RESEARCH OF N,N′-HEXAMETHYLENE BIS-[(O-CRESOLYL)-CARBAMATE] IN INTERNATIONAL CHEMICALS DATABASES

Eldor Mashayev
Senior teacher of the Department of Chemical Technology of Oil Refining, Tashkent Institute of Chemical Technology
Boburbek Ismailov
Associate Professor of the Department of Chemical Technology of Gas Processing, Tashkent Institute of Chemical Technology, Doctor of Philosophy (PhD) in Technical Sciences
Jasurbek Ergashev
Trainee teacher of the Department of Chemical Technology of Gas Processing, Tashkent Institute of Chemical Technology
Sherzod Omonov
Trainee teacher of the Department of Chemical Technology of Gas Processing, Tashkent Institute of Chemical Technology
Abdukhamid Makhsumov
Professor of the Department of Chemical Technology of Oil Refining, Tashkent Institute of Chemical Technology, Honored Inventor of the Republic of Uzbekistan, valid member of the healing academy of Uzbekistan, Academician of the Academy of Sciences “Turon”, doctor of chemical sciences, professor, Tashkent, Republic of Uzbekistan
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Abstract. In this scientific work, studies of bis-carbamate were carried out in modern electronic databases, including elemental analysis, PMR, IR and mass spectra. For example, if we look only at the IR spectra of N,N'-hexamethylene-bis-[(o-cresolyl)-carbamate], we can see functional carbamate groups such as N-H, -C-N, C=O, N-(CO)-O and proves that this is exactly the substance.

Keywords. Bis-carbamate, electronic database, structure-activity, physicochemical analysis, IUPAC, PMR, IR, Mass spectrum.

INTRODUCTION.

With the advent of globalization, the search process on the Internet was automated, information search systems and electronic databases were created. Today, chemists must have the skills to search, differentiate and analyze the right information on giant search platforms such as Google and Yandex [1, 3-6, 8].

Searching for chemical substances not only in scientific journals and databases, but also in electronic databases based on the principle of “structure-activity” in Chemspider, Chemspider Synthetic Pages, Pubchem, E-molecules, Chemicalize, Properties viewer, Chem Search, Organic Syntheses" and many other electronic databases they can get important information about chemicals, their preparation, physico-chemical properties, spectra [2, 7, 9-10]. We named, characterized, and obtained YMR, IR, and mass spectra of newly synthesized N,N′-hexamethylene bis-[(o-cresolyl)-carbamate], i.e., MEE-1, based on these bases.

MATERIAL AND METHODS. In these electronic databases, the solution to the problem of the uniqueness of the chemical language is systems, rules for the precise description of the composition and structure of the molecules of substances. One such system is the

specification of a simplified representation of molecules in a line - SMILEs. Another international text chemical identifier is the InChi code, developed by experts from IUPAC and NIST. From the InChi code comes a new hashed format, the fixed-length InChiKey, which is more convenient for indexing in information retrieval systems. It should be noted that SMILES has advantages over InChi, such as better human understanding of formulas, simpler software support related to a broad theoretical framework - graph theory. We studied the structure of newly synthesized N,N′-hexamethylene bis-[(o-cresolyl)-carbamate], MEE-1, in MOL file.

RESULTS AND DISCUSSION

In order to find out the initial physicochemical properties of the obtained compounds, we included them in PubChem, a public domain database of chemical compounds and mixtures maintained by the US National Center for Biotechnology Information, a division of the US National Library of Medicine. https://pubchem.ncbi.nlm.nih.gov/. In this, the database suggested that we name MEE-1 as:

1. IUPAC Name- (4-methylphenyl) N-[6-[(4-methylphenoxy)carbonylamino]hexyl]carbamate
2. N,N'-(Hexamethylene)bis(carbamic acid p-tolyl) ester.

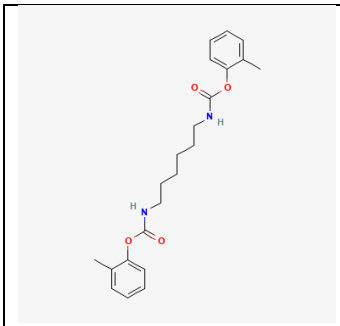
In order to find out the initial physico-chemical properties of the obtained compounds, we included them in the "ChemSpider" database of chemical compounds and mixtures belonging to the British Royal Society of Chemistry. http://www.chemspider.com/ In this, the database suggested us to name the compound MEE-1 in different languages as follows:

1. [ACD/IUPAC Name] [French] 1,6-Hexanediylbiscarbamate de bis(2-méthylphényle)
2. [ACD/IUPAC Name] Bis(2-methylphenyl) 1,6-hexanediylbiscarbamate
3. [ACD/IUPAC Name] [German] Bis(2-methylphenyl)-1,6-hexandiylbiscarbamat
4. [ACD/Index Name] Carbamic acid, N,N'-1,6-hexanediylbis-, bis(2-methylphenyl) ester and etc.

The ACD/Labs Percepta Platform predictions processed using the PhysChem module are then presented in Table 1 below.

Table 1

Preliminary description of the compound MEE-1



Compound MEE-1

Formula		$C_{22}H_{28}N_2O_4$
Molecular mass		384.5 u
Hydrogen of the garden donors the number		2
Hydrogen of the garden acceptors _ the number		4
Percentage composition		
C	12.0107 u × 22	68.727 %
H	1.00794 u × 28	7.3406 %
N	14.0067 u × 2	7.2863 %
O	15.9994 u × 4	16.646 %

Next, the predicted data generated using the US Environmental Protection Agency's EPISuite™ is presented below.

https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface.

Prediction of MEE-1 in the US Environmental Protection Agency's EPISuite™ program

Melting point: 172.95 (average MP)
Quick biological decay potential (BIOWIN v4.10):
Biowin1 (linear model): 0.8329 / Biowin2 (non-linear model): 0.6731
Biological decay probability MITI:
Biowin5 (linear model MITI): -0.0735 / Biowin6: 0.0270
Anaerobic biological decay probability :
Biowin7 (linear anaerobic model): - 0,5150
A tmosphere at oxidation (25°C) [AopWin v1.92]:
Half-life = 0.297 days (12- hour day ; 1.5E6 OH/cm ^{3})
Adsorb ts ion coefficient of soil (PCKOCWIN v1.66):
Koch: 3.82E+005 / Log Koch : 5,582
To the water based on acid-catalyzed hydrolysis (25°C) [HYDROWIN v1.67]:
For total Kb pH > 8 at 25°C : 9.359E+000 l/ mol -sec
Kb half-life pH 8: 20,571 hours
Kb half-life pH 7: 8.571 days

PMR and IR predicted spectra of compound MEE-1 were obtained from the SpectraBase™ open online spectral library of John Wiley & Sons, Inc. and interpreted Figures 1,2. https://spectrabase.com/ .

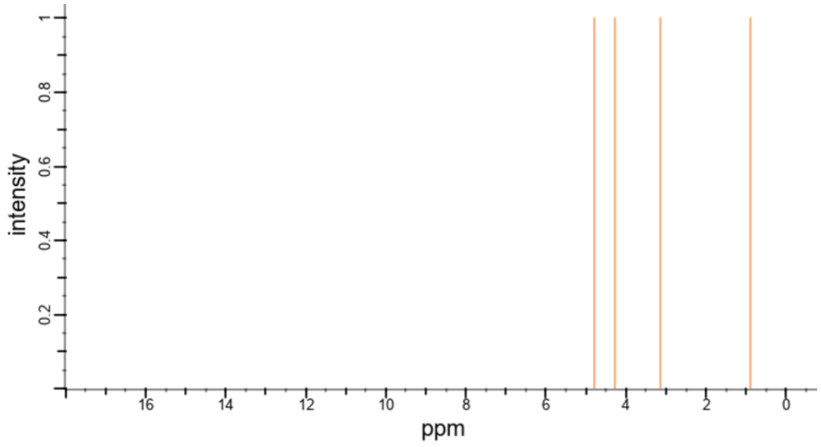


Figure 1. PMR spectrum of compound MEE-1. Device brand Varian CFT-20 solvent $CDCl_3$.

In the MEE-1 PMR spectrum, the signal of hexane appeared in the region near 1 ppm, and the signal of the methylene group appeared in the region after 3 ppm. Aromatic ring signals were observed in areas after 4 ppm.

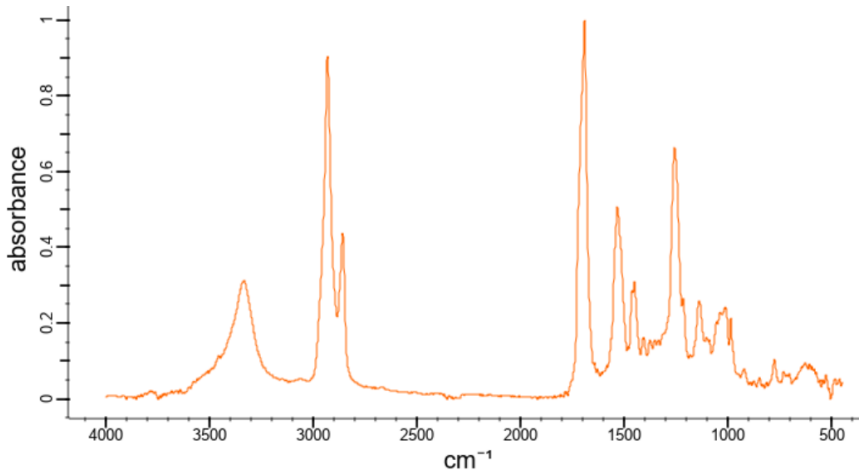


Figure 2. IR spectrum of compound MEE-1. in a KBr tablet.

In the IR spectrum of the compound MEE-1, the amine group NH valence vibrations of carbamates are in the region of 3500-3250 cm^{-1} , and the valence vibration characteristic of the -CN bond is in the region of 1100 cm^{-1} , the carbonyl group C=O is at 1750-1680 cm^{-1} , amine NH deformation vibrations of the group were observed in the region of 1650-1500 cm^{-1} , asymmetric valence vibrations of the N-(CO)-O carbamate group were observed in the region of 1270-1210 cm^{-1}. The ring vibration of the aromatic ring was in the range of 1200-1300 cm^{-1} , the valence vibration of the CH bond of the ring was in the range of 3000-2840 cm^{-1} , and the deformation vibration was manifested in the range of 900-650 cm^{-1}. Skeletal vibration of the methyl group in the aromatic ring was observed in the 1250-800 cm^{-1} region. The valence vibration of the carbonyl group - C -O- was observed in the region of 1200-1080 cm^{-1} . And the vibration of the methylene group of alkanes was observed in the region of 770-720 cm^{-1}.

To perform mass spectroscopic analysis of MEE-1, an estimated mass spectrum of MEE-1 was obtained based on the structure of the compound using Open Access EPFL MStoolbox software. and analyzed Figure 3 and Table 2.

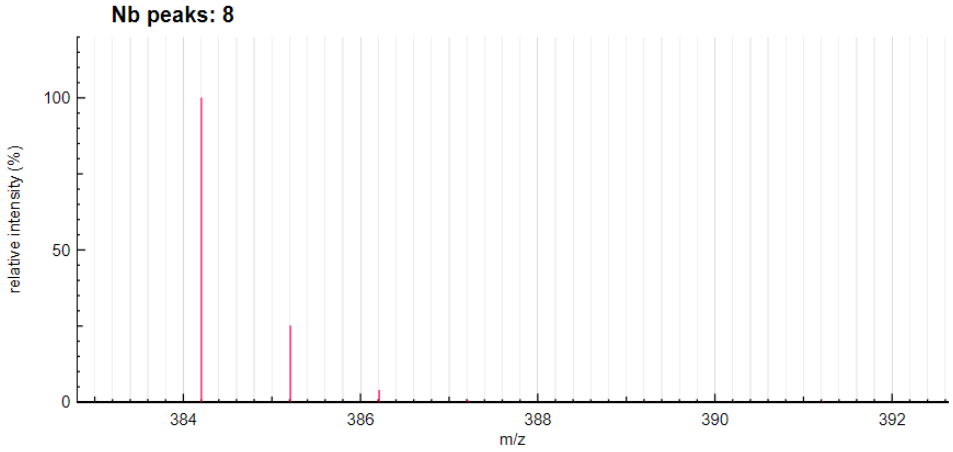


Figure 3. Mass spectrum of compound MEE-1

Table 2 .

Mass spectrum analysis of compound MEE-1

Molecular formula	Molecular mass	Monoisotopic mass _	m/z	Ionization	Insatiability	Charge	Code
$C_{22}H_{28}N_2O_4$	384.47	384.2049	385.2122	H+	10	1	A

CONCLUSION.

We first studied IR, YMR, mass spectra of N,N′-hexamethylene bis-[(o-cresolyl)-carbamate] i.e. MEE-1 in these programs and then conducted physico-chemical analyzes in real devices. the similarity was 80% and these obtained results were of great help in the interpretation of the spectra. We believe that it will be useful for chemists to study the newly synthesized substances in the above-mentioned and other electronic databases before real analysis.

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