

## Prof. DURAN KARAKAŞ

### Personal Information

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### International Researcher IDs

ORCID: 0000-0002-6770-3726

Yoksis Researcher ID: 24380

### Education Information

Doctorate, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Fen Bilimleri Enstitüsü, Turkey 1994 - 2000

Postgraduate, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Fen Bilimleri Enstitüsü, Turkey 1991 - 1993

Undergraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 1985 - 1989

### Foreign Languages

English, B2 Upper Intermediate

### Dissertations

Doctorate, Oktahedral metal karboniller ve türevlerinin IR spektrumlarının çözümlenmesinde yeni bir yöntem, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Fen Bilimleri Enstitüsü, 2000

Postgraduate, Fotokimyasal metatez ile polimerlerin degradasyonu, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Fen Bilimleri Enstitüsü, 1993

### Research Areas

Boron Chemistry, Chemistry, Inorganic Chemistry, Bioinorganic Chemistry, Transition Metals, Coordination Chemistry, Metal Carbene Complexes, Metal olefin complexes, Organometallic Chemistry, Natural Sciences

### Academic Titles / Tasks

Professor, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2021 - Continues

Associate Professor, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2016 - 2021

Assistant Professor, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2003 - 2016

Research Assistant, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 1990 - 2003

## Academic and Administrative Experience

Head of Department, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2018 - Continues  
Assistant Director of the Institute, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Fen Bilimleri Enstitüsü, 2019 - 2022  
Fakülte Kurulu Üyesi, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2018 - 2021  
Fakülte Yönetim Kurulu Üyesi, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2010 - 2013  
Vice Dean, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2010 - 2012  
Deputy Head of Department, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2009 - 2012

## Courses

Genel Kimya II, Undergraduate, 2018 - 2019  
Seminer Dersi, Doctorate, 2019 - 2020  
Spektroskopiye Giriş, Undergraduate, 2018 - 2019  
Anorganik Kimyanın İlkeleri, Postgraduate, 2019 - 2020  
Anorganik Kimya Lab., Undergraduate, 2019 - 2020  
Anorganik Kimyanın İlkeleri, Postgraduate, 2019 - 2020  
Genel Kimya, Undergraduate, 2019 - 2020  
Genel Kimya, Undergraduate, 2019 - 2020  
Uzmanlık Alan Dersi, Postgraduate, 2019 - 2020  
Uzmanlık Alan Dersi, Postgraduate, 2019 - 2020  
İnorganik Kimya, Undergraduate, 2019 - 2020  
Uzmanlık Alan Dersi, Doctorate, 2019 - 2020  
Anorganik Kimya, Undergraduate, 2019 - 2020  
Anorganik Kimya Lab, Undergraduate, 2019 - 2020  
Genel Kimya I, Undergraduate, 2018 - 2019  
Uzmanlık Alan Dersi, Doctorate, 2019 - 2020  
Bitirme Ödevi/Tezi, Undergraduate, 2019 - 2020  
Moleküler Orbital Kuram ve Uygulamaları, Postgraduate, 2018 - 2019  
Moleküler Spektroskopi, Postgraduate, 2018 - 2019  
Organometalik Kimya, Postgraduate, 2018 - 2019  
Tez Çalışması, Postgraduate, 2018 - 2019  
Genel Kimya, Undergraduate, 2018 - 2019  
Seminer Dersi, Postgraduate, 2017 - 2018  
Kimya, Undergraduate, 2018 - 2019  
Koordinasyon Kimyası, Postgraduate, 2017 - 2018  
Geçiş Metal Komplekslerinin Elektronik Spektrumları, Postgraduate, 2018 - 2019  
Bitirme Ödevi/Tezi, Undergraduate, 2017 - 2018  
Spektroskopiye Giriş, Undergraduate, 2015 - 2016  
Bilimsel Hazırlık, Undergraduate, 2015 - 2016  
Halkalı İnorganik Bileşikler, Postgraduate, 2015 - 2016  
Bilimsel Hazırlık, Undergraduate, 2015 - 2016  
Genel Kimya Laboratuvarı, Undergraduate, 2015 - 2016  
Bilimsel Hazırlık Teknolojileri, Undergraduate, 2015 - 2016  
Koordinasyon Kimyasına Giriş, Undergraduate, 2013 - 2014  
Koordinasyon Kimyasına Giriş, Undergraduate, 2013 - 2014  
Temel Kimya, Associate Degree, 2014 - 2015  
Temel Kimya, Associate Degree, 2014 - 2015  
Genel Kimya Lab. - II, Undergraduate, 2012 - 2013  
Genel Kimya II, Undergraduate, 2012 - 2013

İleri Anorganik Kimya-I, Postgraduate, 2013 - 2014  
Genel Kimya I, Undergraduate, 2012 - 2013  
Anorganik Kimya-II, Undergraduate, 2012 - 2013  
Genel Kimya Laboratuvarı II, Undergraduate, 2011 - 2012  
Anorganik Kimya-I, Undergraduate, 2011 - 2012  
Organometalik Kimya, Undergraduate, 2011 - 2012  
Organometalik Kimya, Undergraduate, 2011 - 2012  
Genel Kimya Laboratuvarı I, Undergraduate, 2009 - 2010  
Moleküler Simetri, Undergraduate, 2008 - 2009  
Moleküler Simetri, Undergraduate, 2007 - 2008  
Genel Kimya II, Undergraduate, 2005 - 2006  
Anorganik Kimya-I, Undergraduate, 2006 - 2007  
Anorganik Kimya Lab, Undergraduate, 2006 - 2007  
Kimya-II, Undergraduate, 2003 - 2004  
Kimya-I, Undergraduate, 2003 - 2004

## Advising Theses

Karakaş D., Schiff baz metal komplekslerinin hesapsal karakterizasyonu ve antikanser-antibakteriyel özelliklerinin incelenmesi, Doctorate, S.KAYA(Student), 2021  
Karakaş D., Kanser tedavisinde ilaç olarak kullanılan platin temelli kompleksler üzerine kuantum kimyasal hesaplamalar, Postgraduate, M.TAŞTAN(Student), 2020  
Karakaş D.,  $[Tp(CO)_2Mo(C-Ph)]_2^+$  ve  $[L(CO)_2Mo(C-Ph)]^+$  alkilidin komplekslerinin hesaplamalı kimya ile incelenmesi, Postgraduate, Z.ZAİM(Student), 2019  
Karakaş D., Alkoksitürevli disiyandiamid ligandlarını içeren nikel (II) komplekslerinin yapısal, elektronik ve moleküler özelliklerinin kuantum kimyasal hesaplamalar ile araştırılması, Postgraduate, T.ALAGÖZ(Student), 2019  
Karakaş D., İzosiyano temelli üç çekirdekli altın (I) kompleksleri üzerine kuantum kimyasal çalışmalar, Postgraduate, N.ÖZKAN(Student), 2017  
Karakaş D.,  $Mo(CO)_5[C(OEt)Me]$  ve  $Mo(CO)_5[C(OMe)Et]$  kompleksleri üzerine kuantum kimyasal çalışmalar, Postgraduate, N.GÖVDELİ(Student), 2017  
Karakaş D., Hesaplamalı kimya yöntemleriyle bazı bor komplekslerinin yapısal ve elektronik özelliklerinin incelenmesi, Doctorate, K.SAYIN(Student), 2017  
Karakaş D., Yoğunluk fonksiyonel teori temelinde schrock tipi  $Mo(CO)_5(CMe_2)$  ve  $Mo(CO)_5(CMeEt)$  alkiliden kompleksleri üzerine hesapsal çalışmalar, Postgraduate, H.ÖZÇİFTÇİ(Student), 2017  
Karakaş D., Alkin birimli piridil ligantları içeren bazı dinükleer metal karbonillerin kuantum kimyasal hesaplama yöntemleriyle yapısal, spektroskopik ve optik özelliklerinin incelenmesi, Doctorate, S.ERKAN(Student), 2016  
Karakaş D., İki vanadyum(IV) Schiff baz kompleksi üzerine kuantum kimyasal hesaplamalar, Postgraduate, M.NEŞAT(Student), 2015  
Karakaş D., Hesaplamalı kimya yöntemleri ile bazı platin(II) oksim komplekslerinin moleküler yapısının ve moleküler özelliklerinin araştırılması, Postgraduate, K.SAYIN(Student), 2014  
Karakaş D., Ab initio moleküler orbital yöntemleri ile  $CO_2(CO)_8$  izomerlerinin moleküler yapı parametrelerininve titreşim frekanslarının hesaplanması, Postgraduate, S.ERKAN(Student), 2013

## Jury Memberships

Doctorate, Doctorate, Tokat Gaziosmanpaşa Üniversitesi, June, 2020  
Doctorate, Doctorate, Tokat Gaziosmanpaşa Üniversitesi, June, 2020  
Doctoral Examination, Doctoral Examination, Kahramanmaraş Sütçü İmam Üniversitesi, November, 2019  
Post Graduate, Post Graduate, Fırat Üniversitesi, July, 2019

Post Graduate, Post Graduate, Kahramanmaraş Sütçü İmam Üniversitesi, June, 2019

Appointment to Academic Staff-Assistant Professorship, Appointment Academic Staff, Sivas Cumhuriyet Üniversitesi, November, 2018

## Taught Courses And Trainings

Karakaş D., I. Kanser Günleri, 2019 - 2019

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

- I. **Modeling, spectroscopic structural properties of platinum-II complexes of 2-((phenylimino)methyl)phenolate-based ligands and research of nonlinear optical, organic light emitting diode and solar cell performances**  
ERKAN S., KARAKAŞ D.  
Materials Today Communications, vol.37, 2023 (SCI-Expanded)
- II. **Investigation of substituent effect on rhenium complexes by DFT methods: Structural analysis, IR spectrum, quantum chemical parameter, NLO and OLED properties, molecular docking**  
Yıldız C. A., Güney E., Nasif V., KARAKAŞ D., ERKAN S.  
Journal of Molecular Structure, vol.1278, 2023 (SCI-Expanded)
- III. **Computational design and characterization of platinum-II complexes of some Schiff bases and investigation of their anticancer-antibacterial properties**  
Kaya S., ERKAN S., KARAKAŞ D.  
APPLIED ORGANOMETALLIC CHEMISTRY, vol.36, no.9, 2022 (SCI-Expanded)
- IV. **Investigations substituent effect on structural, spectral and optical properties of phenylboronic acids**  
Çöpçü B., SAYIN K., KARAKAŞ D.  
Journal of Molecular Structure, vol.1227, 2021 (SCI-Expanded)
- V. **Computational investigation of molecular structures, spectroscopic properties and antitumor-antibacterial activities of some Schiff bases**  
Kaya S., ERKAN S., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.244, 2021 (SCI-Expanded)
- VI. **Computational structure characterization, nonlinear optical properties and antitumor activities of Nickel(II) complexes containing alkoxy-derived dicyandiamide ligands**  
Alagöz Sayın T., Karakaş D.  
INDIAN JOURNAL OF CHEMISTRY - SECTION A INORGANIC, PHYSICAL, THEORETICAL AND ANALYTICAL CHEMISTRY, vol.60, pp.51-61, 2021 (SCI-Expanded)
- VII. **Research on structural, spectral (IR, UV-Vis, H-1- and C-13-NMR) and light emitting properties of triisocyano-based trinuclear Au(I) complexes**  
Ozkan N., ERKAN S., SAYIN K., KARAKAŞ D.  
CHEMICAL PAPERS, vol.74, no.8, pp.2415-2425, 2020 (SCI-Expanded)
- VIII. **A theoretical study on cyclometalated iridium (III) complexes by using a density functional theory**  
ERKAN S., KARAKAŞ D.  
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, vol.19, no.2, 2020 (SCI-Expanded)
- IX. **Computational investigation of structural, nonlinear optical and anti-tumor properties of dinuclear metal carbonyls bridged by pyridyl ligands with alkyne unit**  
Erkan S., Karakaş D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1199, 2020 (SCI-Expanded)
- X. **Structural, spectral characterization and molecular docking analyses of mer-ruthenium (II)**

**complexes containing the bidentate chelating ligands**

Erkan S., Kaya S., Sayin K., Karakaş D.

SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.224, 2020 (SCI-Expanded)

- XI. **DFT investigation and molecular docking studies on dinuclear metal carbonyls containing pyridyl ligands with alkyne unit**  
Erkan S., Karakaş D.  
CHEMICAL PAPERS, vol.73, pp.2387-2398, 2019 (SCI-Expanded)
- XII. **New azo-azomethine-based transition metal complexes: Synthesis, spectroscopy, solid-state structure, density functional theory calculations and anticancer studies**  
Sahan F., Kose M., HEPOKUR C., KARAKAŞ D., Kurtoglu M.  
APPLIED ORGANOMETALLIC CHEMISTRY, vol.33, no.7, 2019 (SCI-Expanded)
- XIII. **Tribological behavior and quantum chemical calculations of protic ionic liquids: synthesis, spectroscopic, and thermal properties**  
Karadag A., Akbas H., KARAKAŞ D., Tekin K. C., Korkmazer E.  
TURKISH JOURNAL OF CHEMISTRY, vol.43, no.3, pp.766-786, 2019 (SCI-Expanded)
- XIV. **Investigations of structural, spectral, electronic and biological properties of N-heterocyclic carbene Ag(I) and Pd(II) complexes**  
Sayin K., Kariper S. E., Tastan M., Sayin T. A., Karakaş D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1176, pp.478-487, 2019 (SCI-Expanded)
- XV. **Investigation of structural, electronic properties and docking calculations of some boron complexes with norfloxacin: A computational research**  
SAYIN K., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.202, pp.276-283, 2018 (SCI-Expanded)
- XVI. **Quantum chemical studies on hypothetical Fischer type Mo(CO)(5)[C(OEt)Me] and Mo(CO)(5)[C(OMe)Et] carbene complexes**  
Govdeli N., KARAKAŞ D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1163, pp.94-102, 2018 (SCI-Expanded)
- XVII. **Quantum chemical investigation of levofloxacin-boron complexes: A computational approach**  
SAYIN K., KARAKAŞ D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1158, pp.57-65, 2018 (SCI-Expanded)
- XVIII. **Computational study of some fluoroquinolones: Structural, spectral and docking investigations**  
SAYIN K., KARAKAŞ D., ERKAN KARİPER S., Sayin T. A.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1156, pp.172-181, 2018 (SCI-Expanded)
- XIX. **Computational investigations of trans platinum(II) oxime complexes used as anticancer drug**  
SAYIN K., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.188, pp.537-546, 2018 (SCI-Expanded)
- XX. **Multi-properties of a new azo-Schiff base and its binuclear copper(II) chelate: Preparation, spectral characterization, electrochemical, potentiometric and modeling studies**  
Sarigul M., ERKAN KARİPER S., DEVECİ P., Atabey H., KARAKAŞ D., KURTOĞLU M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1149, pp.520-529, 2017 (SCI-Expanded)
- XXI. **Theoretical study on the antitumor properties of Ru(II) complexes containing 2-pyridyl, 2-pyridine-4-carboxylic acid ligands**  
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1149, pp.473-486, 2017 (SCI-Expanded)
- XXII. **Investigation of Structural, Electronic and Biological Properties of Two Zn(II) Complexes with Pentaaza Macrocyclic Schiff-Base Ligand: A DFT Approach**  
SAYIN K., KARAKAŞ D.  
JOURNAL OF CLUSTER SCIENCE, vol.28, no.6, pp.3075-3086, 2017 (SCI-Expanded)

- XXIII. **Determination of structural, spectral, electronic and biological properties of tosufloxacin boron complexes and investigation of substituent effect**  
SAYIN K., KARAKAŞ D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1146, pp.191-197, 2017 (SCI-Expanded)
- XXIV. **Structural, computational and cytotoxic studies of square planar copper(II) complexes derived from dicyandiamide**  
KÖSE M., HEPOKUR C., KARAKAŞ D., McKee V., KURTOĞLU M.  
POLYHEDRON, vol.117, pp.652-660, 2016 (SCI-Expanded)
- XXV. **Computational and experimental studies of 2-[(E)-hydrazinylidenemethyl]-6-methoxy-4-[(E)-phenyldiazenyl]phenol and its tautomers**  
SAYIN K., KURTOĞLU N., KÖSE M., KARAKAŞ D., KURTOĞLU M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1119, pp.413-422, 2016 (SCI-Expanded)
- XXVI. **Synthesis, characterization and non-linear optical properties of two mononuclear Cu(II) complexes of 2,6-bis(1-butylbenzimidazol-2-yl)pyridine**  
KÖSE M., CEYHAN G., KARAKAŞ D.  
JOURNAL OF COORDINATION CHEMISTRY, vol.69, no.3, pp.497-507, 2016 (SCI-Expanded)
- XXVII. **Pd(II) complexes of novel phosphine ligands: Synthesis, characterization, and catalytic activities on Heck reaction**  
ALTAN O., Serindag O., SAYIN K., KARAKAŞ D.  
PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS, vol.191, no.7, pp.993-999, 2016 (SCI-Expanded)
- XXVIII. **Structural, spectral, NLO and MEP analysis. of the [MgO<sub>2</sub>Ti<sub>2</sub>(OPri)<sub>6</sub>], [MgO<sub>2</sub>Ti<sub>2</sub>(OPri)<sub>2</sub>(acac)<sub>4</sub>] and [MgO<sub>2</sub>Ti<sub>2</sub>(OPri)<sub>2</sub>(bzac)<sub>4</sub>] by DFT method**  
SAYIN K., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.144, pp.176-182, 2015 (SCI-Expanded)
- XXIX. **Spectroscopic investigation, FMOs and NLO analyses of Zn(II) and Ni(II) phenanthroline complexes: A DFT approach**  
SAYIN K., Karaka D., KARAKUŞ N., Sayin T. A., Zaim Z., ERKAN KARİPER S.  
POLYHEDRON, vol.90, pp.139-146, 2015 (SCI-Expanded)
- XXX. **Theoretical spectroscopic study of seven zinc(II) complex with macrocyclic Schiff-base ligand**  
SAYIN K., ERKAN KARİPER S., Sayin T. A., KARAKAŞ D.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.133, pp.348-356, 2014 (SCI-Expanded)
- XXXI. **The investigation of the solvent effect on coordination of nicotinato ligand with cobalt(II) complex containing tris(2-benzimidazolylmethyl) amine: A computational study**  
SAYIN K., KARAKAŞ D.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1076, pp.244-250, 2014 (SCI-Expanded)
- XXXII. **Spectral, structural and quantum chemical computational and dissociation constant studies of a novel azo-enamine tautomer**  
Gozel A., KÖSE M., KARAKAŞ D., Atabey H., McKee V., KURTOĞLU M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1074, pp.449-456, 2014 (SCI-Expanded)
- XXXIII. **Theoretical investigation on the vibrational and electronic spectra of three isomeric forms of dicobalt octacarbonyl**  
KARAKAŞ D., ERKAN KARİPER S.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1062, pp.77-81, 2014 (SCI-Expanded)
- XXXIV. **Synthesis, characterization and antimicrobial studies of 2-[(E)-[(2-hydroxy-5-methylphenyl)imino]methyl]-4-[(E)-phenyldiazenyl] phenol as a novel azo-azomethine dye**  
KÖSE M., KURTOĞLU N., Gumussu O., Tutak M., McKee V., KARAKAŞ D., KURTOĞLU M.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1053, pp.89-99, 2013 (SCI-Expanded)
- XXXV. **Quantum chemical studies on the some inorganic corrosion inhibitors**

- SAYIN K., KARAKAŞ D.  
CORROSION SCIENCE, vol.77, pp.37-45, 2013 (SCI-Expanded)
- XXXVI. **Determination of structural and electronic properties of Ni(NQSC)<sub>2</sub> and Ni(NQTS)<sub>2</sub> complexes with DFT method**  
Sayın K., Karakaş D.  
Journal of New Results in Science, vol.2, pp.47-53, 2013 (SCI-Expanded)
- XXXVII. **DFT and TD-DFT studies on copper(II) complexes with tripodal tetramine ligands**  
KARAKAŞ D., SAYIN K.  
INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL & ANALYTICAL CHEMISTRY, vol.52, no.4, pp.480-485, 2013 (SCI-Expanded)
- XXXVIII. **A new approach to predicting the carbonyl stretching frequencies of Co<sub>2</sub>(CO)<sub>8</sub> with D<sub>3d</sub> symmetry**  
KAYA C., KARAKAŞ D., Üstün E.  
Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry, vol.46, no.9, pp.1388-1392, 2007 (SCI-Expanded)
- XXXIX. **Force constant calculations for Hg[Co(CO)<sub>4</sub>]<sub>2</sub> from the CO-factored force field**  
KAYA C., KARAKAŞ D.  
Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry, vol.46, no.1, pp.33-38, 2007 (SCI-Expanded)
- XL. **A new method for assigning the C-O stretching bands in cis-disubstituted octahedral metal carbonyl complexes**  
Kaya C., Karakas D.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, vol.660, no.1, pp.116-120, 2002 (SCI-Expanded)
- XLI. **Force constant calculations for octahedral complexes of the type M(CO)<sub>5</sub>L, based on the CO-factored force field**  
Karakas D., Kaya C.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, vol.640, pp.37-40, 2001 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Investigation of the Effect of Main Components of Wild Thyme on Covid-19 by Computational Methods**  
KAYA S., ERKAN S., KARAKAŞ D.  
CUMHURİYET SCIENCE JOURNAL, vol.44, 2023 (Peer-Reviewed Journal)
- II. **Investigation of Antiviral Activities of Nickel and Copper Complexes with Macrocyclic Ligands against Crimean-Congo Hemorrhagic Fever by In Silico Calculations**  
ERKAN S., BULUT N., KARAKAŞ D.  
CUMHURİYET SCIENCE JOURNAL, vol.44, 2023 (Peer-Reviewed Journal)
- III. **Computational spectroscopic investigation of the effect of nitrosyl bonding type on molecular properties in iron tetracarbonyl nitrosyl complex**  
Özதாகçi Ö., KARAKAŞ D.  
Indian Journal of Chemistry (IJC), vol.62, no.10, pp.1030-1039, 2023 (Scopus)
- IV. **Investigations of structural, spectral (IR and NMR) and in silico analyses of boron compounds as SERM inhibitor**  
KAYA S., SAYIN K., ERKAN S., KARAKAŞ D.  
Chemical Data Collections, vol.37, 2022 (Peer-Reviewed Journal)
- V. **Computational study on the structural, electronic, molecular and thermochemical properties of hypothetical [Tp(CO)<sub>2</sub>Mo≡C-Ph]<sub>2</sub><sup>+</sup> and [L(CO)<sub>2</sub>Mo≡C-Ph]<sup>+</sup> carbyne complexes**  
ZAIM Z., KARAKAŞ D.  
Cumhuriyet Science Journal, vol.42, pp.45-59, 2021 (Peer-Reviewed Journal)
- VI. **Computational study on molecular structure, vibrational spectrum analysis and acidity strength of**

#### **P4On (n = 6-10) phosphorus oxides with cage structure**

Karakaş D.

Cumhuriyet Science Journal, vol.41, no.3, pp.659-664, 2020 (Peer-Reviewed Journal)

- VII. **Structural, spectroscopic and activity calculations on methanesulfonylhydrazone derivative chromium pentacarbonyl complexes**  
ERKAN S., SAYIN K., KARAKAŞ D.  
Journal of the Turkish Chemical Society, Section A: Chemistry, vol.5, no.3, pp.1193-1204, 2018 (Scopus)
- VIII. **Determination of The Best Method (HF, MP2 and B3LYP) in Calculation of Chemical Hardness**  
ZAIM Z., ALAGÖZ SAYIN T., SAYIN K., KARAKAŞ D.  
Turkish Computational and Theoretical Chemistry, vol.2, no.2, pp.7-15, 2018 (Scopus)
- IX. **Theoretical Investigation of Temperature Effect on the Formation of Sulphuric Acid Rain**  
SAYIN K., KARAKAŞ D.  
Turkish Computational and Theoretical Chemistry, vol.1, pp.11-16, 2017 (Scopus)
- X. **Theoretical investigation on electrophilicity indexes and proton affinities of some boron-nitrogen open-chain species**  
KARAKAŞ D.  
Turkish computational and theoretical chemistry, vol.1, no.1, pp.1-10, 2017 (Scopus)
- XI. **Ab-Initio and DFT Calculations on Some Inorganic InhibitorsComputaional Study on Inorganic Corrosion Inhibitors**  
SAYIN K., KARAKAŞ D.  
Journal of new results in science, vol.6, no.1, pp.20-31, 2017 (Peer-Reviewed Journal)
- XII. **Theoretical Studies on Oxovanadium(IV) Complexes with Sterically Crowded Schiff Base Ligands**  
KARAKAŞ D., SAYIN K.  
Cumhuriyet Science Journal, vol.38, pp.1-12, 2017 (Peer-Reviewed Journal)
- XIII. **Method and basis set investigations and computational spectral studies for oximato bridged trans platinum II dimer used as anticancer drug**  
SAYIN K., KARAKAŞ D.  
Journal of new results in science, no.8, pp.1-12, 2015 (Peer-Reviewed Journal)
- XIV. **Method and basis set investigation for trans platinum II oxime complex**  
SAYIN K., KARAKAŞ D.  
Cumhuriyet University Faculty of Science Science Journal (CSJ), vol.36, no.2, pp.1-10, 2015 (Peer-Reviewed Journal)
- XV. **Theoretical Studies on EightOxovanadium IV Complexes withSalicylaldehyde and Aniline Ligands**  
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- I. **Investigation of Substituent Effect on Rhenium Complexes by DFT Methods: Structural Analysis, IR Spectrum, Quantum Chemical Parameter, NLO and OLED Properties, Molecular Docking**  
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- II. **Quantum chemical calculations o some platinum-based complexes used as drugs in cancer treatment**  
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- XVIII. **New azo azomethine based copper II and zinc II complexes experimental and theoretical studies**  
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- XIX. **2-E-3, 4-dimethylphenyl imino methyl-4-E-4 ethylphenyl diazenyl phenol Schiff base and its properties of corrosion**  
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- XXII. **Alkin birimli pridil ligantlarıyla köprülenmiş iki çekirdekli metal karboniller üzerine kuantum kimyasal çalışmalar**  
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- XXIII. **Makrosiklik schiff baz ligandlı çinko II kompleksleri üzerine hesaplamalı kimya çalışmaları**  
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2. ULUSAL HESAPLAMALI KİMYA KONGRESİ, Turkey, 2 - 05 June 2015
- XXIV. **Yoğunluk fonksiyon teori metoduyla MgO<sub>2</sub>Ti<sub>2</sub> OPri 6 MgO<sub>2</sub>Ti<sub>2</sub> OPri 2 Acac 4 ve MgO<sub>2</sub>Ti<sub>2</sub> OPri 2 bzac 4 kompleksleri üzerine hesapsal çalışmalar**  
Sayın K., Karakaş D., Sultan E. K.  
Mersin Üniversitesi, V. Ulusal Anorganik Kimya Kongresi, Turkey, 22 - 25 April 2015
- XXV. **Bazı çinko II komplekslerinin biyolojik aktiflik sıralamasının hesapsal yöntemlerle belirlenmesi**  
Sayın K., Sultan E. K., Tuba A. S., Karakaş D.  
Mersin Üniversitesi, V. Ulusal Anorganik Kimya Kongresi, Turkey, 22 - 25 April 2015
- XXVI. **Metansülfonilhidrazon temelli krompentakarbonil kompleksleri üzerine yapısal spektroskopik ve aktivite hesaplamaları**

- SULTAN E. K., SAYIN K., KARAKAŞ D.  
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- XXVII. **Bazı lactam inhibitörleri üzerine kuantum kimyasal çalışmalar**  
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- XXIX. **Oksimato köprülü trans platin II kompleksi üzerine kuantum kimyasal çalışmalar**  
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- XL. **Theoretical studies on zinc complexes with schiff base ligand**  
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**XLI. D3d simetrisindeki Co<sub>2</sub> CO<sub>8</sub> in karbonil gerilme bölgesindeki titreşim spektrumunun analizi**

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Karakaş D., Erkan S., Project Supported by Higher Education Institutions, Anti-kanser özelliği taşıyan siklometalat iridyum(III) kompleksleri üzerine yapısal, spektroskopik ve kuantum kimyasal hesaplamalar, 2016 - 2020

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Karakaş D., Zaim Z., Project Supported by Higher Education Institutions, [Tp(CO)<sub>2</sub>Mo(CPh)]<sub>2</sub> ve [Tp(CO)<sub>2</sub>Mo(CPh)] alkilidin komplekslerinin hesaplamalı kimya ile incelenmesi, 2018 - 2019

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## Activities in Scientific Journals

Cumhuriyet Science Journal, Committee Member, 2018 - Continues

Turkish Computational and Theoretical Chemistry, Committee Member, 2017 - Continues

Cumhuriyet Üniversitesi Fen-Edebiyat Fakültesi Fen Bilimleri Dergisi, Committee Member, 2017 - 2018

## Scientific Refereeing

Turkish Computational and Theoretical Chemistry, Other Indexed Journal, February 2021

Project Supported by Higher Education Institutions, BAP PhD, Kahramanmaraş Sutcu Imam University, Turkey, February 2021

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, February 2021

JOURNAL OF MOLECULAR STRUCTURE, SCI Journal, August 2020

Project Supported by Higher Education Institutions, BAP PhD, Kahramanmaraş Sutcu Imam University, Turkey, August 2020

Süleyman Demirel Üniversitesi Fen Bilimleri Enstitüsü Dergisi, Other Indexed Journal, May 2020

Cumhuriyet Science Journal (CSJ), Other Indexed Journal, May 2020

Cumhuriyet Science Journal (CSJ), Other Indexed Journal, March 2020

Project Supported by Higher Education Institutions, BAP Research Project, Kahramanmaraş Sutcu Imam University, Turkey, October 2019

International Journal of Advances in Engineering and Pure Sciences, Other Indexed Journal, September 2019

JOURNAL OF MOLECULAR STRUCTURE, SCI Journal, June 2019

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, May 2019

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, May 2019

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, October 2018

Project Supported by Higher Education Institutions, BAP Research Project, Kahramanmaraş Sutcu Imam University, Turkey, October 2018

Turkish Computational and Theoretical Chemistry, Other Indexed Journal, June 2018

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, June 2018

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, April 2018

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, April 2018

Turkish Computational and Theoretical Chemistry, Other Indexed Journal, March 2018

Cumhuriyet Science Journal (CSJ), Other Indexed Journal, December 2017

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, December 2017

Turkish Computational and Theoretical Chemistry, Other Indexed Journal, November 2017

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, August 2017

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, June 2017

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, November 2016

Project Supported by Higher Education Institutions, BAP Research Project, Kahramanmaraş Sutcu Imam University, Turkey, October 2016

Project Supported by Higher Education Institutions, BAP MSc, Sivas Cumhuriyet University, Turkey, March 2016

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, February 2016

Project Supported by Higher Education Institutions, BAP MSc, Sivas Cumhuriyet University, Turkey, November 2015

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, June 2015

Project Supported by Higher Education Institutions, BAP Research Project, Sivas Cumhuriyet University, Turkey, May 2015

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## **Metrics**

Publication: 102

Citation (WoS): 551

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H-Index (Scopus): 16

## **Non Academic Experience**

MİLLİ EĞİTİM BAKANLIĞI