

MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE

V.N. KARAZIN KHARKIV NATIONAL UNIVERSITY (T. N. ROMAN 13PT)

**Inorganic chemistry department**

UDC 541.35

*Allow for defense*

« \_\_\_\_ » \_\_\_\_ 2024

Head of the department  
Last name FIRST NAME of  
Head of the department

**DIPLOMA BACHELOR THESIS**

Bachelor thesis  
of the School of Chemistry  
**WANG Xiaoming** ( LAST name First  
name)

Supervisor  
PhD, assoc. prof  
PhD, assoc. prof  
name First name)

Oleg KALUGIN  
ZHOU Jielun( LAST

KHARKIV 2024

(separated by 1 line below)

## ABSTRACT (Times New Roman 13pt)

Body (Times New Roman 13pt, 1.5 line spacing, paragraph indent -1.25 cm)

The abstract should contain (in sequence):

- information on the scope of the qualification (course) work, on the number of sections, illustrations, tables, appendices, sources according to the list of references (including appendices data);
- abstract text;
- list of keywords.

*Key words:* italics, separated by commas, 1 space for each word, at least 5 main terms for the topic (Times New Roman 13pt)

The text of the abstract should reflect the information presented in the work and, as a rule, in the following sequence:

- object of research or development;
- the purpose of the work;
- research methods and equipment;
- results and their novelty;
- basic structural, technological and operational characteristics and indicators;
- degree of implementation;
- relationship with other works;
- recommendations on the use of work results;
- field of application;
- significance of work and conclusions;
- predictive assumptions about the development of the object of research or development.

(separated by 1 line below)

CONTENT(Times New Roman 13pt, separated by 1 line below)

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(separated by 1 line below)

## INTRODUCTION(Times New Roman 13pt, separated by 1 line below)

In the introduction to the work, an assessment of the current state of the solved problem is briefly presented. It is necessary to show the novelty and relevance of this work, its main purpose, the scientific and technical significance of the research, the initial data for conducting the work, and global trends in solving the tasks. If there is an experimental (calculation) part in the work, the introduction justifies the advisability of setting up and performing relevant research.

An introduction of 2-3 pages starts on a separate page.

Body (Times New Roman, 13pt, 1.5 line spacing, paragraph indent – 1.25 cm)

(separated by 1 line above)

## **Chapter I** (Times New Roman 13pt)

**TITLE** (Times New Roman 13pt, separated by 1 line below)

### **1.1 title**×× (Times New Roman 13pt, separated by 1 line below)

Body (Times New Roman 14pt, Indent the first line by 2 characters and 1.5 line spacing)

The review is compiled by the student independently based on the study of literary sources.

The text of the work should be printed following such margins: **top and bottom - at least 20 mm, right - at least 10 mm, left - at least 30 mm.**

The sections of the work must have sequential numbering within the framework of the presentation of the essence of the work and be marked with Arabic numerals without a period. For example, 1, 2, 3, etc.

Subsections must be sequentially numbered within each section. The subdivision number consists of the section number and the serial number of the subdivision, separated by a dot. For example, 1.2, 1.3, 1.4, etc.

(separated by 1 line above)

## **Chapter II**

### **TITLE**

#### **2.1 TITLE××**

Each chapter needs a separate page

(separated by 1 line above)

## CONCLUSIONS (Times New Roman 13pt, separated by 1 line below)

The results of the work should contain short conclusions based on the results of the work.

Their volume should not exceed 1.5 pages

should be indicated how the work ended:

- obtaining scientific results about new objects, processes, phenomena, patterns;
- development of scientific foundations of new research methods and principles;
- obtaining qualitative and quantitative characteristics of objects and phenomena;
- development instructions, recommendations, methods (calculations, measurements, tests, etc.);
- production of laboratory and experimental samples of products.

(separated by 1 line above)

LIST OF REFERENCES (T.N.Roman 13pt, separated by 1 line below, at least 15-30)

1. Walla P. J., Single-biomolecule techniques. In *Modern Biophysical Chemistry*, Wiley-VCH Verlag GmbH & Co. KGaA: 2014; pp 203-256.
2. Walsh T. R. Pathways to structure–property relationships of peptide–materials interfaces: Challenges in predicting molecular structures. *Acc. Chem. Res.* **2017**, 50 (7), 1617-1624.
- 3.
- 4.
- ...



**Examples of compiling a bibliographic description  
for a list of sources used**

(based on the American Chemical Society ACS style format)

Source	Styling example
<b>Books:</b>	
– single author	Walla P. J., Single-biomolecule techniques. In <i>Modern Biophysical Chemistry</i> , Wiley-VCH Verlag GmbH & Co. KGaA: 2014; pp 203-256.
– two authors	Šachl R., Johansson L. B. Å., Heterogeneous lipid distributions in membranes as revealed by electronic energy transfer. In <i>Reviews in Fluorescence</i> 2015, Geddes, C. D., Ed. Springer International Publishing: 2016; Vol. 8, pp 171-187.
– three authors	Hermann E., Ries J., García-Sáez A., Scanning fluorescence correlation spectroscopy on biomembranes. In <i>Methods in Membrane Lipids</i> , Owen, D. M., Ed.; Springer New York: 2015; Vol. 1232, pp 181-197.
<b>Dissertation:</b>	Chandrakanth J.S. Effects of ozone on the colloidal stability of particles coated with natural organic matter. Ph.D. Dissertation, University of Colorado, Boulder, CO, 1994.
<b>Multi-volume documents:</b>	
– single volume reference	Annual Review of Physical Chemistry; Leone S.R., McDermott A.E., Paul A., Eds.; Annual Reviews: Palo Alto, CA, 2005; Vol. 56.
	Wiberg, K. In <i>Investigations of Rates and Mechanisms of Reactions</i> ; Lewis, E.S., Ed.; Techniques of Chemistry, Vol. VI, Part I; Wiley & Sons: New York, 1974; p 764.
<b>Reference books:</b>	Advanced Inorganic Chemistry; Wiley, 1999; p. 532.
<b>Journal article:</b>	
- single author	Walsh T. R. Pathways to structure–property relationships of peptide–materials interfaces: Challenges in predicting molecular structures. <i>Acc. Chem. Res.</i> <b>2017</b> , 50 (7), 1617-1624.
- two authors	Shao Q., Hall C. K. Allosteric effects of gold nanoparticles on human serum albumin. <i>Nanoscale</i> <b>2017</b> , 9 (1), 380-390.
- three authors	Pan, X. J.; Kadla, J. F.; Ehara, K. Organosolv Ethanol Lignin from Hybrid Poplar as a Radical Scavenger: Relationship Between Lignin Structure, Extraction Conditions, and Antioxidant Activity. <i>J. Agric. Food Chem.</i> <b>2006</b> , 54 (16), 5806-5813. DOI: 10.1021/jf0605392
- four authors	Caetano D. L. Z., de Carvalho S. J., Metzler R., Cherstvy A. G. Critical adsorption of periodic and random polyampholytes onto charged surfaces. <i>Phys. Chem. Chem. Phys.</i> <b>2017</b> , 19 (22), 23397-23413.

- five or more authors	Foster, J. C.; Varlas, S.; Couturaud, B.; Coe, J.; O'Reilly, R. K. Getting into Shape: Reflections on a New Generation of Cylindrical Nanostructures' Self-Assembly Using Polymer Building Block. <i>J. Am. Chem. Soc.</i> <b>2019</b> , <i>141</i> (7), 2742–2753. DOI: 10.1021/jacs.8b08648
<b>Conference proceedings:</b>	
– single author	Aleksandrov S.V. Problems of oil-contaminated land reclamation. In <i>Problems of Life Safety and Industrial Ecology</i> , Proceedings of the III-th International Scientific and Practical Conference, Ulyanovsk, Russia, June 3-4 2010; Savinykh V.V., Krasnogorskaya N.N., Silina E.K., Ed.; UIGTU, 2010; pp. 29-30.
– two authors	Garrone E., Ugliengo P. In <i>Structure and reactivity of surfaces</i> , Proceedings of the European Conference, Trieste, Italy, Sept 13–20, 1988; Zecchina A., Cost G., Morterra C., Eds.; Elsevier: Amsterdam, 1988.

<b>Conference paper:</b>	
– single author	Kaplan L.J. <i>Books of Abstracts, Part 2</i> , 213 <sup>th</sup> ACS National Meeting, San Francisco, CA, April 13-17, 1997; American Chemical Society: Washington, DC, 1997; CHED-824.
– two author	Ierapetritou, M. G.; Androulakis, I. P.; Monas, D. S.; Floudas, C. A. Structure Prediction of Binding Sites of MHC Class II Molecules Based on the Crystal HLA-DRB1 and Global Optimization. In <i>Optimization in Computational Chemistry and Molecular Biology: Local and Global Approaches</i> : Proceedings, 1999, Princeton University, Princeton, NJ, May 7-9, 1999; Floudas, C. A., Pardalos, P. M., Eds.; Kluwer, 2000; pp 157-190.
<b>Online resources:</b>	CARO Analytical Services. <i>Soil Testing Capabilities</i> . <a href="https://www.caro.ca/soil-testings/">https://www.caro.ca/soil-testings/</a> (accessed 2020-09-14).
<b>Patents:</b>	1. Lenssen K.C., Jantscheff P., Kiedrowski G., Massing U. Cationic lipids with serine backbone for transfecting biological molecules. Eur. Pat. Appl. 1457483, 2004. 2. Langhals H., Wetzel F. Perylene pigments with metallic effects. Ger. Offen. DE 10357978.8, Dec 11, 2003; <i>Chem. Abstr.</i> <b>2005</b> , <i>143</i> , 134834.

Figure styling example

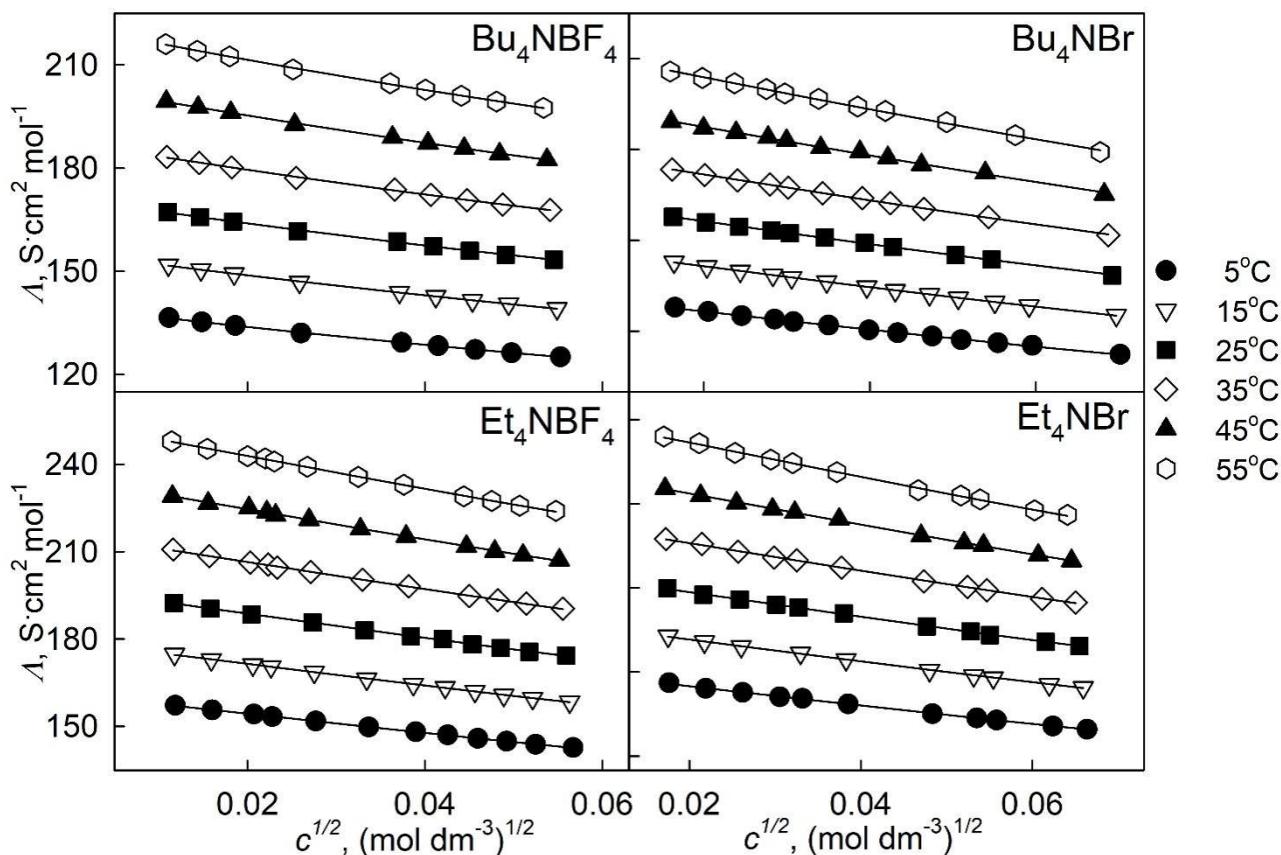


Figure 1.7 Concentration dependence of molar electrical conductivity of tetraalkylammonium salts in acetonitrile at different temperatures. Lines on the figure represent theoretical function of electrical conductance obtained by the f Lee-Wheaton equation.

Example:

"The movement of an electron in an atom is described by a wave function, which is a solution to the Schrödinger equation

$$-\frac{h^2}{8\pi^2m}\nabla^2\psi + U\psi = E\psi \quad (4.1)$$

where

$h$  - Planck's constant,

$\psi$  - the wave function,

$m$  - mass of the electron,

$U$  - potential energy of the interaction of the electron with the nucleus,

$E$  - full energy."

## Table styling example

Table 3.2 Physico-chemical properties of non-aqueous solvents  
 ( $P=101.325$  kPa,  $T=298.15$  K)

Solvent	$M$ , g/mol	$T_b$ , K	$T_m$ , K	$\mu_v$ , D	DN	$\eta_0 \cdot 10^3$ , Pa·s	$\epsilon$
Methanol	32.04	337.66	175.66	1.70	19.1	0.5409	32.6
Ethanol	46.07	351.45	158.65	1.69	19.2	1.087	24.3
Propanol-1	60.11	370.35	146.15	1.66	19.8	1.967	20.1
Butanol-1	74.12	390.95	183.15	1.66	19.5	2.571	17.1
Pentanol-1	88.15	411.15	192.56	1.66	20.4	3.335	14.6
Hexanol-1	102.18	430.25	225.75	1.66	20.5	4.470	12.9
Hheptanol-1	116.21	449.45	240.35	1.66	-	5.675	11.1
Octanol-1	130.23	468.25	256.85	1.66	20.3	7.260	9.7
Nonanol-1	144.26	486.65	268.15	1.66	-	10.27	8.8
Acetonitrile	41.05	354.65	227.45	3.97	14.1	0.347	36.7
DMSO	78.09	462.15	291.35	3.96	29.8	1.963	46.3
Ethylene glycol	62.07	470.35	259.35	2.28	19.1	16.72	37.7
Acetone	58.1	329.39	177.80	2.85	17.0	0.304	20.7

## A sample of computer program source styling

### Appendix A.1

#### A program for computer simulation of fluids by the methods of Brownian and molecular dynamics

```
// file: BDHMAIN.CPP

// "Brownian and molecular Dynamics" after Heerman D.W.
// Author: O.N. Kalugin , September 2005
// updating 20.01.06
// .....
#include <time.h>
#include <math.h>
#include <string.h>
#include <complex.h>
#include "BDH.H"

int Analyse(int argc, char *argv[]);
int FileNames(int argc, char *argv[]);

FILE *in, *out, *store, *key, *par, *lgn;
char *fk, *fp, *fi, *fo, *fs, *fl, *fomd, *fobd;

int key_init = 1,      // Key for start new calculation or read previous
one

                        // { x, vh, f } from "in" file *.str
key_eqv  = 0,          // Nonequilibrium or equilibrium calculation
key_RDF  = 0,          // (1) for RDF calculation (0) for opposite case
key_trans= 0,          // (1) for VACF and square disp. calculation
                        // (0) for opposite case
key_BDH  = 1;          // (1) for VACF and square disp. calculation
                        // (0) for opposite case

time_t t;
clock_t starttime, endtime;
float elapsed_time;

double x[n3]={0},vh[n3]={0},f[n3]={0},
den    = 0.83134,
side   = 6.75284, // side length of the cubical box in sigma units
tref   = 0.722,   // reduced temperature
rcoff  = 2.5,     // cutoff of the potential in sigma units
ek,ekin,epot,etot,pres,vel,rp,vir,sideh,
hsq,hsq2,rcoffs,tscale,vaver,temp;

//
MAIN .....
int main(int argc, char *argv[])
{
int i;
double E_total;
```

### **Rules for the dissertation designing**

Volume	Bachelor's qualification work - at least 20 pages
Interval	After 1.5 intervals
Font	Font Times New Roman 13
Fields	Margin dimensions: top and bottom - at least 20 mm, right at least 10 mm, left - at least 30 mm
	Only the customary terms recommended by existing standards should be used. Abbreviations and abbreviations should also be generally accepted
	It is advisable to use only one name for a certain substance or phenomenon.
Nomenclature	Give the names of chemical compounds in accordance with the accepted nomenclature. They are capitalized in headings and at the beginning of sentences. It is not allowed to use professional scientific jargon when writing a qualification paper.
	Names and designations of measurement units should be given in the system of units SI.
	When describing methods of synthesis, measurements, calculations, etc. you should use uniform methods of writing defining words throughout the work.
	Mathematical quantities should be denoted by the usual symbols and names of physical and other quantities
Designing	When designing the work, it is necessary to observe the uniform writing of the text, contrast and clear image of the letters throughout the entire work. Lines, letters, numbers and other signs must be clear and not vague.
Structural elements	Structural elements "ABSTRACT", "CONTENTS", "LIST OF TERMS, SYMBOLS, UNITS, ABBREVIATIONS AND TERMS", "INTRODUCTION", "CONCLUSIONS", "REFERENCE LIST", "APPENDICES", etc. are not numbered, and their names follow the headings of structural elements.
Sections	Sections and subsections must have headings. Items and sub-items can have headings.
Paragraph	Paragraph indentation must be the same throughout the text and equal to five characters
	The distance between the title and the text should be: not less than two lines.
	The distance between the lines of the title, as well as between two titles, is taken as the same as in the text.
The pages	The pages of the qualification (coursework) should be numbered with Arabic numerals, adhering to the numbering throughout the entire text of the work. The page number is placed in the upper right corner of the page without a period at the end. The title page is included in the total page numbering. Number pages on the title page are not inserted.

Chapters	<p>Chapters, subsections, items and sub-items of the work should be numbered with Arabic numerals.</p> <p>The sections of the work must have sequential numbering within the framework of the presentation of the essence of the work and be marked with Arabic numerals without a period. For example, 1, 2, 3, etc.</p>
Illustrations	<p>Illustrations should be numbered with Arabic numerals in sequential numbering within the chapter, except for illustrations that are given in the appendices.</p>
The table	<p>The table number consists of the section number and the serial number of the table, separated by a dot. For example, table 3.1 is the first table of the third section. If there is one table in the work, it should also be numbered.</p>
Mandatory elements	<p>The qualification (coursework) must contain the following mandatory elements.</p> <ol style="list-style-type: none"> <li>1. Title page.</li> <li>2. Abstract in two languages (English and another language).</li> <li>3. Content.</li> <li>4. List of conventions, symbols, units, abbreviations and terms</li> <li>5. Introduction.</li> <li>6. Literary (analytical) review.</li> <li>7. Experimental part.</li> <li>8. Labor protection (if necessary and/or important).</li> <li>9. Conclusions (summaries of the work).</li> <li>10. List of used sources (list of references).</li> <li>11. Appendix (if necessary)</li> </ol>