

## Prof. CEMAL KAYA

### Personal Information

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### Education Information

Doctorate, Hacettepe University, Fen Bilimleri Enstitüsü, Kimya (Dr), Turkey 1978 - 1982

Postgraduate, Hacettepe University, Fen Fakültesi, Kimya Bölümü, Turkey 1976 - 1978

### Foreign Languages

English, C1 Advanced

### Dissertations

Postgraduate, Friedel crafts ürünlerinin incelenmesi, Hacettepe Üniversitesi, Fen Fakültesi, Kimya Bölümü, 1978

### Academic Titles / Tasks

Professor, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 1983 - Continues

### Academic and Administrative Experience

Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 1982 - Continues

Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 1998 - 2001

Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 1993 - 1998

Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 1990 - 1992

### Courses

Anorganik Kimya-II, Undergraduate, 2018 - 2019

Anorganik Kimya-I, Undergraduate, 2019 - 2020

Anorganik Kimya-II, Undergraduate, 2018 - 2019

Anorganik Kimyanın İlkeleri, Postgraduate, 2017 - 2018

Asit - Baz Kimyası, Undergraduate, 2018 - 2019

Anorganik Kimya-I, Undergraduate, 2018 - 2019

Uzmanlık Alan Dersi, Doctorate, 2017 - 2018

Moleküler Simetri, Undergraduate, 2016 - 2017

Simetri ve Spektroskopi, Postgraduate, 2017 - 2018

Anorganik Kimya Lab, Undergraduate, 2017 - 2018

Uzmanlık Alan Dersi, Postgraduate, 2017 - 2018  
İleri Anorganik Kimya-I, Postgraduate, 2017 - 2018  
Bitirme Ödevi/Tezi, Undergraduate, 2016 - 2017  
Koordinasyon Kimyası, Postgraduate, 2015 - 2016  
Grup Teori ve Kimyasal Uygulamaları, Postgraduate, 2016 - 2017  
İleri İnorganik Kimya-II, Postgraduate, 2015 - 2016  
Bitirme Ödevi/Tezi, Undergraduate, 2015 - 2016  
Seminer Dersi, Postgraduate, 2015 - 2016  
Geçiş Elementleri Kimyası, Doctorate, 2013 - 2014  
Asit - Baz Kimyası, Undergraduate, 2014 - 2015  
Seminer Dersi, Doctorate, 2014 - 2015  
Anorganik Kimya Lab, Undergraduate, 2014 - 2015  
Moleküler Simetri, Undergraduate, 2013 - 2014  
Genel Kimya Laboratuvarı I, Undergraduate, 2013 - 2014  
Genel Kimya Laboratuvarı II, Undergraduate, 2011 - 2012  
Genel Kimya Lab. - II, Undergraduate, 2010 - 2011  
Organometalik Kimya, Undergraduate, 2010 - 2011  
Organometalik Kimya, Undergraduate, 2009 - 2010  
Spektroskopiye Giriş, Undergraduate, 2007 - 2008  
Spektroskopiye Giriş, Undergraduate, 2008 - 2009

## Advising Theses

KAYA C., Kohesif enerjinin kimyasal sertlikle ilişkisinin araştırılması, Postgraduate, İ.UĞURLU(Student), 2017  
KAYA C., Kimyasal sertlik ve elektronegatiflik kavramlarına ilişkin dengelenme ilkelerinin kimyadaki bazı yeni uygulamaları, Doctorate, S.KAYA(Student), 2017  
KAYA C., İzoelektronik serilerde kimyasal sertlik ve mutlak elektronegatifliğin incelenmesi, Postgraduate, S.KAYA(Student), 2013  
KAYA C., Pd(II), Ni(II) ve Ru(II) metallerinin azol komplekslerinin sentezi ve katalitik özellikleri, Doctorate, N.ŞAHİN(Student), 2012  
KAYA C.,  $M(CO)\{=C=CH(R)\}(NO)Tp^*$  (M = Mo, W, R = H, Me, Pr, Ph)viniliden komplekslerinin sentezi, Doctorate, H.MARŞAN(Student), 2011  
KAYA C.,  $C_{2v}$  ve  $C_{3v}$  simetrisindeki tek çekirdekli tetra karbonillerin  $^{13}C$  izotopomerlerinin karbonil gerilme bölgesindeki titreşim spektrumlarının analizi, Postgraduate, M.KILIÇ(Student), 2009  
KAYA C.,  $C_s$  simetrisindeki trikarbonil komplekslerinin seküle denklemlerinin çözümü için yeni yaklaşımların geliştirilmesi ve co-gerilme bölgesindeki IR spektrumlarının analizi, Doctorate, E.ÜSTÜN(Student), 2009  
KAYA C.,  $Fe_2(CO)_4(?5-C_5H_5)_2$  kompleksinin  $^{13}C$ -izotopomerlerinin karbonil gerilme bölgesindeki titreşim spektrumlarının analizi, Postgraduate, A.ÜNGÖRDÜ(Student), 2007  
KAYA C., Oktahedral metal karboniller ve türevlerinin IR spektrumlarının çözümlenmesinde yeni bir yöntem, Doctorate, D.KARAKAŞ(Student), 2000  
KAYA C.,  $M(CO)_5-nLn$  ( $n=0,1,2,3,4$ ) tipi komplekslerde C-O gerilme kuvvet sabitlerinin hesaplanması ve titreşim spektrumlarının cotton-kraihanzel kuvvet alanı yaklaşımıyla çözümlenmesi, Doctorate, N.ZENGİN(Student), 1999  
KAYA C.,  $(M(CO)_4X)_2$  tipi dinükleer (İki çekirdekli) metal karbonillerin CO gerilme bölgesindeki spektrumlarının analizi, Postgraduate, G.ÜNAL(Student), 1998  
KAYA C., Fotokimyasal metatez ile polimerlerin degradasyonu, Postgraduate, D.KARAKAŞ(Student), 1993  
KAYA C., W (CO) $_6$ /CHC $_{13}$  sistemi ile 1-oktenin metatezi, Postgraduate, N.GÜLER(Student), 1991  
KAYA C., Bazı molibden karbonil türevlerinin sentezi ve stereokimyası, Postgraduate, H.MARŞAN(Student), 1988

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

- I. **Quantum Chemical Studies on the Corrosion Inhibition of Fe78B13Si9 glassy alloy in Na2SO4 Solution of Some Thiosemicarbazone Derivatives**  
SARAÇOĞLU M., Elusta M. I. A., KAYA S., KAYA C., KANDEMİRLİ F.  
INTERNATIONAL JOURNAL OF ELECTROCHEMICAL SCIENCE, vol.13, no.8, pp.8241-8259, 2018 (SCI-Expanded)
- II. **Quantum chemical calculations, molecular dynamic (MD) simulations and experimental studies of using some azo dyes as corrosion inhibitors for iron. Part 2: Bis-azo dye derivatives**  
Madkour L. H., KAYA S., Guo L., KAYA C.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1163, pp.397-417, 2018 (SCI-Expanded)
- III. **Anticorrosive Effects of Some Thiophene Derivatives Against the Corrosion of Iron: A Computational Study**  
Guo L., Safi Z. S., KAYA S., Shi W., TÜZÜN B., ALTUNAY N., KAYA C.  
FRONTIERS IN CHEMISTRY, vol.6, 2018 (SCI-Expanded)
- IV. **Theoretical insight into an empirical rule about organic corrosion inhibitors containing nitrogen, oxygen, and sulfur atoms**  
Guo L., Obot I. B., Zheng X., Shen X., Qiang Y., KAYA S., KAYA C.  
APPLIED SURFACE SCIENCE, vol.406, pp.301-306, 2017 (SCI-Expanded)
- V. **A computational study on corrosion inhibition performances of novel quinoline derivatives against the corrosion of iron**  
ERDOĞAN Ş., Safi Z. S., KAYA S., ÖZBAKIR İŞİN D., Guo L., KAYA C.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1134, pp.751-761, 2017 (SCI-Expanded)
- VI. **New insights from the relation between lattice energy and bond stretching force constant in simple ionic compounds**  
KAYA S., Chamorro E., Petrov D., KAYA C.  
POLYHEDRON, vol.123, pp.411-418, 2017 (SCI-Expanded)
- VII. **An alternative approach on the calculation of cohesive energy density and isothermal compressibility of alkali metal halides**  
KAYA S., KAYA C.  
MOLECULAR PHYSICS, vol.115, no.24, pp.3136-3142, 2017 (SCI-Expanded)
- VIII. **A novel lattice energy calculation technique for simple inorganic crystals**  
KAYA C., KAYA S., Banerjee P.  
PHYSICA B-CONDENSED MATTER, vol.504, pp.127-132, 2017 (SCI-Expanded)
- IX. **Quantum chemical calculations, molecular dynamics simulation and experimental studies of using some azo dyes as corrosion inhibitors for iron. Part 1: Mono-azo dye derivatives**  
Madkour L. H., KAYA S., KAYA C., Guo L.  
JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS, vol.68, pp.461-480, 2016 (SCI-Expanded)
- X. **Quantum chemical and molecular dynamic simulation studies for the prediction of inhibition efficiencies of some piperidine derivatives on the corrosion of iron**  
KAYA S., Guo L., KAYA C., TÜZÜN B., Obot I. B., Tourir R., Islam N.  
JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS, vol.65, pp.522-529, 2016 (SCI-Expanded)
- XI. **Quantum chemical and molecular dynamics simulation studies on inhibition performances of some thiazole and thiadiazole derivatives against corrosion of iron**  
KAYA S., KAYA C., Guo L., KANDEMİRLİ F., TÜZÜN B., Ugurlu I., Madkour L. H., SARAÇOĞLU M.  
JOURNAL OF MOLECULAR LIQUIDS, vol.219, pp.497-504, 2016 (SCI-Expanded)
- XII. **Density Functional Theory (DFT) modeling and Monte Carlo simulation assessment of inhibition performance of some carbohydrazide Schiff bases for steel corrosion**  
Obot I. B., KAYA S., KAYA C., TÜZÜN B.  
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, vol.80, pp.82-90, 2016 (SCI-Expanded)
- XIII. **Reply to the "Comment on "A new equation based on ionization energies and electron affinities of atoms for calculating of group electronegativity" by S. Kaya and C. Kaya [Comput. Theoret. Chem. 1052 (2015) 42-46]"**

- KAYA S., KAYA C., Islam N.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1083, pp.75-76, 2016 (SCI-Expanded)
- XIV. **Theoretical evaluation of triazine derivatives as steel corrosion inhibitors: DFT and Monte Carlo simulation approaches**  
Obot I. B., KAYA S., KAYA C., TÜZÜN B.  
RESEARCH ON CHEMICAL INTERMEDIATES, vol.42, no.5, pp.4963-4983, 2016 (SCI-Expanded)
- XV. **Maximum hardness and minimum polarizability principles through lattice energies of ionic compounds**  
KAYA S., KAYA C., Islam N.  
PHYSICA B-CONDENSED MATTER, vol.485, pp.60-66, 2016 (SCI-Expanded)
- XVI. **The nucleophilicity equalization principle and new algorithms for the evaluation of molecular nucleophilicity**  
KAYA S., KAYA C., Islam N.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1080, pp.72-78, 2016 (SCI-Expanded)
- XVII. **Theoretical evaluation of some benzotriazole and phosphono derivatives as aluminum corrosion inhibitors: DFT and molecular dynamics simulation approaches**  
KAYA S., Banerjee P., Saha S. K., TÜZÜN B., KAYA C.  
RSC ADVANCES, vol.6, no.78, pp.74550-74559, 2016 (SCI-Expanded)
- XVIII. **Determination of corrosion inhibition effects of amino acids: Quantum chemical and molecular dynamic simulation study**  
KAYA S., TÜZÜN B., KAYA C., Obot I. B.  
JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS, vol.58, pp.528-535, 2016 (SCI-Expanded)
- XIX. **Copper-Catalysed Allylic Substitution Using 2,8,14,20-Tetrapentylresorcinarenyl-Substituted Imidazolium Salts**  
Kaloglu M., Sahin N., Semeril D., Brenner E., Matt D., ÖZDEMİR İ., KAYA C., Toupet L.  
EUROPEAN JOURNAL OF ORGANIC CHEMISTRY, no.33, pp.7310-7316, 2015 (SCI-Expanded)
- XX. **A Simple Method for the Calculation of Lattice Energies of Inorganic Ionic Crystals Based on the Chemical Hardness**  
KAYA S., KAYA C.  
INORGANIC CHEMISTRY, vol.54, no.17, pp.8207-8213, 2015 (SCI-Expanded)
- XXI. **A new equation for calculation of chemical hardness of groups and molecules**  
KAYA S., KAYA C.  
MOLECULAR PHYSICS, vol.113, no.11, pp.1311-1319, 2015 (SCI-Expanded)
- XXII. **A new method for calculation of molecular hardness: A theoretical study**  
KAYA S., KAYA C.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1060, pp.66-70, 2015 (SCI-Expanded)
- XXIII. **A new equation based on ionization energies and electron affinities of atoms for calculating of group electronegativity**  
KAYA S., KAYA C.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.1052, pp.42-46, 2015 (SCI-Expanded)
- XXIV. **Palladium-catalysed Suzuki-Miyaura cross-coupling with imidazolylidene ligands substituted by crowded resorcinarenyl and calixarenyl units**  
Sahin N., Semeril D., Brenner E., Matt D., KAYA C., Toupet L.  
TURKISH JOURNAL OF CHEMISTRY, vol.39, no.6, pp.1171-1179, 2015 (SCI-Expanded)
- XXV. **Subtle Steric Effects in Nickel-Catalysed Kumada-Tamao-Corriu Cross-Coupling Using Resorcinarenyl-Imidazolium Salts**  
Sahin N., Semeril D., Brenner E., Matt D., ÖZDEMİR İ., Kaya C., Toupet L.  
EUROPEAN JOURNAL OF ORGANIC CHEMISTRY, vol.2013, no.20, pp.4443-4449, 2013 (SCI-Expanded)
- XXVI. **Resorcinarene-Functionalised Imidazolium Salts as Ligand Precursors for Palladium-Catalysed SuzukiMiyaura Cross-Couplings**  
Sahin N., Semeril D., Brenner E., Matt D., ÖZDEMİR İ., KAYA C., Toupet L.

- CHEMCATCHEM, vol.5, no.5, pp.1116-1125, 2013 (SCI-Expanded)
- XXVII. **Synthesis and use of trans-dichlorido-tetrakis-(N-R-imidazole)nickel(II) complexes in Kumada-Tamao-Corriu cross-coupling reactions**  
Sahin N., El Moll H., Semeril D., Matt D., ÖZDEMİR İ., KAYA C., Toupet L.  
POLYHEDRON, vol.30, no.12, pp.2051-2054, 2011 (SCI-Expanded)
- XXVIII. **Calculating the CO-factored force constants of tricarbonyl complexes with C-s symmetry**  
ÜSTÜN E., KAYA C.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, vol.695, pp.2273-2276, 2010 (SCI-Expanded)
- XXIX. **The Nature of the Crustal Structure of the Eastern Anatolian Plateau, Turkey**  
YILMAZ A., YILMAZ H., KAYA C., BOZTUĞ D.  
GEODINAMICA ACTA, vol.23, no.4, pp.167-183, 2010 (SCI-Expanded)
- XXX. **Deep crustal structure of northwestern part of Turkey**  
Kaya C.  
TECTONOPHYSICS, vol.489, pp.227-239, 2010 (SCI-Expanded)
- XXXI. **A new approach to predicting the carbonyl stretching frequencies of Co-2(CO)(8) with D-3d symmetry**  
Kaya C., Karakas D., Uestuen E.  
INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL & ANALYTICAL CHEMISTRY, vol.46, no.9, pp.1388-1392, 2007 (SCI-Expanded)
- XXXII. **Force constant calculations for Hg[CO(CO)(4)](2) from the CO-factored force field**  
Kaya C., Karakas D.  
INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL & ANALYTICAL CHEMISTRY, vol.46, no.1, pp.33-38, 2007 (SCI-Expanded)

## Articles Published in Other Journals

- I. **New triazepine carboxylate derivatives: correlation between corrosion inhibition property and chemical structure**  
Alaoui K., El Kacimi Y., Galai M., Serrar H., Touir R., KAYA S., KAYA C., Touhami M. E.  
INTERNATIONAL JOURNAL OF INDUSTRIAL CHEMISTRY, vol.11, no.1, pp.23-42, 2020 (ESCI)
- II. **A New Method for Analyzing the Force Constants of Tricarbonyl Complexes with CS Symmetry**  
ÜSTÜN E., KAYA C.  
Ordu University Journal of Science and Technology, 2018 (Peer-Reviewed Journal)
- III. **Derivation of ionization energy and electron affinity equations using chemical hardness and absolute electronegativity in isoelectronic series**  
KAYA S., KAYA C.  
Journal of Physical and Theoretical Chemistry, pp.155-163, 2015 (Peer-Reviewed Journal)

## Metrics

Publication: 37

Citation (WoS): 1598

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H-Index (Scopus): 16