

Prof. DURAN KARAKAŞ

Personal Information

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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

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

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

Assistant Director of the Institute, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Fen Bilimleri Enstitüsü, 2019 - Continues

Head of Department, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2018 - Continues
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., Kanser tedavisinde ilaç olarak kullanılan platin temelli kompleksler üzerine kuantum kimyasal hesaplamalar, Postgraduate, M.TAŞTAN(Student), 2020
Karakaş D., $[Tp(CO)_2Mo\eta^5-C-Ph]_2^+$ ve $[L(CO)_2Mo\eta^5-C-Ph]^+$ alkilidin komplekslerinin hesaplamalı kimya ile incelenmesi, Postgraduate, Z.ZAİM(Student), 2019
Karakaş D., Alkoxi türevli 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 hesaplamalı 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 parametrelerinin ve 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 Academic Staff, Appointment Academic Staff, Sivas Cumhuriyet Üniversitesi, November, 2018

Taught Courses And Trainings

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

Articles Published in Journals That Entered SCI, SSCI and AHCI Indexes

- I. **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 (Journal Indexed in SCI Expanded)
- II. **Computational structure characterization, nonlinear optical properties and antitumor activities of Nickel(II) complexes containing alkoxy-derived dicyandiamide ligands**
ALAGÖZ SAYIN T., KARAKAŞ D.
Indian Journal of Chemistry, vol.60, pp.51-61, 2021 (Journal Indexed in SCI Expanded)
- III. **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 (Journal Indexed in SCI)
- IV. **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 (Journal Indexed in SCI)
- V. **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 (Journal Indexed in SCI)
- VI. **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 (Journal Indexed in SCI)
- VII. **Structural, spectral characterization and molecular docking analyses of mer-ruthenium (II) complexes containing the bidentate chelating ligands**
Erkan S., Kaya S., Sayın K., Karakaş D.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.224, 2020 (Journal Indexed in SCI)
- VIII. **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 (Journal Indexed in SCI)
- IX. **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 (Journal Indexed in SCI)
- X. **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 (Journal Indexed in SCI)
- XI. **Investigations of structural, spectral, electronic and biological properties of N-heterocyclic carbene Ag(I) and Pd(II) complexes**
Sayın K., Kariper S. E. , Tastan M., Sayın T. A. , Karakaş D.
JOURNAL OF MOLECULAR STRUCTURE, vol.1176, pp.478-487, 2019 (Journal Indexed in SCI)

- XII. **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
(Journal Indexed in SCI)
- XIII. **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 (Journal Indexed in SCI)
- XIV. **Quantum chemical investigation of levofloxacin-boron complexes: A computational approach**
SAYIN K., KARAKAŞ D.
JOURNAL OF MOLECULAR STRUCTURE, vol.1158, pp.57-65, 2018 (Journal Indexed in SCI)
- XV. **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 (Journal Indexed in SCI)
- XVI. **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
(Journal Indexed in SCI)
- XVII. **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 (Journal Indexed in SCI)
- XVIII. **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 (Journal Indexed in SCI)
- XIX. **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 (Journal Indexed in SCI)
- XX. **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 (Journal Indexed in SCI)
- XXI. **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 (Journal Indexed in SCI)
- XXII. **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 (Journal Indexed in SCI)
- XXIII. **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 (Journal Indexed in SCI)
- XXIV. **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 (Journal

Indexed in SCI)

- XXV. **Structural, spectral, NLO and MEP analysis. of the [MgO₂Ti₂(OPri)(6)], [MgO₂Ti₂(OPri)(2)(acac)(4)] and [MgO₂Ti₂(OPri)(2)(bzac)(4)] by DFT method**
SAYIN K., KARAKAŞ D.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.144, pp.176-182, 2015
(Journal Indexed in SCI)
- XXVI. **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 (Journal Indexed in SCI)
- XXVII. **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
(Journal Indexed in SCI)
- XXVIII. **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 (Journal Indexed in SCI)
- XXIX. **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 (Journal Indexed in SCI)
- XXX. **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 (Journal Indexed in SCI)
- XXXI. **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 (Journal Indexed in SCI)
- XXXII. **Quantum chemical studies on the some inorganic corrosion inhibitors**
SAYIN K., KARAKAŞ D.
CORROSION SCIENCE, vol.77, pp.37-45, 2013 (Journal Indexed in SCI)
- XXXIII. **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 (Journal Indexed in SCI)
- XXXIV. **A new approach to predicting the carbonyl stretching frequencies of Co₂(CO)₈ with D_{3d} 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 (Journal Indexed in SCI Expanded)
- XXXV. **Force constant calculations for Hg[Co(CO)₄]₂ 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 (Journal Indexed in SCI Expanded)
- XXXVI. **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 (Journal Indexed in SCI)
- XXXVII. **Force constant calculations for octahedral complexes of the type M(CO)₅L, based on the CO-factored force field**

Articles Published in Other Journals

- I. **Computational study on the structural, electronic, molecular and thermochemical properties of hypothetical $[\text{Tp}(\text{CO})_2\text{Mo}\equiv\text{C-Ph}]_2^+$ and $[\text{L}(\text{CO})_2\text{Mo}\equiv\text{C-Ph}]^+$ carbyne complexes**
ZAIM Z., KARAKAŞ D.
Cumhuriyet Science Journal, vol.42, pp.45-59, 2021 (Refereed Journals of Other Institutions)
- II. **Computational study on molecular structure, vibrational spectrum analysis and acidity strength of P4O_n ($n = 6-10$) phosphorus oxides with cage structure**
Karakas D.
Cumhuriyet Science Journal, vol.41, no.3, pp.659-664, 2020 (National Refreed University Journal)
- III. **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 (Refereed Journals of Other Institutions)
- IV. **Detemination 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 (Refereed Journals of Other Institutions)
- V. **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 (Refereed Journals of Other Institutions)
- VI. **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 (Refereed Journals of Other Institutions)
- VII. **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 (Refereed Journals of Other Institutions)
- VIII. **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 (Refereed Journals of Other Institutions)
- IX. **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 (Refereed Journals of Other Institutions)
- X. **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 (Refereed Journals of Other Institutions)
- XI. **Theoretical Studies on EightOxovanadium IV Complexes withSalicylaldehyde and Aniline Ligands**
ERKAN KARİPER S., SAYIN K., KARAKAŞ D.
Hacettepe Journal of Biology and Chemistry, vol.42, no.3, pp.337-342, 2014 (Other Refereed National Journals)
- XII. **Determination of structural and electronic properties of $\text{Ni}(\text{NQSC})_2$ and $\text{Ni}(\text{NQTS})_2$ complexes with DFT method**

SAYIN K., KARAKAŞ D.

Spectrochimica Acta Part A-Molecular And Biomolecular Spectroscopy, vol.2, pp.47-53, 2013 (Refereed Journals of Other Institutions)

XIII. **Quantum chemical studies on Co ntb pic complex ion**

SAYIN K., KARAKAŞ D.

Journal of New Results in Science, vol.2, pp.54-59, 2013 (Refereed Journals of Other Institutions)

XIV. **W(CO)6/CCl4/hv katalizör sistemi ile bazı polimerlerin bozunması**

KARAKAŞ D., KAYA C.

C.Ü Fen-Edebiyat Fakültesi, Fen Bilimleri Dergisi, vol.21, pp.147-153, 1999 (Other Refereed National Journals)

XV. **[M(CO4)X]2 tipi metal karbonillerin C-O gerilme bantlarının simetri etiketlemesi**

Gülcan Ü., KARAKAŞ D., KAYA C.

C.Ü Fen-Edebiyat Fakültesi, Fen Bilimleri Dergisi, vol.21, pp.177-186, 1999 (Other Refereed National Journals)

Books & Book Chapters

I. **Moleküler Simetri**

Karakaş D., Kaya C.

Palme Yayın Dağıtım, Ankara, 2010

Refereed Congress / Symposium Publications in Proceedings

I. **Computational research on the molecular properties and anti-tumor activity of Pt (II) complexes with a chiral halogenated Schiff base ligand**

Kaya S., ERKAN S., KARAKAŞ D.

I. International Cancer Days, 19 - 21 September 2019, pp.455

II. **Quantum chemical calculations o some platinum-based complexes used as drugs in cancer treatment**

Taştan M., Karakaş D.

I. International Cancer Days, Sivas, Turkey, 19 - 21 September 2019, pp.184

III. **Computational Analysis of Structural, Spectroscopic and NLO Properties on Molybdenum Carbonyl Complexes with 4,4'-xx-Dipyridylacetylene Bridge Ligand and Triphenyl Phosphine and Triphenoxy Phosphine Terminal Ligand**

ERKAN S., KARAKAŞ D.

2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), Nevşehir, Turkey, 25 - 27 June 2019, pp.8

IV. **NLO Properties and Molecular Docking Study Molybdenum Carbonyl Complexes with Pyridyl Ligands with Alkyne Unit**

ERKAN S., KARAKAŞ D.

2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), Nevşehir, Turkey, 25 - 27 June 2019, pp.15

V. **Quantum Chemical Calculations on Manganese Complexes with Penta-Amine Macrocyclic Schiff Base Ligand: Computational and Molecular Docking Analyses**

ERKAN S., SAYIN K., KARAKAŞ D.

2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), Nevşehir, Turkey, 25 - 27 June 2019, pp.21

VI. **Quantum Chemical Calculations on Ag and Pb Complexes withPenta-Amine Macrocyclic Schiff Base Ligand: Computational andMolecular Docking Analyses**

SAYIN K., ERKAN S., KARAKAŞ D.

2nd International Conference on Physical Chemistry and Functional Materials (PCFM'xx19), 25 - 27 June 2019, pp.82

- VII. **Computational study on molybdenum-based metal carbonyl complexes**
ERKAN S., KARAKAŞ D.
2nd International Conference on Physical Chemistry and Functional Materials(PCFM'19), 25 - 27 June 2019, pp.1
- VIII. **Computational studies on Schrock type Mo(CO)₅(Cme₂) and Mo(CO)₅(Cmeet) alkyliden complexes based on density functional theory**
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