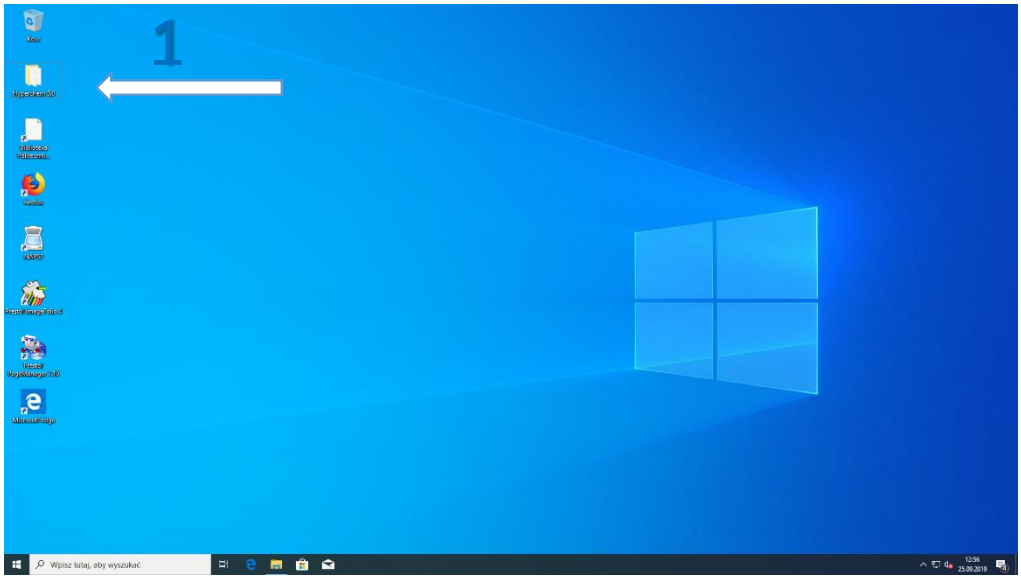
Hyperchem - Characteristics of the software

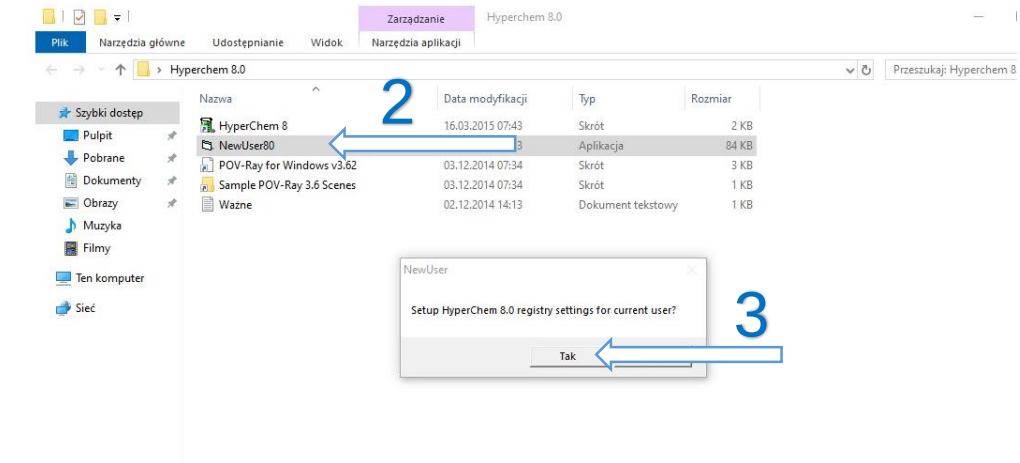
Content:

HyperChem is a molecular modeling software. It enables users to prepare and carry out calculations and visualize the results. With the use of this software, you can predict the chemical and physical properties of molecules, model large systems such as proteins in force fields, study interaction mechanisms and chemical reaction mechanisms, and simulate spectroscopic spectra (UV, IR, NMR). The program enables you to carry out calculations using popular methods in theoretical calculations, including simple and molecular mechanics, semi-empirical, computational quantum chemistry (ab initio), calculations based on DFT density functions and methods of molecular dynamics.

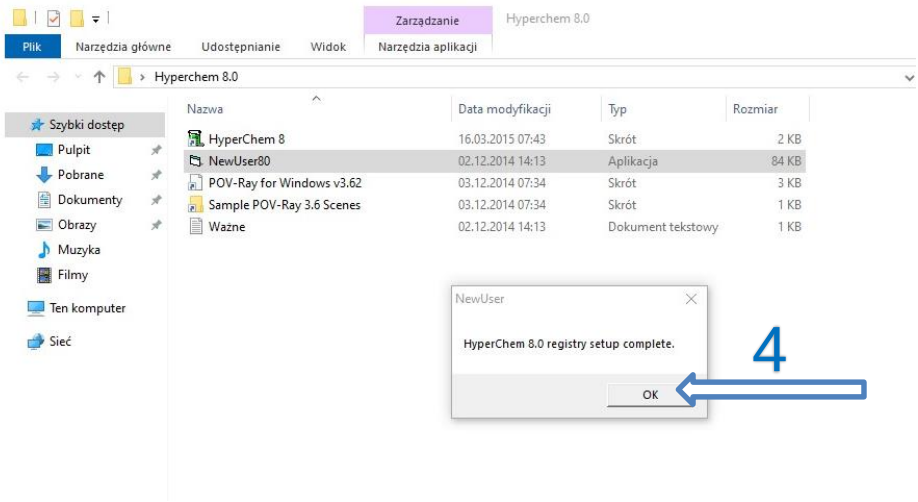
Launching the software:

Before running Hyperchem 8, you need to start the application **New User 80 HyperChem** located in the folder on the desktop (see the picture below).





PhD Beata Korzystka
Scientific Information Department
Email: Beata.Korzystka@put.poznan.pl
Phone: 61 665 3522



Access:

You can use the software **in the Reading Room (1st floor)** and **at the Faculty of Chemical Technology** (within the IP range of Poznan University of Technology).

30 August 2022

LIBRARY
POZNAN UNIVERSITY OF TECHNOLOGY

PhD Beata Korzystka
Scientific Information Department
Email: Beata.Korzystka@put.poznan.pl
Phone: 61 665 3522