window opens.
- 2. In the *Component* window, select from the list a conditionally constant component.
- 3. In the *Concentration* field, enter the molar fraction value (in %).
- 4. In the *Expanded uncertainty* field, enter the absolute expanded uncertainty value.

14.2. Conditionally Constant Components

- 5. Click **Save**.
- 6. To edit the parameters of the added component, double-click in the corresponding cell of the table.
- 7. (Optional) To remove the selected component, click **Remove.**

Chromatograms	Calibration	Components	Calculation	Methane number	Report	Export	Mixtures	Aliases	Conditionally constant	Shewhart map	Settings	About		
											I	Add		Remove
Component										Concentrati	on	Exp	anded	uncertainty
C6										0.00	34			0.00098

Fig. 13: Conditionally constant components

To configure the software, in the *Settings* tab (Fig. 14), do the following:

- 1. Set calibration parameters:
 - In the *Method* field, select the calibration method from the list:

- *Method* A – is designed to measure the molar fraction of nitrogen, oxygen, helium, hydrogen, carbon dioxide, saturated hydrocarbons up to C5, benzene and toluene individually; the molar fraction of heavy hydrocarbon isomers is measured in total as pseudo-components C6, C7 and C8;

- *Method B* – is designed to measure the mole fraction of nitrogen, oxygen, helium, hydrogen, carbon dioxide, hydrocarbons from C1 to C5 individually; all hydrocarbons heavier than n-pentane are considered as a single pseudo-component C6+, and its mole fraction is measured in total using the total peak area of hydrocarbons heavier than n-pentane;

- *Method C1* – is designed to measure the molar fraction of individual components: helium, hydrogen, nitrogen, oxygen, carbon dioxide, methane, ethane, propane, isobutane, i-butane, isopentane, neopentane, n-pentane, benzene, toluene and the molar fraction of heavy hydrocarbon isomers in total in the form of pseudo-components C6, C7 and C8;

- *Method* C2 – is designed to measure the molar fraction of nitrogen, oxygen, helium, hydrogen, carbon dioxide, hydrocarbons from C1 to C5 individually and the molar fraction of all heavy hydrocarbons as a single pseudo-component C6+; its molar fraction is measured in total using the total peak area of hydrocarbons heavier than n-pentane.

- If the detector is linear for carbon dioxide, nitrogen or oxygen, check the option next to the corresponding component;
- To carry out calibration control in accordance with clause 9.5.2.5. of GOST 31371.7-2020, check the *Calibration Control* option;
- To check for compliance of calibration mixtures with the requirements of GOST 31371.7-2020 Appendix B, check the *Check the compliance with GOST 31371.7-2020* option.
- 2. Set calculation parameters:
 - To make a correction for changes in atmospheric pressure during the measurement, check the *Correction by pressure* option;
 - To make a correction for changes in ambient temperature during the measurement, check the *Correction by temperature* option;
 - In the *Measure* field, select the temperature of measurement value from the list (0, 15, 15.55, 20 °C);
 - In the *Combustion* field, select the temperature of combustion value from the list (0, 15, 15.55, 20, 25 °C);
 - To calculate the mole fraction of methane by difference, check the *Methane by difference* option;
 - To use the identity matrix for calculation of correlation factors, check the *Identity matrix of correlation factor* option;

- To compare actual measurements with calibration ones, check the *Mixture compliance check* option;
- In the *Chromatograph* field, select the chromatograph type from the list (laboratory, process);
- To carry out the control of calculation results in accordance with clause 12.3 of GOST 31371.7-2020, check the *Measurement results correctness check* option;
- To carry out the measurement of the mole fraction of components in the range from 0.001% to 0.005% using a standard sample of appropriate composition and the accuracy specifications of Method A, check the *Extended range (Method B)* option.

Chromatograms Calibration Components Calculation M	ane number Report Export Mixtures Aliases Conditionally	constant Shewhart map Settings About
Chromatograms Calibration Calculation M Calibration Method Method A Carbon dioxide (linear) Mitrogen (linear) Oxygen (linear) Calibration control	ane number Report Export Mixtures Aliases Conditionally Calculation Correction by pressure Correction by temperature Measure 20 Combustion 25	constant Shewhart map Settings About View Chromatograms Settings Calibration Settings Calculation Settings Methane Settings
Check the compliance with GOST 31371.7-2020		

Fig. 14: Settings

- 3. Set display parameters:
 - To set up the chromatograms display parameters, opposite the *Chromatograms* line, click **Settings**. A dialog window opens (Fig. 15).
 - 1. To display a column in the table, check the corresponding option.
 - 2. In the *Atm. pressure* field, enter the number of decimals (integer value).
 - 3. To save the changes, click **OK**.

View: Chromatograms	×
✓ Time	
Method	
└ Mixture	
Atm. pressure	3
ОК	Cancel

Fig. 15: View: Chromatograms

• To set up the calibration display parameters, opposite the *Calibration* line, click **Settings**. A dialog window opens (Fig. 16).

- 1. To display a column in the table, check the corresponding option.
- 2. To set the number of decimals, in the corresponding *Accuracy* field, enter an integer value.
- 3. To round values in accordance with GOST 31371.7-2020, opposite the corresponding parameter, check the *GOST* option.
- 4. To save the changes, click **OK**.

View: Calibration		×
	GOST	Accuracy
CRM concentration		
✓ C1, C2, C3	\checkmark	4
Cal. factor (Method A, B)	\checkmark	4
Cal. factor (Method C)	\checkmark	4
🗸 Area	\checkmark	4
Acceptability of cal. factor values	\checkmark	4
Cal. factor control. Range	\checkmark	4
Cal. factor control. Acceptability	\checkmark	4
RSD of detector response values	\checkmark	4
	ОК	Cancel

Fig. 16: *View: Calibration*

- To set up the components display parameters, opposite the *Components* line, click **Settings**. A dialog window opens (Fig. 17).
 - 1. To display a column in the table, check the corresponding option.
 - 2. To set the number of decimals, in the corresponding *Accuracy* field, enter an integer value.
 - 3. To round values in accordance with GOST 31371.7-2020, opposite the corresponding parameter, check the *GOST* option.
 - 4. To save the changes, click **OK**.

View: Components		×
	GOST	Accuracy
✓ Time	\checkmark	4
Area	\checkmark	4
✓ Height	\checkmark	4
Unnormalized conc. (mol. %)	\checkmark	4
✓ Conc.(mol. %)	\checkmark	4
Conc.(mass %)		4
Conc.(vol. %)		4
Acceptability		4
X1, X2		4
	ОК	Cancel

Fig. 17: View: Components

- To set up the calculation display parameters, opposite the *Calculation* line, click **Settings**. A dialog window opens (Fig. 18).
 - 1. To display a column in the table, check the corresponding option.
 - 2. To set the number of decimals, in the corresponding *Accuracy* field, enter an integer value.
 - 3. To round values in accordance with GOST 31369-2021, opposite the corresponding parameter, check the *GOST* option.
 - 4. To display ideal gas parameters, check the *Show ideal gas parameters* option.
 - 5. To save the changes, click **OK**.

View: Calculation		×
Show ideal gas properties		
	GOST	Accuracy
☑ Mixture molar mass [kg/kmol]	\checkmark	4
Compressibility factor	\checkmark	4
Molar heat of combustion [kJ/mol]	\checkmark	4
Mass heat of combustion [MJ/kg]	\checkmark	4
✓ Volumetric heat of combustion [MJ/m³]	\checkmark	4
Volumetric heat of combustion [kcal/m³]		7
└─ Density [kg/m³]	\checkmark	4
✓ Wobbe index [MJ/m³]	\checkmark	4
Wobbe index [kcal/m³]		7
	ОК	Cancel

Fig. 18: View: Calculation

- To set up the methane number display parameters, opposite the *Methane number* line, click **Settings**. A dialog window opens (Fig. 19).
 - 1. To display a column in the table, check the corresponding option.
 - 2. To set the number of decimals, in the corresponding *Accuracy* field, enter an integer value.
 - 3. To round values in accordance with GOST 31371.7-2020, opposite the corresponding parameter, check the *GOST* option.
 - 4. To save the changes, click **OK**.

View: Methane number		×
	GOST	Accuracy
Methane	\checkmark	4
Simplified mixture		4
Initial methane number values		4
Natural gas compounds		4
	ОК	Cancel

Fig. 19: View: Methane number

16. Hotkeys

16. Hotkeys

The software uses keyboard shortcuts for quick access to actions:

Ctrl + A	Select all
Ctrl + C	Copy to clipboard
Ctrl + D	Delete selected chromatograms
Ctrl + G	Add calibration chromatograms
Ctrl + H	Add assay chromatograms
Ctrl + J	Add control chromatograms
Ctrl + R	Refresh chromatogram list
Ctrl + T	Open chromatogram
Ctrl + E	Copy areas of selected chromatograms to clipboard
Shift + ↑/↓	Select lines above/below

17. Program Identification

The identification data of the software «Chromos: Natural Gas» is placed on the *About...* tab (Fig. 20). In the software «Chromos: Natural Gas», the metrologically significant part is allocated in the form of separate calculation modules protected from intentional changes:

- CalcLibPlugin.dll does not contain metrologically significant functions;
- CalcLib31371720.dll contains metrologically significant functions in accordance with GOST 31371.7-2020;
- CalcLib3136921.dll contains metrologically significant functions in accordance with GOST 31369-2021 (ISO 6976:2016);
- CalcLib3470420.dll contains metrologically significant functions in accordance with GOST 34704-2020.

The identification data of the certified calculation modules are specified in the certificate of metrological certification of the software «Chromos: Natural Gas».



Fig. 20: Program identifier