

# Prof. ŞENAY YURDAKUL

## Personal Information

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## International Researcher IDs

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ScopusID: 7004632268

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## Education Information

Doctorate, Hacettepe University, Mühendislik Fakültesi, Fizik Mühendisliği Bölümü, Turkey 1980 - 1985

Postgraduate, Hacettepe University, Mühendislik Fakültesi, Fizik Mühendisliği Bölümü, Turkey 1979 - 1980

Undergraduate, Hacettepe University, Mühendislik Fakültesi, Fizik Mühendisliği Bölümü, Turkey 1974 - 1979

## Research Areas

Natural Sciences

## Academic Titles / Tasks

Professor, Gazi University, Fen Fakültesi, Fizik, 1996 - Continues

Associate Professor, Gazi University, Fen Fakültesi, Fizik, 1989 - 1996

Assistant Professor, Gazi University, Fen Fakültesi, Fizik, 1988 - 1989

Research Assistant, Middle East Technical University, Faculty Of Arts And Sciences, Department Of Chemistry, 1986 - 1988

Research Assistant, Hacettepe University, Mühendislik Fakültesi, Fizik Mühendisliği Bölümü, 1979 - 1986

## Academic and Administrative Experience

Fakülte Kurulu Üyesi, Gazi University, Fen Fakültesi, Fizik, 2021 - Continues

Head of Department, Gazi University, Fen Fakültesi, Fizik, 2020 - Continues

## Advising Theses

Yurdakul Ş., Theoretical and experimental vibrational spectroscopic studies of some drug molecules, Doctorate, M.ALP(Student), 2023

Yurdakul Ş., Experimental and theoretical vibrational spectroscopic study of biological active ligand and compounds, Doctorate, C.KÜÇÜK(Student), 2023

Yurdakul Ş., INVESTIGATION OF 3-ACETYL PYRIDINE AND 4-ACETYL PYRIDINE ACTIVE MOLECULES BY EXPERIMENTAL

AND THEORETICAL VIBRATIONAL SPECTROSCOPY, Doctorate, A.ATILGAN(Student), 2022

YURDAKUL Ş., EXPERIMENTAL AND THEORETICAL INVESTIGATION OF THE STRUCTURAL AND VIBRATIONAL PROPERTIES OF 6-METHOXYQUINOLINE MOLECULE, Postgraduate, M.Nurhan(Student), 2021

YURDAKUL Ş., Experimental And Theoretical Investigation Of Urasil Molecular DmsO Production Solution, Postgraduate, T.ÖZTAN(Student), 2017

YURDAKUL Ş., Experimental And Theoretical Investigations On Structural And Physical Properties Of Several Ligand Compounds Used In Drug Design By Using Molecular Vibrational Spectroscopy, Doctorate, M.TUĞFAN(Student), 2016

YURDAKUL Ş., Experimental and theoretical study on vibrations of oxazole and its zinc halide complexes, Postgraduate, L.ÖZKURT(Student), 2014

YURDAKUL Ş., Structural analysis of the tautomeric forms and isomers of 3-hydroxy-2- uinoxalinecarboxylic acid and 8-hydroxy-2-quinolinecarboxylic acid molecules by using vibrational spectroscopy and quantum chemical calculations, Doctorate, S.BADOĞLU(Student), 2013

YURDAKUL Ş., Investigation of 2,2'-dipyridylamine molecule and its palladium and platinum complexes by experimental and theoretical vibrational spectroscopy, Postgraduate, M.TUĞFAN(Student), 2013

YURDAKUL Ş., Experimental and theoretical investigation on spectroscopic properties of some nitrogen-ended ligands, Doctorate, S.TANRIBUYURDU(Student), 2013

YURDAKUL Ş., ?-acetylpyridine ketone'un ve argerol'lü bileşiminin titreşimlerinin deneysel ve teorik olarak incelenmesi, Postgraduate, A.ATILGAN(Student), 2013

YURDAKUL Ş., Experimental and theoretical study on vibrations of free : &#945;- acetylpyridine ketone and it's argerol complex, Postgraduate, A.Atılgan(Student), 2013

YURDAKUL Ş., BAZI BİYOLOJİK AKTİF LİGANDLARIN TİTREŞİMSSEL SPEKTROSKOPİ İLE İNCELENMESİ, Postgraduate, Y.GÜLEŞCİ(Student), 2012

YURDAKUL Ş., Experimental and theoretical study on vibrations of 4-(imidazol-1-yl) phenol, Postgraduate, G.SELCİK(Student), 2012

YURDAKUL Ş., Study of the structures of free nipecotic acid and nipecotamide molecules and their complexes by using vibrational spectroscopy, Doctorate, N.ÇİĞDEM(Student), 2011

YURDAKUL Ş., Theoretical and experimental investigation of 2- hydroxyquinoxaline and 4-hydroxyquinazoline, Doctorate, T.POLAT(Student), 2010

YURDAKUL Ş., EXPERIMENTAL AND THEORETICAL STUDY ON VIBRATIONS OF FREE IMIDAZO(1,2-A)PYRIDINE, Postgraduate, S.BADOĞLU(Student), 2008

YURDAKUL Ş., THE CALCULATION OF THE VIBRATIONAL SPECTRA OF 1,2- BIS(2-PYRIDYL)ETHYLENE AND TRANS 1,2-BIS(4-PYRIDYL)ETHYLENE AND THE METAL COMPLEXES OF THEM, Doctorate, Z.ÖZHAMAM(Student), 2007

YURDAKUL Ş., Bazı metal 2,2'-dipyridyl'in halojen birleşiklerinin infrared spektroskopisi ile incelenmesi, Postgraduate, H.KÜÇÜK(Student), 2007

YURDAKUL Ş., 1,2-BİS(2-piridil)etilen ve trans 1,2- BİS(4-piridil etilen moleküllerinin serbest halde ve kompleks yapıdaki titreşim frekanslarının hesaplanması, Doctorate, Z.ÖZHAMAM(Student), 2007

YURDAKUL Ş., Bazı metal(II) halojenür 3-acetylpyridine bileşiklerinin titreşimsel spektroskopisi ile incelenmesi, Postgraduate, Z.DEMİRKAPI(Student), 2007

YURDAKUL Ş., Bazı metal 2-asetilpridin bileşiklerinin infrared spektroskopisi yöntemi ile incelenmesi, Postgraduate, E.ÖZGE(Student), 2006

YURDAKUL Ş., Bazı metal (II) halojenür 2-aminopyrimidine bileşiklerinin titreşimsel spektroskopisi ile incelenmesi, Postgraduate, N.ÇİĞDEM(Student), 2005

YURDAKUL Ş., Bazı metal (II) 2,2' bikiolin bileşiklerinin infrared spektroskopisi yöntemi ile incelenmesi, Postgraduate, F.KUŞTAN(Student), 2004

YURDAKUL Ş., Teorik ve deneysel titreşim spektroskopisi yardımıyla bazı molekül ve bileşiklerin incelenmesi, Doctorate, K.ARICI(Student), 2004

YURDAKUL Ş., Bazı metal (II) halejenür kinazolin bileşiklerinin titreşimsel spektroskopisi, Postgraduate, D.YASA(Student), 2004

YURDAKUL Ş., Bazı metal 4-tert-butylpyridine ve phenazine bileşiklerinin infrared spektroskopisi yöntemi ile incelenmesi, Postgraduate, M.OTHMAN(Student), 2004

YURDAKUL Ş., Bazı metal(II) phthalazine bileşiklerinin infrared spektroskopisi yöntemiyle araştırılması ve phthalazine

molekülünün titreşim spektrumunun teorik olarak incelenmesi, Postgraduate, M.AYASLAN(Student), 2003

YURDAKUL Ş., Bazı metal(II) benzimidazol bileşiklerinin yapılarının kırmızı altı spektroskopisi yöntemiyle araştırılması ve 1,2-bis(4-pyridyl) ethane molekülünün titreşim spektrumunun teorik olarak incelenmesi, Doctorate, M.KURT(Student), 2003

YURDAKUL Ş., Bazı metal(II) nikotinamid ve izonikotinamid bileşiklerinin yapılarının incelenmesi, Doctorate, A.ATAÇ(Student), 2002

YURDAKUL Ş., Bazı metal (II) phthalazine tetraşyanonikel bileşiklerinin titreşimsel spektroskopi ile incelenmesi, Postgraduate, C.BARDAKÇI(Student), 2001

YURDAKUL Ş., Bazı metal (II) benzimidazol tetraşyanonikel bileşiklerinin titreşimsel spektroskopi ile incelenmesi, Postgraduate, C.YILMAZ(Student), 1999

YURDAKUL Ş., Kadmiyum (II) ve nikel (II)'li 3 klor 4 metil anilin tetraşyanonikel ve klorür bileşiklerinin infra-red ve raman spektroskopileri ile incelenmesi, Postgraduate, A.İLHAN(Student), 1996

YURDAKUL Ş., Bazı bileşiklerin kırmızı-altı ve raman spektroskopisiyle titreşim frekans ve kiplerinin saptanması, Postgraduate, D.KÜÇÜKGÜLDAL(Student), 1995

YURDAKUL Ş., Metal ( II ) 4-tersiyer butil pridin tetraşyanonikel ( II ) komplekslerinin titreşimsel spektroskopi ile incelenmesi, Postgraduate, M.BAHAT(Student), 1995

YURDAKUL Ş., Bazı bileşiklerin kırmızı-altı ve raman spektroskopileri ile titreşim frekans ve kiplerinin saptanması, Doctorate, A.ÖZBAY(Student), 1995

YURDAKUL Ş., Kadmiyum (II) ve nikel (II)li kinoksalin tetraşyanonikel komplekslerin infrared ve raman spektroskopileri ile incelemesi, Postgraduate, M.GÜLLÜOĞLU(Student), 1995

YURDAKUL Ş., Geçiş metallerinin akridin ile yaptığı komplekslerin infrared spektroskopisi ile incelenmesi, Postgraduate, M.TAŞDELEN(Student), 1995

YURDAKUL Ş., 3,5 lutidin metal tetraşyanonikel komplekslerinin infra-red spektroskopisi ve DTA tekniği ile incelenmesi, Postgraduate, G.SAĞLAM(Student), 1994

## Jury Memberships

Appointment to Academic Staff-Professorship, Appointment to Academic Staff-Professorship, Türk Hava Kurumu Üniversitesi, October, 2023

Appointment to Academic Staff-Professorship, Appointment to Academic Staff-Professorship, İstanbul Üniversitesi, August, 2023

Post Graduate, Post Graduate, Gazi Üniversitesi, June, 2022

Appointment to Academic Staff - Associate Professorship, Appointment to Academic Staff - Associate Professorship, Gazi Üniversitesi, June, 2022

Appointment to Academic Staff-Professorship, Appointment to Academic Staff-Professorship, Gazi Üniversitesi, June, 2022

Appointment to Academic Staff-Assistant Professorship, Appointment to Academic Staff-Assistant Professorship, Gazi Üniversitesi, June, 2022

Doctorate, Doctorate, Gazi Üniversitesi, March, 2022

Post Graduate, Post Graduate, Gazi Üniversitesi, January, 2022

## Published journal articles indexed by SCI, SSCI, and AHCI

- I. **An experimental and computational studies, evaluating the in vitro antidiabetic and antioxidant activity, in silico prediction ADMET properties of 5-chloro-1H-benzimidazole and its newly synthesized silver(I) complex**  
Kucuk C., Celik S., YURDAKUL Ş., Coteli E.  
Applied Organometallic Chemistry, vol.38, no.6, 2024 (SCI-Expanded)
- II. **Characterization of the synthesized diaqua-bis(indazole-κN2)bis(nitrato-κO)zinc(II) complex and**

## DFT calculations

Kucuk C., Celik S., Yurdakul S., Özdemir N., Bülbül H.

Journal of Molecular Structure, vol.1304, 2024 (SCI-Expanded)

- III. **Spectroscopic characterization, DFT calculations, antimicrobial activity, and molecular docking studies of 5-methoxy-1H-benzo[d]imidazole and its Ag(I) complex**  
Kucuk C., Celik S., Yurdakul S., Erdem B.  
Polyhedron, vol.251, 2024 (SCI-Expanded)
- IV. **Synthesis, crystal structure and spectroscopic studies of a new silver complex derived from [1-(3-pyridinyl) ethanone]**  
Celik S., ATILGAN A., Alp M., YURDAKUL Ş., Demircioğlu Z., Özdemir N., Büyükgüngör O.  
Journal of Molecular Structure, vol.1294, 2023 (SCI-Expanded)
- V. **Synthesis, characterization, thermal, DFT study, antioxidant and antimicrobial in vitro investigations of indazole and its Ag(I) complex**  
Kucuk C., Celik S., YURDAKUL Ş., Cotel E., Erdem B.  
Polyhedron, vol.241, 2023 (SCI-Expanded)
- VI. **Structural and spectroscopic characterization, electronic properties, and biological activity of the 4-(3-methoxyphenyl)piperazin-1-ium 4-(3-methoxyphenyl)piperazine-1-carboxylate monohydrate**  
Kucuk C., YURDAKUL Ş., Özdemir N., Erdem B.  
Chemical Papers, vol.77, no.5, pp.2793-2815, 2023 (SCI-Expanded)
- VII. **An experimental vibrational spectroscopic and density functional theory computational study on 2,4-dioxypyrimidine in solvation phase**  
Badoğlu S., YURDAKUL Ş.  
International Journal of Quantum Chemistry, vol.123, no.8, 2023 (SCI-Expanded)
- VIII. **Experimental and theoretical vibrational spectroscopic, quantum chemical analysis, and electronic properties investigations of novel ruthenium complexes (RuLC12·2H2O; L: 4,4'-Dimethoxy-2,2'-Bipyridine, 4,4'-Dimethyl-2,2'-Bipyridine)**  
Alp M., YURDAKUL Ş.  
Polyhedron, vol.234, 2023 (SCI-Expanded)
- IX. **Crystal structure, vibrational spectroscopy, 1H NMR, and DFT analyses with antibacterial activity studies on silver nitrate complex of 5-iodoindole**  
Kucuk C., YURDAKUL Ş., Özdemir N., Erdem B.  
Inorganic Chemistry Communications, vol.150, 2023 (SCI-Expanded)
- X. **Copper(I) iodide complex with 4-pyridinecarboxaldehyde ligand: Synthesis, spectroscopic characterisation, AIM and NCI analysis combined with molecular docking and antibacterial activity studies**  
Celik S., YURDAKUL Ş., Erdem B.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1273, 2023 (SCI-Expanded)
- XI. **Combined Experimental and Theoretical Spectroscopic Properties (FT-IR, FT-Ra, Uv-Vis, and NMR), DFT Studies, Biological Activity, Molecular Docking, and Toxicity Investigations of 3-methoxy-1-piperazinylbenzene**  
Kucuk C., YURDAKUL Ş., Erdem B.  
Letters in Organic Chemistry, vol.20, no.5, pp.457-480, 2023 (SCI-Expanded)
- XII. **Experimental and DFT studies of 2-methyl-quinoxaline and its silver (I) complex: Non-covalent interaction analysis, antimicrobial activity and molecular docking study**  
Kucuk C., YURDAKUL Ş., Celik S., Erdem B.  
Inorganic Chemistry Communications, vol.145, 2022 (SCI-Expanded)
- XIII. **New silver(I) complex as antibiotic candidate: Synthesis, spectral characterization, DFT, QTAIM and antibacterial investigations and docking properties**  
Celik S., YURDAKUL Ş., ERDEM B.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1261, 2022 (SCI-Expanded)
- XIV. **Experimental and Theoretical Vibrational Spectroscopic Investigations, DFT quantum chemical**

- analysis, Biological activities and Molecular docking on 4,4'-Dimethoxy-2,2'-Bipyridine
- Alp M., YURDAKUL Ş., ERDEM B.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1260, 2022 (SCI-Expanded)
- XV. **Synthesis, theoretical and experimental spectroscopic properties, molecular docking, ADMET, and RDG analysis of copper(II) complex of dichloro(1,10-phenanthroline)(1,2,4-triazole-3-carboxylic acid)**  
Celik S., Badoglu S., YURDAKUL Ş.  
CHEMICAL PAPERS, vol.76, pp.4099-4114, 2022 (SCI-Expanded)
- XVI. **Experimental and theoretical Fourier transform infrared and Raman spectroscopy, density functional theory, antibacterial activity and molecular docking studies on 1-(4-methoxyphenyl)-1H-imidazole**  
Kucuk C., YURDAKUL Ş., ERDEM B.  
CHEMICAL PAPERS, vol.76, no.5, pp.2833-2854, 2022 (SCI-Expanded)
- XVII. **Spectroscopic characterization, DFT calculations, and microbiological activity of 5-iodoindole**  
Kucuk C., YURDAKUL Ş., ERDEM B.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1252, 2022 (SCI-Expanded)
- XVIII. **Synthesis, crystal structure, Hirshfeld surface analysis and molecular docking analysis of new cadmium(II) iodide complex with the pyridine, 4-(1,1-dimethylethyl)**  
Celik S., DEMİRCİOĞLU Z., YURDAKUL Ş., BÜYÜKGÜNGÖR O.  
JOURNAL OF COORDINATION CHEMISTRY, vol.75, pp.84-106, 2022 (SCI-Expanded)
- XIX. **Synthesis, spectroscopic characterization (FT-IR, PL), DFT calculations and antibacterial activity of silver(I) nitrate complex with nicotinaldehyde**  
Celik S., YURDAKUL Ş., ERDEM B.  
INORGANIC CHEMISTRY COMMUNICATIONS, vol.131, 2021 (SCI-Expanded)
- XX. **A combined experimental and theoretical study on vibrational spectra of 3-pyridyl methyl ketone**  
Celik S., Alp M., YURDAKUL Ş.  
SPECTROSCOPY LETTERS, vol.53, no.4, pp.234-248, 2020 (SCI-Expanded)
- XXI. **Crystal structure, spectroscopic characterization, thermal properties and theoretical investigations on [Ag(methyl 4-pyridyl ketone)2NO3]**  
YURDAKUL Ş., TEMEL E., BÜYÜKGÜNGÖR O.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1191, pp.301-313, 2019 (SCI-Expanded)
- XXII. **Electronic [UV-Visible] and vibrational [FT-IR] investigation and NMR spectroscopic analysis of some halogen substituted chromone (6-Fluorochromone, 6-Chlorochromone, 6-Bromochromone)**  
Erdođdu Y., Yurdakul Ş., Badoglu S., Gulluoglu M. T.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1184, pp.364-374, 2019 (SCI-Expanded)
- XXIII. **Experimental and Theoretical Study on New Zn(II) Halide Complexes of 3,5-Diazaindole**  
Badoglu S., Yurdakul Ş.  
JOURNAL OF STRUCTURAL CHEMISTRY, vol.59, no.5, pp.1010-1021, 2018 (SCI-Expanded)
- XXIV. **FT-IR and Raman Spectroscopy and Computation of 5-Methylfurfural**  
ERDOĐDU Y., Sertbakan T. R., Gulluoglu M. T., Yurdakul Ş., Guvenir A.  
JOURNAL OF APPLIED SPECTROSCOPY, vol.85, no.3, pp.517-525, 2018 (SCI-Expanded)
- XXV. **DFT simulation, quantum chemical electronic structure, spectroscopic and structure-activity investigations of 4-acetylpyridine**  
ATILGAN A., Yurdakul Ş., ERDOĐDU Y., Gulluoglu M. T.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1161, pp.55-65, 2018 (SCI-Expanded)
- XXVI. **Vibrational spectroscopic and density functional study on 1,2,4-triazolo-[1,5-a]pyrimidine**  
Celik S., BADOĐLU S., YURDAKUL Ş.  
VIBRATIONAL SPECTROSCOPY, vol.92, pp.280-286, 2017 (SCI-Expanded)
- XXVII. **Experimental and theoretical studies on molecular structures and vibrational modes of novel compounds containing silver**  
BİLKAN M. T., Yurdakul A.

- RUSSIAN JOURNAL OF INORGANIC CHEMISTRY, vol.62, no.7, pp.910-924, 2017 (SCI-Expanded)
- XXVIII. **Experimental and DFT studies of solvent effects on molecular structure and physical properties of Dipyriddyamine pyridine based ligand**  
Bilkan M. T., ŞAHİN O., YURDAKUL Ş.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1133, pp.580-590, 2017 (SCI-Expanded)
- XXIX. **An experimental and theoretical investigation of free Oxazole in conjunction with the DFT analysis of Oxazole center dot center dot center dot (H<sub>2</sub>O)(n) complexes**  
YURDAKUL Ş., Badoglu S., Ozkurt L.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.162, pp.48-60, 2016 (SCI-Expanded)
- XXX. **Crystal structure, FT-IR, FT-Raman and DFT studies on a novel compound [C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>](4)AgNO<sub>3</sub>**  
Bilkan M. T., YURDAKUL Ş., Demircioglu Z., BÜYÜKGÜNGÖR O.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, vol.805, pp.108-116, 2016 (SCI-Expanded)
- XXXI. **An FT-IR and DFT study of the free and solvated 4-(imidazol-1-yl)phenol**  
YURDAKUL Ş., Badoglu S.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.150, pp.614-622, 2015 (SCI-Expanded)
- XXXII. **Spectroscopic and structural properties of 2,2'-dipyridylamine and its palladium and platinum complexes**  
Yurdakul A., Bilkan M. T.  
OPTICS AND SPECTROSCOPY, vol.119, no.4, pp.603-619, 2015 (SCI-Expanded)
- XXXIII. **Experimental and theoretical study on free 5-nitroquinoline, 5-nitroisoquinoline, and their zinc(II) halide complexes**  
YURDAKUL Ş., Badoglu S., Gulesci Y.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.137, pp.945-956, 2015 (SCI-Expanded)
- XXXIV. **FTIR, Raman and NMR spectroscopic and DFT theoretical studies on poly(N-vinylimidazole)**  
Talu M., Derniroglu E. U., YURDAKUL Ş., Badoglu S.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.134, pp.267-275, 2015 (SCI-Expanded)
- XXXV. **Quantum chemical and spectroscopic (FT-IR and FT-Raman) investigations of 3-methyl-3h-imidazole-4-carbaldehyde**  
POLAT T., YURDAKUL Ş.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.133, pp.683-696, 2014 (SCI-Expanded)
- XXXVI. **DFT study of solvent effects on 3-hydroxy-2-quinoxalinecarboxylic acid tautomers**  
Badoglu S., Yurdakul Ş.  
OPTICS AND SPECTROSCOPY, vol.117, no.2, pp.201-212, 2014 (SCI-Expanded)
- XXXVII. **FT-IR, FT-Raman Spectra and Quantum Mechanical Study of Piperidine-3-carboxylic Acid and Its Tautomers, Isomers**  
YURDAKUL Ş., Yasayan N. C., Badoglu S.  
OPTICS AND SPECTROSCOPY, vol.116, no.6, pp.906-918, 2014 (SCI-Expanded)
- XXXVIII. **FT-IR, FT-Raman spectra, and DFT computations of the vibrational spectra and molecular geometry of chlorzoxazone**  
YURDAKUL Ş., Yurdakul M.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.126, pp.339-348, 2014 (SCI-Expanded)
- XXXIX. **A Combined Experimental and Theoretical Study on 8-Hydroxy-2-quinolinecarboxylic Acid**  
Badoglu S., YURDAKUL Ş.  
OPTICS AND SPECTROSCOPY, vol.116, no.2, pp.196-206, 2014 (SCI-Expanded)
- XL. **DFT, FT-IR and FT-Raman investigations of 1-methyl-2-imidazolecarboxaldehyde**

- POLAT T., YURDAKUL Ş.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1053, pp.27-37, 2013 (SCI-Expanded)
- XLII. **Vibrational and electronic structural study of dinuclear Zn(II) halide complexes with 4-azabenzimidazole**  
Badoglu S., YURDAKUL Ş.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, vol.745, pp.363-372, 2013 (SCI-Expanded)
- XLIII. **DFT, FT-Raman, FT-IR and FT-NMR studies of 4-phenylimidazole**  
Gulluoglu M. T., ERDOĞDU Y., Karpagam J., Sundaraganesan N., Yurdakul Ş.  
JOURNAL OF MOLECULAR STRUCTURE, vol.990, pp.14-20, 2011 (SCI-Expanded)
- XLIV. **Molecular structure and vibrational spectra of piperidine and 4-methylpiperidine by density functional theory and ab initio Hartree-Fock calculations**  
Gulluoglu M. T., Erdoğan Y., Yurdakul Ş.  
JOURNAL OF MOLECULAR STRUCTURE, vol.834, pp.540-547, 2007 (SCI-Expanded)
- XLV. **Vibrational frequencies and structural determination of 2,2'-biquinoline**  
Yurdakul Ş., Yurdakul M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.834, pp.555-560, 2007 (SCI-Expanded)
- XLVI. **HF and DFT studies and vibrational spectra of 1,2-bis(2-pyridyl) ethylene and its zinc (II) halide complexes**  
Ozhamam Z., Yurdakul M., Yurdakul Ş.  
VIBRATIONAL SPECTROSCOPY, vol.43, no.2, pp.335-343, 2007 (SCI-Expanded)
- XLVII. **DFT studies and vibrational spectra of trans 1,2-bis(4-pyridyl)ethylene and its zinc(II)halide complexes**  
Ozhamam Z., Yurdakul M., Yurdakul Ş.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.761, pp.113-118, 2006 (SCI-Expanded)
- XLVIII. **Synthesis and vibrational spectroscopic studies of isonicotinamide metal(II) halide complexes**  
Atac A., Yurdakul Ş., İDE S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.783, pp.79-87, 2006 (SCI-Expanded)
- XLIX. **Molecular structure and vibrational spectra of lepidine and 2-chlorolepidine by density functional theory and ab initio Hartree-Fock Calculations**  
Kurt M., Yurdakul Ş.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.730, pp.59-67, 2005 (SCI-Expanded)
- L. **Vibrational spectra of phthalazine by density functional theory calculations and assignment of its metal complexes**  
Kurt M., Yurdakul Ş.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.717, pp.171-178, 2005 (SCI-Expanded)
- LI. **HF and DFT studies of the structure and vibrational spectra of 8-hydroxyquinoline and its mercury(II) halide complexes**  
Arici K., Yurdakul M., Yurdakul Ş.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.61, pp.37-43, 2005 (SCI-Expanded)
- LII. **Molecular structure and vibrational spectra of 3-chloro-4-methyl aniline by density functional theory and ab initio Hartree-Fock calculations**  
Kurt M., Yurdakul M., Yurdakul Ş.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.711, pp.25-32, 2004 (SCI-Expanded)
- LIII. **Fourier transform-infrared spectroscopic study of isonicotinamide metal(II) tetracyanonickelate and halide complexes**  
Yurdakul Ş., Atac A.  
SPECTROSCOPY LETTERS, vol.37, no.1, pp.33-42, 2004 (SCI-Expanded)
- LIV. **Coordination behaviour of nicotinamide: an infrared spectroscopic study**  
Bayari S., Atac A., Yurdakul Ş.  
JOURNAL OF MOLECULAR STRUCTURE, vol.655, no.1, pp.163-170, 2003 (SCI-Expanded)

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XXVI. AN INFRARED AND RAMAN SPECTROSCOPIC STUDY OF THE TRANSITION STATE OF THE  
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XXI. EUROPEAN CONGRESS ON MOLECULAR SPECTROSCOPY, 23 - 28 August 1992

## Supported Projects

YURDAKUL Ş., Project Supported by Higher Education Institutions, Urasil molekülünün yapısal, titreşimsel ve elektronik özellikleri üzerinde çözücü etkisinin deneysel titreşimsel spektroskopi ve teorik kuantum kimyasal hesaplamalar ile incelenmesi, 2016 - 2018

YURDAKUL Ş., Project Supported by Higher Education Institutions, Nipekotik asit molekülünün tautomerik yapılarının deneysel ve teorik titreşimsel spektroskopi ile incelenmesi, 2012 - 2013

YURDAKUL Ş., Project Supported by Higher Education Institutions, Nipekotamid molekülünün deneysel ve teorik titreşimsel spektroskopi ile incelenmesi, 2011 - 2012

YURDAKUL Ş., Project Supported by Higher Education Institutions, 4-quinazolinol molekülünün tautomerik yapılarının ve bazı bileşiklerinin deneysel ve teorik titreşimsel spektroskopi ile incelenmesi, 2010 - 2012

YURDAKUL Ş., Project Supported by Higher Education Institutions, 2-hidroksikinoksalin molekülünün tautomerik yapılarının deneysel ve teorik titreşimsel spektroskopi ile incelenmesi, 2009 - 2011

YURDAKUL Ş., Project Supported by Higher Education Institutions, İmidazo(1,2-Alpha)Pyridine Metal (I) Halojenür Bileşiklerin Yapılarının Deneysel ve Ligandın Teorik Titreşimsel Spektroskopi İle Araştırılması, 2008 - 2009

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YURDAKUL Ş., Project Supported by Higher Education Institutions, Metal (II) 3-Klor-4-Metilanilin Halojenür Bileşiklerinin Yapılarının Titreşimsel Spektroskopi ile İncelenmesi, 2005 - 2007

YURDAKUL Ş., Project Supported by Higher Education Institutions, Metal (II) 1,2-bis (4-pyridyl) Etan Halojenür Bileşiklerinin Yapılarının Titreşimsel Spektroskopi ile incelenmesi, 2003 - 2004

YURDAKUL Ş., Project Supported by Higher Education Institutions, Bazı Metal Halojenür Phatalazin Bileşiklerinin Yapılarının Titreşimsel Spektroskopi ile İncelenmesi, 2002 - 2003

YURDAKUL Ş., Project Supported by Higher Education Institutions, Metod halojenür izonikotinamid bileşiklerinin infrared spektroskopisi ile inc., 2001 - 2002

Yurdakul Ş., TUBITAK Project, Ab initio yöntemler ile bazı moleküllerin yapısal parametrelerinin ve Titreşimsel spektrumlarının incelenmesi, 2000 - 2001

YURDAKUL Ş., Project Supported by Higher Education Institutions, Bazı izonikotinamid ve kınozalin metal (II) bileşiklerinin yapılarının titreşimsel spektroskopi ile incelenmesi, 2000 - 2000

YURDAKUL Ş., Project Supported by Higher Education Institutions, Bazı piperidin metal (II) bileşiklerinin yapılarının titreşimsel spektroskopisi ile araştırılması, 1999 - 1999

YURDAKUL Ş., Project Supported by Higher Education Institutions, 4-acetylpyridine halojenür bileşiklerinin titreşimsel spektroskopisi ile yapılarının incelenmesi, 1998 - 1998

YURDAKUL Ş., Project Supported by Higher Education Institutions, Hofman tipi çeşitli benzimidazol bileşiklerinin titreşimsel spektroskopisi ile incelenmesi, 1997 - 1997

YURDAKUL Ş., Project Supported by Higher Education Institutions, 3-Cl 4-metil Anilin Metal Tetrasiyononnikel bileşiklerinin titreşimsel spektroskopisi ile incelenmesi, 1996 - 1996

YURDAKUL Ş., Project Supported by Higher Education Institutions, Bazı organometalik bileşiklerin infrared ve raman spektroskopisi yöntemiyle incelenmesi, 1995 - 1995

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YURDAKUL Ş., Project Supported by Higher Education Institutions, Bazı tetrasiyononnikel metal bileşiklerinin titreşimsel spektroskopisi ile incelenmesi, 1993 - 1993

## **Scientific Refereeing**

JOURNAL OF MOLECULAR STRUCTURE, SCI Journal, December 2022  
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JOURNAL OF MOLECULAR STRUCTURE, SCI Journal, June 2022  
JOURNAL OF MOLECULAR STRUCTURE, SCI Journal, May 2022  
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## **Congress and Symposium Activities**

International Conferences on Science and Technology, Natural Science and Technology Prizren, Invited Speaker, Prizren, Kosovo, 2019  
32th European Congress on Molecular Spectroscopy, 2014, DUSSELDORF, Attendee, Düsseldorf, Germany, 2014