



Conf.dr. Ionel HUMELNICU

Domenii de competență:

Chimie teoretică, structură moleculară, chimie cuantică, spectroscopie, modelare moleculară, dinamică moleculară, mecanisme de reactive, reactivitate moleculară

Cursuri predate:

Dinamică moleculară și reactivitate, Reactivitate și spectroscopie moleculară, Biochimie cuantică, Chimie cuantică, Dinamica interacțiunilor intermoleculare, Chimie fizică (Structură), Modelarea proceselor fizico-chimice din mediu, Spectroscopie computațională, Structură și simetrie moleculară, Dinamica sistemelor chimie, Modelare moleculară, Chimie cuantică și structură, Chimie computațională

Lucrări științifice - selecție

1. I. Druță, Rodica Dinică, Elena Bâcu and **I. Humelnicu**, Synthesis of 7,7'-Bisindolizines by the Reaction of 4,4'-Bipyridinium-Ylides with Activated Alkynes, *Tetraherdon*, **54**, 10811-10818 (1998).
2. **I. Humelnicu**, M. Constantinescu, Iuliana Voicu and C. Ghirvu, „On the Interaction Between the H Atom and HCl Molecule”, *Revue Roumaine de Chimie*, vol.**47** nr.8-9, 817-823 (2002).
3. N. Heße, R. Fröhlich, **I. Humelnicu** and E-U Würthwein, „1,3,5-Triazapentadienes as Chelating Ligands: 1,2,4-Triphenyl-1,3,5-triazapentadiene Complexes of Cobalt(II), Nickel(II), Palladium(II), Copper(II) and Zinc(II)”, *Eur. J. Inorg. Chem.* **11**, 2189–2197 (2005)
4. M. Dimitriu, E. Filip, **I. Humelnicu**, „Theoretical Study of some benzene derivatives in water”, *Rev. Chim. Bucharest*, **59** (9), 1009-1013 (2008).
5. Josette Weinberg, F. Cimpoesu, D. Lerner and **I. Humelnicu** „The Association of Dehydro-Epiandrosterone and Adenosine Triphosphate Acid. A DFT Study of Interactions between Prototypic Biologically Active Molecules” *Journal of Molecular Structure: THEOCHEM*, (2009) **912** (1-3) 32-37
6. C. Nadejde, D.E. Creanga, **I. Humelnicu**, E. Filip, D.O. Dorohoi, ”Study on the Intermolecular Interactions in Rifampicin Ternary Solutions – Calculation of Microscopic Parameters of Rifampicin Molecules”, *Journal of Molecular Liquids*; (2009) **150** (1-3) 51-55;
7. Lucia Odochian, Lorela Iancu, **I. Humelnicu**, Anca Mihaela Mocanu, Adriana Băiceanu, „Contributions to the reaction mechanism of photochemical decomposition of hydrogen peroxide in aqueous solution”, *Rev. Chim. (Bucharest)*, (2011) **62**, No. 10, 1012-1016
8. **I. Humelnicu**, E-U Würthwein, G. Haufe, „The Conformers of 3-Fluoroalanine. A Theoretical Study Influence of a Fluorine Substituent on the Physicochemical Properties and Chemical Reactivity of Fluorinated Amino Acids. Part 1”, *Organic & Biomolecular Chemistry*, (2012) **10** (10), 2084-2093
9. C. Oprea, P. Panait, F. Cimpoesu, **I. Humelnicu**, Marilena Ferbințeanu, M. Gîrțu, „Broken symmetry DFT calculations of exchange coupling constants for manganese-porphyrin quasi-one-



dimensional molecular magnets”, *Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta)*, *Theor Chem Acc* (2012) **131** (7) 1249-1261

10. D. Maftai, Gh. Zbancioc, **I. Humelnicu**, I. Mangalagiu “Conformational Effects on the Lowest Excited States of Benzoyl-Pyrrolopyridazine. Insights from PCM Time- Dependent DFT” *The Journal of Physical ChemistryA*, (2013) **117** (15) pp 3165–3175.