Executive Summary of the Biodata of Dr. Eluvathingal D. Jemmis

Education: Indian Institute of Technology Kanpur (**MSc 1973**); Princeton University (**Ph.D.1978**, with Profs Paul Schleyer and John Pople, 1998 Nobel Laureate).
Employment: Cornell University (**Research Associate 1978-80**, with Prof Roald Hoffmann, 1981 Nobel Laureate). **University of Hyderabad**, India, **Lecturer 1980**; **Reader 1984**; **Professor 1990**; **Indian Institute of Science**, Bangalore, **Professor 2005-2017**, **Hon Professor 2017-2022**. **Year of Science Chair Professor (SERB) 2019-2014.**
Institution Building; administrative engagements: Univ. of Hyderabad**, Dean of the School, 2002-5.**
Established a **Centre for Modeling Simulation and Design** at the Univ. of Hyderabad in 2002, as a project grant from the Department of Science and Technology, New Delhi. (http://cmsd.uohyd.ac.in).
Founding Director 2008-13, Indian Institute of Science Education and Research Thiruvananthapuram, a project of the Ministry of Human Resource Development, Govt of India, on a 5 year deputation from IISc Bangalore (http://www.iisertvm.ac.in).
Member, International Board: WATOC, World Association of Theoretical and Computational Chemists; **APATCC**, Asia Pacific Association of Theoretical and Computational Chemists; **IMEBORON**, International Meeting on Boron Chemistry.

Research: His research aims to bring general understanding of structure, bonding and reactions of molecules, clusters, and solids, using Quantum Chemistry, searching for transferable models from numbers. Transition metal organometallic reactions involving C-C fond formation, and C-H activation, structural chemistry boranes and of allotropes of elemental boron, generalization of Hydrogen-Bonds to similar weak interactions in main group and transition metal chemistry, three dimensional aromaticity, electron counting rules, broron equivalents of graphenes and fullerenes, and unusual structural variations in heavier main group elements are topics that have received particular attention in his laboratory. The Jemmis mno Rule helped to relate beta-rhombohedral boron to polyhedral 'a la benzene to graphite and methane diamond. These ideas in the chemistry of boron has got into general chemistry textbooks and is taught in Inorganic chemistry courses across the world. Efforts are on to study borophene bilayers and multilayers on metal templates which may have more promising properties as materials of the future in areas where graphene is found wanting.

Jemmis has been recognized for his contributions with many awards, prizes and fellowships. He was selected as a student with special talent early on as a National Science Talent Search Scholar in the 12th Class. He received the highest science recognition of India for scientists below 45 years, the Shanti Swarup Bhatnagar Prize. The Government of India awarded the civilian honor of Padma Shree to Dr. Jemmis in the area of Science and Engineering for his many contributions. He has been a member of the advisory board of several international journals in chemistry. He received funding continuously from the DST, UGC, and BRNS of DAE Govt of India.

Biodata of Dr. Eluvathingal D. Jemmis

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Full Name, Place & Date of Birth

Eluvathingal Devassy Jemmis
Chevoor (Kerala, India)
31-10-1951

Maried: to Alice; two Children: Sebastian and Lilly.

Education

Degree	Year	Particulars
B.Sc.	1971	First Rank, University of Calicut (Specialization: Chemistry)
M.Sc.	1973	Indian Institute of Technology, Kanpur (Specialization: Chemistry)
A.M.	1974	Princeton University (Specialization: Chemistry)
Ph.D.	1978	Applied Theoretical Chemistry, Princeton University (with Professors Paul von R Schleyer, John Pople (1998 Nobel Laureate), and Lee Allen)

Employment

Position Held	Year	Particulars
Research Associate	1978–80	Cornell University (with Professor Roald Hoffmann, 1981 Nobel Laureate)
Lecturer	1980	University of Hyderabad
Reader	1984	University of Hyderabad
Professor	1990	University of Hyderabad
Visiting Fellow	1991, Jan-Dec	Research School of Chemistry, Institute for Advanced Study, Australian National University, Canberra.
Visiting Professor	2000, May-Jul	Centre for Computational Quantum Chemistry, University of Georgia, Athens.

Dean	2002-05	School of Chemistry, University of Hyderabad
Honorary Professor	2003-2017	Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore.
Professor (super-annuated in 2017)	2005-17	Inorganic and Physical Chemistry Dept, Indian Institute of Science, Bangalore.
Hon. Prof. (with no emoluments)	2017-22	Inorganic and Physical Chemistry Dept, Indian Institute of Science, Bangalore.
Founding Director	2008-13	Indian Institute of Science Education and Research Thiruvananthapuram
Adjunct Professor	2008-11	International Centre for Theoretical Sciences, TIFR, Bangalore
Year of Science Professor, SERB	2019-24	Inorganic and Physical Chemistry Dept, Indian Institute of Science, Bangalore.

Teaching Experience

Graduate Courses

1. Structure and Bonding
2. Advanced Inorganic Chemistry
3. Introduction to Quantum Chemistry
4. Chemical Binding
5. Theoretical Organic Chemistry
6. Theoretical Inorganic Chemistry
7. Computational Chemistry:Understanding Numbers

Under Graduate Courses

1. Chemistry of the Main Group Elements, to third year UG students at IISc (every year from 2013).

Grants for Research

Obtained research grants on a continuing basis from:

(a) Department of Science & Technology (DST), New Delhi.
(b) Council of Scientific & Industrial Research (CSIR), New Delhi.
(c) University Grants Commission (UGC), New Delhi.
(d) Board of Research in Nuclear Studies (DAE), Mumbai
(e) Year of Science Chair; SERB, DST, New Delhi

Fellowships of Academies and other Professional Affiliations.

(a) Fellow, Indian Academy of Sciences, Bangalore (1992)
(b) Fellow, Indian National Science Academy, New Delhi (1998)
(c) Fellow, Andhra Pradesh Akademi of Sciences, Hyderabad (2003)
(d) Fellow, National Academy of Sciences India, Allahabad (2004)
(e) Fellow, Third World Academy of Sciences, Trieste, Italy (2004)

(f) Fellow, Asia Pacific Association of Theoretical and Computational Chemists, (2016).
(f) Member, American Chemical Society
(g) Elected Member, Scientific Advisory Board of World Association of TheoreticallyOriented Chemists (WATOC) (2008)
(h) Member, Chemical Research Society of India (2000)
(i) Member, Indian Science Congress Association (2001)
(j) Elected Member, Advisory Board, Asia Pacific Association of Theoretical and Computational Chemists, 2008.
(k) Elected Member, Advisory Board, IMEBORON, International Meeting on Boron Chemistry, 2017.

Honors, Awards etc

1. National Science Talent Search Scholarship, NCERT, 1968.
2. University Gold Medal, BSc first rank, Calicut, 1971.
3. Young Scientist Award, Indian National Science Academy, 1982.
4. Young Associate, Indian Academy of Sciences, 1984.
5. Anil Kumar Bose Memorial Award, Indian National Science Academy, 1988.
6. Member, Ed Board, Proceedings of the Indian Academy of Sciences, 1989.
7. Member, Ed Board, Indian Journal of Chemistry, 1993.
8. Shanti Swarup Bhatnagar Prize, Council of Scientific and Industrial Research, New Delhi, 1994.
9. Dr. Swaminathan Memorial Lecture, Osmania University, 1995.
10. Dr. Jagdish Shankar Memorial Lecture, INSA, 2000.
11. Millennium Medal, Indian Science Congress, CSIR, New Delhi, 2000.
12. Prof. K. Venkataraman Lecture, University Department of Chemical Technology, University of Bombay, Mumbai, 2001.
13. Platinum Jubilee Lecture in Chemistry, Indian Science Congress, 2002.
14. Silver Medal, Chemical Research Society of India, 2002.
15. Member, Ed Board, Journal of Computational Chemistry, 2002.
16. Andhra Pradesh Scientist Award -2003 of the Andhra Pradesh Council of Science and Technology.
17. Guest Editor for Proceedings of Indian National Science Academy, New Delhi, 2003.
18. Third World Academy of Sciences (TWAS) Prize in Chemistry, 2003.
19. Robert S. Mulliken Lecture of the University of Georgia, August, 2004.
20. Prof Priyadaranjan Ray Memorial Award, Indian Chemical Society, 2005.
21. J.C. Bose National Fellowship, DST, 2006-2019.
22. Member, Advisory Board, Asia Pacific Association of Theoretical and Computationa Chemists, 2008.
23. UGC Hari Om Ashram Trust National Awards - Meghanand Saha Award in Theoretical Sciences, New Delhi, 2009.
24. Member, Editorial Board, Interdisciplinary Reviews: WIRES- Computational Molecular Science 2011.
25. Member, International Advisory Board, Chemistry An Asian Journal, 2013.
26. Padma Shri, civilian award, by the Government of India, in Science and Engineering, 2014.
27. Swadeshi Sasthra Puraskaram, 2014 of the Swadeshi Science Movement,

6 Nov 2014.
28. Goyal Prize in Chemistry, Kurukshetra University, Haryana, 23, April, 2015.
29. Editorial Advisory Board, J. Chemical Sciences, 2015.
30. Editorial Advisory Board, ChemPlusChem, 2015.
31. P. C. Ray Memorial Award, Indian Science Congress, 2016.
32. Fukui Medal, Asia Pacific Association of Theoretical and Computational Chemists, 2016.
33. Linus Pauling Lecture Award, Mahatma Gandhi Univ, Kottayam, Kerala, 2016.
34. Professor R. P. Mitra Memorial Lecture Award, University of Delhi, 2018, delivered on 12th January 2018.
35. Year of Science Chair Professorship, SERB-DST, Nw Delhi, 2019-2024.
36. Sir Devaprasad Sarvadhikari Medal, Calcutta University, 2020

Research Interests: Applied Theoretical Chemistry; Structure, Bonding and Reactions of molecules, Clusters and Solids; Aromaticity and Electron Counting Rules; Structure of Elemental Boron and Boron-rich Solids.

Special emphasis is placed in weaving threads between problems in one area to another; between polymorphs of elements and their compounds, between organic and organometallic chemistry, amongst the chemistry of various main group elements; Bonding, Structure and Reactions across the Periodic Table of Elements.

Summary of recent results:

Novel Ideas in Structure and Bonding

The accepted concepts of structure and bonding is tested to its limits so that these could be broken and novel arrangements of atoms which are contrary to the chemical commonsense can be designed. Six valence electron tri-coordinate pyramidal arrangements have been stabilized for boron and aluminum. A comparison of the bonding capabilities of heavier main group elements indicate that the rules of bonding that are taken as standard for the lighter elements, exemplified by carbon, is more of an exception than the rule. The general idea that bond length is proportional to bond strength and that sigma bonds are stronger than pi bonds is common in chemistry. Though difficult to see in large numbers, it is reasonable to anticipate short bond lengths if pi-only bonds can be designed. Jemmis group has recently designed aromatic hyper coordinate molecules involving P and S, such a $(PF_3)_3^{-2}$ and $(SF_2H_2)_3$ using qualitative perturbation theory using variations in electronegativity of substituents as a perturbation.

Transition Metal Organometallics

The bis-cyclopentadienyl titanium and zirconium groups help in several catalytic processes involving C-C bond formation and sigma-bond metathesis. The details of the ways in which these fragments stabilize strained molecular structures are being studied. The C-C coupling reactions of bridging acetylides of Cp_2Zr and Cp_2Ti complexes are being generalised to the metals of the main group, Actinides and Lanthanides.

Just about any transition metal is shown to help in C-H bond activation. This is remarkable for the following reason. The energy of a C-H bond remains approximately constant in most organic ligands. On the other hand the energy of the atomic orbitals of the metal from Sc to Ni varies substantially. A general understanding of the ways in which different ligand combinations work together to make any transition metal fragment to activate C-H bond and in some instances, stabilize them on the way as agostic structures, is being pursued. Similar studies are planned for other single bond activation processes. Jemmis group also collaborates with experimentalists in these areas.

The idea of isolobal connections that exist between apparently unrelated species is being studied in a variety of contexts. Double insertion reactions of benzynes to naphthalenes are used as models for similar reactions in carborynes. Analogues of olefin metathesis in the chemistry of boron is also being followed. We are currently looking at ways of stabilizing boron equivalents of $Cp_2Zr(C_4H_2)$ where C_4H_2 is replaced by B_4R_2.

Electron Counting Rules, Elemental Boron, Boron-Rich Solids, boron-fullerenes and boron-nanotubes

One of the first benefits of quantum mechanics to organic chemistry came in the form of pi MO theory and the Hückel 4n+2 pi electron rule. In addition to generating a large area of chemistry of the condensed aromatics, the Hückel 4n+2 rule brought a conceptual relationship between benzene, naphthalene and other condensed aromatics on the one hand and graphite on the other. A similar understanding of the structure of boranes and the allotropes of boron is lacking. An electron counting rule to condense polyhedral boranes and its application to relate polycondensed boranes to beta-rhombohedral boron is being sought. This process helps in bringing conceptual links between carbon and boron chemistry and an understanding of the structure of boron-rich solids. This has also led to the design of boron based stuffed fullerenes and boron nanotubes. Borospherenes, tau-boron and boron-rich metal borides are amongst the current areas of research.

Jemmis group has begun the study of boron equivalents of graphenes. The inevitability of hexagonal holes in the triangular boron network of borophenes is demonstrated. The effect of metal templates and multilayers of borophenes are currently being probed. We also study the structure and reactions of smaller molecules of boron and heavier main group elements with unusual multiple bonds.

Weak Hydrogen Bonds and other non-covalent interactions.

Nature of bonding in the weakest of the Weak interactions, viz. the C-H...pi interactions has been a point of interest in recent years. The unexpected shortening of the C-H bond as a consequence of the C-H...pi interactions has been studied by us theoretically and experimentally in collaboration with many research groups. The experimental strategy has been to isolate the system in an argone matrix and and use surface FTIR spectroscopy in collaboration with experimental groups. Theoretically the spectra and the structure of these systems have been studied. Jemmis group

dissected the total interaction energy into various components and now understand, for example, the reasons for the near equal interaction energy of added $CHCl_3$ molecules to HCCH up to four $CHCl_3$ around the HCCH. Implications of the shortening of the C-H bondlengths involved in C-H...pi interaction are being pursued. Dr. Jemmis provided a general understanding for the blue-shifted H-Bonds in X-H---Y and are in the process of generalizing this to any weak bond X-Z---Y where Z is any atom in the periodic table of elements. Examples of the latter such as the Halogen-Bond, and Chalcogen Bonds are now well known. A plethora of other Z-Bonds are waiting to happen. We have started to apply the weak interactions such as the halogen bonds in novel ways, such as strengthening the sextuple bond of Cr_2 and Mo_2.

The attempt by the Jemmis group is not just to get some calculations and a specific answer, nor to work in a contemporary area where many scientists work, but to develop general understanding of a transferable nature in a chosen area to help further the thought processes in chemistry. This has always led to applications in material science and biology. Majority of his former students work in material science or computaional drug design and molecular modelling.

Dr. Jemmis is also involved in a kind of extension work in spreading the message of computational chemistry among experimental chemists. Many visitors come through official and non-official routes to spend varying length of time to learn the art of making explanations from calculations, understanding from numbers.

Supervision of PhD and Postdoctoral Research

Past:		
Ph.D. Students (degree awarded)	:	26
Current: Ph.D. Students	:	4
Postdoctoral Students and senior associates	:	12
Current:		3

Service to Science education, research and administration:

At University of Hyderabad from its inception, in addition to being a member of numerous academic and administrative committees, Jemmis was involved in:

1. Instrumental in reorganizing the Campus School, 1985.
2. Helped in starting e-mail facility at the Univeristy, 1989-90.
3. As Professor-in-Charge of the Computer Centre, helped install a fiber optic network in the Campus, 1999-2001.
4. Established the Centre for Modeling, Simulation and Design (CMSD), a computing facility with state-of-the-art software and hardware at the University of Hyderabad in 2003.
5. As the Dean campaigned successfully for obtaining new faculty and research equipment at the School (2002-2005).

6. As the Head of the CMSD, helped in establishing a High Performance Computing Facility (HPCF) with independent Physical Structure, which can be used by any faculty from DST-FIST-supported departments across the country. http://cmsd.uohyd.ac.in

At the Indian Institute of Science:

Chairman, Advisory Committee, Supercomputer Education and Research Center, SERC, 2006.
Member, Committee on Networking, Internet and Email, 2007.
Member, Committee for Centenary Postdoctoral Fellowship, 2006.
Chair, Faculty Recruitment Committee, IPC Dept, 2015.

Service to National Scientific, Educational and Research Organizations

Served in various decision making bodies for funding research in the country such as the Department of Science and Technology, the Council of Scientific and Industrial Research, and the University Grants Commission. Spearheaded a project to establish a High Performance Computing Facility for University community across the country, as a sponsored project of the Department of Science & Technology in 2003-2005.

Served the Indian Academy of Sciences, Bangalore and Indian National Science Academy, New Delhi in many capacities; Member of Andhra Pradesh and Kerala State Science and Technology Councils; Academic Council of the Homi Bhabha National Institute; Chemical Research Society of India; Steering Committee to establish and run National Institute for Science Education and Research, Bhubaneswar in the first year; Academic Advisory Council of the Indian Association for Cultivation of Science, Kolkota, Executive Council of the Tamil Nadu, Pondicherry and Kerala Central Universities; Member, Academic Council Central University of Rajasthan; Member, Board of Governors of IIT Kanpur, NISER Bhubaneswar, TIFR-Hyderabad.

Institution Development

Dr. Jemmis accepted the challenge of the Ministry of Human Research Development, Govt of India, to start the Indian Institute of Science Education and Research (IISER) Thiruvananthapuram, a research and teaching institute of the Ministry as its Founding Director taking a five year deputation from Indian Institute of Science Bangalore(2008-13). It is a fast developing institute (http://www.iisertvm.ac.in).

Publications of Dr. E. D. Jemmis:

Over 200, in international refereed journals, about 50 of them in the Journal of the American Chemical Society or Angew Chemie. The ideas of Jemmis on the extension of Wades Rules to the Jemmis mno Rule that includes electron counting rules for condensation polyhedral boranes and the relationship established between icosahedral boranes and beta-rhombohedral boron are being taught in Advanced

Inorganic Chemistry Courses in India and around the world. Periodically our results have been highlighted in various popular journals, textbooks and the web.
eg. Inorganic Chemistry text book (2003) by Gary L. Miessler and Donald A. Tarr, Pearson Education Press; Structural Inorganic Chemistry, (2008), by Wai-Kee Li, Gong-Du Zhou, Thomas Mak, Oxford University Press; Molecular Clusters: A Bridge to Solid State Chemistry, (2007) Cambridge Molecular Science series, Thomas Fehlner, and Jean-Francois Halet; Basic Organometallic Chemistry (2010) by B. D. Gupta and Anil J. Elias, Universities Press.

1. J.B. Collins, J.D. Dill, E.D. Jemmis, Y. Apeloig, P.v.R. Schleyer, R. Seeger and J.A. Pople, Stabilization of planar tetracoordinate carbon, J. Am. Chem. Soc., *98*, 5419-5427 (1976).

2. E.D. Jemmis, V. Buss, P.v.R. Schleyer and L.C. Allen, Shape and angle strain in organic intermediates. A model study of alkyl radicals, anions and cations, J. Am. Chem. Soc., *98*, 6483-6489 (1976).

3. S. Lahiri, V. Dabral, V. Bhatt, E.D. Jemmis and M.V. George, Thermal and photochemical transformations of tetraphenyl-p-dioxin and tetraphenyl-p-dithiin, Proc. Indian Acad. Sci., *86A*, 1-14 (1977).

4. E.D. Jemmis, D. Poppinger, P.v.R. Schleyer and J.A. Pople, The curious structure of the lithiocarbon, C_3Li_4, J. Am. Chem. Soc., *99*, 5796-5698 (1977).

5. T. Clark, E.D. Jemmis, P.v.R. Schleyer, J.S. Binkley and J.A. Pople, *ab initio* Structures of allyllithium, J. Organomet. Chem., *150*, 1-6 (1978).

6. P.v.R. Schleyer, E.D. Jemmis and J.A. Pople, CH_3O^+ and $CH_2{=}O^+H$: High barrirs to isomerization, Chem. Commun., 190-191 (1978).

7. E.D. Jemmis, P.v.R. Schleyer and J.A. Pople, Structure and bonding of CH_2Li_2 dimers, J. Organomet. Chem., *154*, 327-335 (1978).

8. E.D. Jemmis, S. Alexandratos, P.v.R. Schleyer, A. Streitwieser, Jr. and H.F. Schaefer, III, *ab initio* SCF-MO study of cyclopentadienylberyllium hydride and of beryllocene, J. Am. Chem. Soc., *100*, 5695-5700 (1978).

9. E.D. Jemmis, J. Chandrasekharand P.v.R. Schleyer, Stabilization of D_3h pentacoordinate carbonium ions. Linear three-center-two-electron bonds. Implications for aliphatic electrophilic substitution reactions, J. Am. Chem. Soc., *101*, 527-533 (1979).

10. J. Chandrasekhar, E.D. Jemmis and P.v.R. Schleyer, Double aromaticity: Aromaticity in orthogonal planes. The 3,5-dehydrophenyl cation, Tetrahedron Lett., 3707-3710 (1979).

11. E.D. Jemmis, J. Chandrasekhar and P.v.R. Schleyer, The unusual structures, energies and bonding of lithium substituted allenes, propynes and cyclopropenes, J. Am. Chem. Soc., *101*, 2848-2856 (1979).

12. E.D. Jemmis and R. Hoffmann, Cleaving CC bonds in cyclopropenium ions, J. Am. Chem. Soc., *102*, 2570-2575 (1980).

13. E.D. Jemmis, A.R. Pinhas and R. Hoffmann, $Cp_2M_2(CO)_4$-Quadruply bridging, doubly bridging, semibridging or nonbridging? J. Am. Chem. Soc., *102*, 2576-2585 (1980).

14. Y. Apeloig, T. Clark, A.J. Kos, E.D. Jemmis and P.v.R. Schleyer, Geometries and energies of dilithioethylene isomers and of vinyl lithium. An *ab initio* study, Israel J. Chem., *20*, 43-50 (1980).

15. R.J. Goddard, R. Hoffmann and E.D. Jemmis, Unusual M-C-H angles, C-H bond activation and α-hydrogen abstraction in transition metal carbene complexes, J. Am. Chem. Soc., *102*, 7667-7676 (1980).

16. H.H. Dunken and E.D. Jemmis, Quantenchemische berechnung der absorption von wasserstoff in tetraedrischenund oktaedrischen clustern des nickels, palladiums und platins, Z. Chem., *20*, 454-455 (1980).

17. E. Wurthwein, J. Chandrasekhar, E.D. Jemmis and P.v.R. Schleyer, The [4.4.4.4]fenestrane and [2.2.2.2]paddlane. Prospects for the realization of planar tetracoordinate carbon? Tetrahedron Lett., 843-846 (1981).

18. A.J. Kos, E.D. Jemmis, P.v.R. Schleyer, R. Gleiter, U. Fischbach and J.A. Pople, 1,2-Dilithioethane. A molecular orbital study, J. Am. Chem. Soc., *103*, 4996-5002 (1981).

19. E.D. Jemmis, J. Chandrasekhar, E.U. Wurthwein, P.v.R. Schleyer, J.W. Chinn, Jr., F.J. Landro, R.J. Lagow, B. Luke and J.A. Pople, Lithiated carbocations. The generation, structureand stability of CLi5<SUP+< sup>, J. Am. Chem. Soc., *104*, 4275-4276 (1982).

20. E.D. Jemmis, Nobel prizes. The course of chemical reactions, Science Today, Jan. 53-54 (1982).

21. E.D. Jemmis and P.v.R. Schleyer, Aromaticity in three dimensions. 4 Influence of orbital compatibility on the geometry and stability of capped annulene rings with six interstitial electrons, J. Am. Chem. Soc., *104*, 4781-4788 (1982).

22. E.D. Jemmis, Overlap control and stability of polyhedral molecules. *closo*-Carboranes, J. Am. Chem. Soc., *104*, 7017-7020 (1982).

23. E.D. Jemmis, Aromaticity, orbital size and relative stability of *closo*-carboranes, Sci. Acad. Medals for Young Scientists - Lectures, Published by Indian National Science Academy, New Delhi, pp.94-103 (1982).

24. P.v.R. Schleyer, B.Tidor, E.D. Jemmis, J. Chandrasekhar, E.U. Wurthwein, A.J. Kos, B.T. Luke and J.A. Pople, Lithium-stabilized methanonium ions, $CLi_{5-n}H_n^+$. A theoretical study, J. Am. Chem. Soc., *105*, 484-488 (1983).

25. E.D. Jemmis, The geometries of tetracoordinate carbon, Current Science, *52*, 1049-1053 (1983).

26. E.D. Jemmis and P.N.V. Pavan Kumar, Stability of polyhedral borane anions and carboranes, Proc. Ind. Acad. Sci. (Chemical Sciences), *93*, 479-489 (1984).

27. E.D. Jemmis, K.S. Sharma and P.N.V. Pavan Kumar, A non-least motion pathway for 1,2-shift in cylic vinyl cations, J. Mol. Struct. (Theochem), *121*, 305-311 (1985).

28. P.v.R. Schleyer, E.D.Jemmis and G.W. Spitznagel, Do anomeric effects involving the second-row substituents Cl, SH, and PH_2 exist? Stabilization energies and structural preferences, J. Am. Chem. Soc., *107*, 6393-6394 (1985).

29. B.V.R.S.S.V. Prasad, A.D. Prasad and E.D. Jemmis, Theoretical studyof the electronic structure and reactions of $R_2W(?\text{-}CR)_2WR_2$, Recent Trends in Inorganic Chemistry, ed. A. Chakravorty, Indian National Science Academy, New Delhi, pp.66-77 (1986). Also published in Proc. Indian Natn. Sci. Acad., *52A*, 764-775 (1986).

30. P.N.V. Pavan Kumar, B. Ashok and E.D. Jemmis, Inevitability of agostic interactions, Recent Advancesin Catalysis and Catalytic Reaction Engineering, ed. P. Kanta Rao, Regional Research Lab., Hyderabad, pp. 285-293 (1986).

31. V. Pitchi Reddy and E.D. Jemmis, A D_{4d} structure for [8]-prismane, Tetrahedron Lett., *27*, 3771-3774 (1986).

32. P.N.V. Pavan Kumar, B. Ashok and E.D. Jemmis, Agostic interactions as an alternative to octahedral ethylenehydride complexes. b-CH Bond activation, J. Organomet. Chem., *315*, 361-367 (1986).

33. E.D. Jemmis, P.N.V.Pavan Kumar and N.R. Sreenivaskumar, Structure and bonding in $Si_2R_4X_2$ molecules, X=0, NH, CH_2, or S; R=H, J. Chem. Soc. Dalton Trans., 271-273 (1987).

34. E.D. Jemmis and B.V. Prasad, Reaction of $L_2W(?\text{-}CR)_2WL_2$ with C_2R_2. A theoretical study, J. Am. Chem. Soc., *109*, 2560-2563 (1987).

35. E.D. Jemmis and B.V. Prasad, The fragment molecular orbital approach in organometallic reactivity. Reactions of the binuclear complexes, Proc. Ind. Acad. Sci. (Chem. Sci.), *99*, 105-111 (1987).

36. G. Granozzi, M. Casarin, F. Edelmann, T.A. Albright and E.D. Jemmis, Experimental and theoretical studies of the bonding in $CpCoS_2N_2$, Organometallics, *6*, 2223-2227 (1987).

37. E.D. Jemmis and G. Leela, On the $\pi 2S + \pi\ 2S$ Pathways toward n-prismanes, Proc. Ind. Acad. Sci. (Chem. Sci.), *99*, 281-282 (1987).

38. A.P. Marchand, C. Huang, R. Kaya, A.D. Baker, E.D. Jemmis and D.A. Dixon, Synthesis of alkene-substituted pentacyclo[5.4.0.02,6.33,10.05,9]undecanes. 2.

Photoelectron spectra and electronic structures of substituted pentacyclo[5.4.0.02,6.03,10.05,9]undecanes, J. Am. Chem. Soc., *109*, 7095-7101 (1987).

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243. H. W. Roesky, S. K. Sarkar, M. M. Siddiqui, S. Kundu, J. Kretsch, P. Stollberg, R. Herbst-Irmer, D. Stalke, M. Ghosh, A. C. Stuckl, S. Ghorai, E. D. Jemmis, B. Schwederski, W. Kaim, Isolation of Base Stabilized Fluoroborylene and its Radical Cation. **Dalton Trans**., DOI: 10.1039/C9DT01899A (2019).

244. S. Balasubramaniam, S. Kumar, A. P. Andrews, B. Varghese, E. D. Jemmis, and A. Venugopal, A Reactive Bismuth Lewis Acid: Si-H Addition to Olefins. **Eur. J. Inorg. Chem.**, DOI: 10.1002/ejic.201900459 (2019).

245. J. Joy, E.D. Jemmis, Designing M-bond (X-M··· Y, M = transition metal): σ-hole and radial density distribution. J. Chem. Sci. 131, 1-8(2019).

246. G. Karir, E.D. Jemmis**,** Continuum in H-bond and Other Weak Interactions (X-Z··Y): Shift in X-Z Stretch from Blue Through Zero to Red. J. Indian Inst. Sci. 100, 127-133(2020).

Delivered numerous Invited Lectures at Symposia, Conferences, and Seminars in India and abroad. Last five year's list is given below.

International:

Fifteen years of the mno Rule in Chemistry, Plenary Lecture, International Conference on Boron Chemistry, IMEBORON-XV, Prague, Czech Republic, 24-28, Aug 2014.

Perspectives on the Structure, Bonding and Reactivity of Metallacyclocumulenes involving Cp_2M (M=Ti, Zr, Hf), Invited Lecture, World Association of Theoretical and Computational Chemists, WATOC2014, Santiago, Chile, 4-9, Oct 2014.

Perspectives on the Structure, Bonding and Reactivity of Metallacyclocumulenes involving Cp_2M (M=Ti, Zr, Hf), Sultan Qaboos University, Muscat, Oman, 29 Oct 2014.

A Journey through Three-Membered Rings, Modelling Chemical and Biological (Re)Activity- Winter School and Conference, Ruprecht Karls University of Heidelberg, Germany, February 17-26, 2015.

A Structural Chemistry for Boron, Institut für Anorganische und Analytische Chemie, Goethe-Universitaet, Frankfurt, Germany, 27 Feb, 2015.

A Structural Chemistry for Boron, Department of Chemistry, Texas A & M University, College Station, Texas, USA, 16th July, 2015.

A Structural Chemistry for Boron: Elemental Boron, Boron Fullerenes and Polyhedral Boranes, Department of Material Science and Nano Engineering, Rice University, Houston, Texas, USA, 17th July, 2015.

A beta-Rhombohedral Boron Route to Stuffed Boron Fullerenes, at the workshop on "Boron: an amazing element, from theory to application", Innovation Campus, University of Wollongong, Australia, 22nd October 2015.

A Structural Chemistry for Boron, Research School of Chemistry, Australian National University, Canberra, Australia, 26th October, 2015.

A Structural Chemistry for Boron, School of Chemistry, University of Sydney, Australia, 27th October 2015.

Hueckel 4n+2, Wade's n+1 and mno Rules, Fukui Medal Lecture, Asia Pacific Conference on Theoretical and Computational Chemistry, APCTCC7, Jan 25-28, 2016, Taiwan.

Transitions: Princeton, Munich and Erlangen, in Theory and Experiment: A Meeting at the Interface - A Symposium Commemorating the Life and Work of Paul Schleyer, Institute of Organic Chemistry, University of Erlangen-Nurnberg, Germany, March 30 – April 1, 2016.

The Contrasting Behavior of Transition Metal Complexes in Noncovalent X-Z···Y Interactions: Z=Transition Metals vs Main Group Elements, in Molecular Quantum Mechanics, MQM2016 – A Celebration of the Swedish School, University of Uppsala, Sweden, 26 June - 1 July 2016.

The Importance of Early Questions, First Julio Palacios International Symposium, University of A Coruna, Spain, 21-22, July 2016.

Boranes, Borospherenes, Borophenes, and Boron, Wuerzburg Summer School 2016 on Molecular Boron Chemistry, University of Wuerzburg, Germany, 25-29 July 2016.

Boranes, Borophenes and Borospherenes, KeyNote Lecture, IMEBORON 2017, Chinese University of Hong Kong, Hong Kong, 9-13 July 2017.

Hydrogen Bond (X-Z···Y, Z=H) and other weak Interactions (Z= any element of the Periodic Table), Invited Lecture, Department of Chemistry, University of Georgia, Athens, Georgia, USA, 18 August 2017.

Borophenes, Borospherenes and Boron, Invited Talk, Theoretical Models of Chemical Bonding & Reactivity Spanning the Periodic Table: A Symposium in Honor of Roald Hoffmann, ACS National Meeting, Washington DC, 20-24, August, 2017.

Borophenes, Borospherenes, Boranes, 3D-Boron Allotropes and Boron-Rich Solids, Invited Talk, WATOC 2017, University of Munich, Munich, 27 August – 1 September, 2017.

Nature Plays Dice with Boron: Inevitability of Uncertainties, Department of Chemistry, CalTech, Pasadena, 9, July 2018.

Nature Plays Dice with Boron: Inevitability of Uncertainties, Invited Lecture, International Conference on Chemical Bonding, Kauai, Hawai, 13-17, July 2018.

Periodic Table of Elements: Known, Unknown and the Novel – a personal selection, Invited Lecture, Ciclo De Conferencias- 2019-Año Internacional de la Tabla Periódica de los Elementos Madrid, 20, June, 2019.

Overlap of radial dangling orbitals controls the relative stabilities of polyhedral B_nH_{nx} isomers (n = 5 to 12, x = 0 to n-1), Keynote Lecture, International Conference on Boron Chemistry-II, Taiyuan, Shanxi, China, 14-17, July 2019.

MECP (Minimum Energy Crossing Point) barrier controls reductive coupling of isocyanides mediated by Cr-Cr quintuple bond: A DFT study, Invited Lecture, APATCC2019-International Conference of Asia Pacific Theoretical and Computational Chemists, Sydney, Australia, 30 Sept – 3 Oct, 2019.

A Structural Chemistry for Boron, Invited Lecture, University of Newcastle, New Southwales, Australia, 2 October 2019.

National:

A Journey through Three-Membered Rings, Symposium on Chemistry with Computers, IICT, Hyderabad, 18-19 Jan 2014.

Lectures on Electronic Structure and Reactions of Moleules at DST-SERB Winter School on Modeling Chemical and Biological Reactivity (MCBR 2014), IICT and IIIT Hyderabad, 20-23 Jan 2014.

Chemistry with Computers, in Recent Developments in Physical Chemistry, Academy workshop, St. Joseph's College, Irinjalakuda, 30 Jan- 1 Feb 2014.

Perspectives on the Structure, Bonding and Reactivity of Metallacyclocumulenes Department of Chemistry, National Institute of Technology, Calicut, 19 March, 2014.

A Structural Chemistry for Boron, University Frontier Lectures, University of Calicut, 20 March, 2014.

A Boron Fullerene Way To Elemental Boron, Chemical Society, Central College, Bangalore University, 28 March 2014.

Perspectives on the Structure, Bonding and Reactivity of Metallacyclocumulenes involving Cp_2M (M=Ti, Zr, Hf), XVI NOST Organic Chemistry Conference, Agra, 4-7, April 2014.

Perspectives on the Structure, Bonding and Reactivity of Metallacyclocumulenes involving Cp_2M (M=Ti, Zr, Hf), NIPER, Mohali, 23 May 2014.

Designing Boron Fullerenes: Role of Electron Counting Rules and Overlap-Matching, Advanced Materials: Current Trends and Future Prospects, Manali, Himachal Pradesh, 28 May – 1 June, 2014.

Computational Chemistry to Help Green Chemistry, in the National Seminar on Green Chemistry, St. Mary's College, Trichur, 24-25 July, 2014.

Perspectives on the Structure, Bonding and Reactivity of Metallacyclocumulenes, Seminar, Indian Institute of Science Education and Research Pune, 10, Nov 2014.
Designing Fullerene-like Boron Nanoclusters, Institute Colloquium, TIFR-Hyderabad, 18 Nov 2014.

The long and short of weak interactions, Theoretical Chemistry Symposium, (TCS2014), National Chemical Laboratory, Pune, 18-21, Dec 2014.

Negative Hyperconjugation and Red-, Blue- or Zero-Shift in X-Z---Y Complexes, Jyothish Joy, Eluvathingal D. Jemmis, Kaipanchery Vidya, Faraday Discussions-77, IISc, Bangalore, 12-14, Jan, 2015.

The Long and Short of Weak Interactions, Hebrew University of Jerusalem Israel – IISc Meeting on Chemical Sciences, Bangalore, March 22 to 24, 2015.
The Importance of Asking Questions, Institute Lecture, Indian Institute of Science Education and Research Bhopal, 30th March, 2015.

Hueckel's 4n+2, Wade's n+1 and mno Rules: 3-D Aromaticity and Chemistry of Boron, Goyal Prize Lecture, Kurukshetra University, 23rd April, 2015.

Importance of Early Questions in Science, DST INSPIRE Science Camp, Central College, Bangalore University, 23rd June 2015.

Evolution of Scientific Inquiry and Importance of Early Questions, Dr. S. R. Anantha Krishna Memorial Lecture, Bangalore Science Forum, The National College Campus, Bangalore 560004, 2nd July, 2015.

Reducing Strain Energy of Fullerenes and Stabilizing Boron Fullerenes, in the National Seminar on Recent Advances in Chemistry, Central University of Kerala, Kasaragodu, 3rd November, 2015.

Institute Colloquium, A structural chemistry for Boron: Boranes, b-Boron, Metal Borides, Boron-Fullerenes and nanotubes, Indian Institute of Science, Bangalore 560012, 12th November, 2015.

Professor Jose Mechery Memorial Lecture, A Structural Chemistry for Boron: Hückel 4n+2, Wade's n+1 and mno Rules, St. Thomas College, Trichure, 13th November 2015.

Lewis Electron Pair Bond, Octet Rule and Other Electron Counting Rules, Workshop on 100 Years of the Chemical Bond, New Chemistry Unit, JNCASR, Bangalore, 29th January, 2016.

Importance of Early Questions in Science, National Seminar on Recent Trends in Chemistry, Jyoti Nivas College Autonomous, Bangalore, 24th February, 2016.

Gilbert Newton Lewis, 2c-2e Bond, Multicentre Bonds, and Beyond, in 100 Years of the Chemical Bond, CSIR-IICT, CRSI, AND INSA, Hyderabad, 4-5 August, 2016.

E. D. Jemmis, Importance of Early Questions, Inaugural lecture, Indian Society for Technical Education-BIET Chapter, Bapuji Institute of Engineering & Technology Davangere-577004, 8th September, 2016.

E. D. Jemmis, Structure of Boron, in Emerging Trends in Analytical Chemistry (ETAC-2016) in association with Indian Society of Analytical Scientists (ISAS) Bangalore Chapter and Atomic and Minerals Division of DAE, Bangalore, 21-23 September 2016.

E. D. Jemmis, A Structural Chemistry for Boron: Borophene, Borospherene and Electron Counting Rules, Linus Pauling Lecture Award, Mahatma Gandhi University, Kottayam, 7th October, 2016.

E. D. Jemmis, Orbital Engineering in Chemistry, in the conference, Computational Modelling of Molecules and Materials, CM3-2016, The River View Retreat, Nainital, 20-22, October, 2016.

Qualitative Molecular Orbital Theory, in the Work shop on Computational Quantum Chemistry, Sacred Hearts College, Thevara, Kerala, 6th January, 2017

A Structural Chemistry for Boron: Borophene, Borospherene and Electron Counting Rules, in UGC sponsored national seminar, Recent Trends in Chemistry, Department of Chemistry, Vimala College, Trichur, Kerala, 9th January, 2017. Inevitability of Holes in Borophenes, Recent Advances in Many-Electron Theory (RAMET-2017), Goa, 10th February 2017.

Understanding Borophenes and Borospherenes, Modeling Chemical and Biochemical (Re)Activity-5 Conference, CLRI, Chennai, 18th Feb 2017.

On the Structure of Borophenes: Boron Equivalent of Graphene in National Seminar on Recent Advances in Chemical Sciences, Department of Chemistry, University College, Thiruvananthapuram, 13th March, 2017.

Boron, Borophenes and Borospherenes, New Chemistry Unit, JNCASR, Bangalore, 28th March, 2017.

Borophenes, Borospherenes, Boranes, 3D-Boron Allotropes and Boron-Rich Solids, Invited Talk, Department of Chemistry, IIT Madras, Chennai, 28th June, 2017.

Recent Developments in Boranes, and allotropes of Boron, Invited Talk at Department of Chemistry, IIT Kanpur, 11th September, 2017.

New Developments in Boranes, Borospherenes and Borophenes, Invited Lecture at the International Conference on Emerging Frontiers in Chemical Sciences, EFCS2017, Farook College, Calicut University, Kerala, 23-24, September, 2017.

Generalization of Structure and Bonding in [L]M(μ-CCR)$_2$M[L] and [L]M(μ-RC$_4$R)M[L] across the Periodic Table: Similarity of Main Group Compounds with Lanthanides and Transition Metal Compounds with Actinides, Indo-US Organometallic Chemistry workshop and Symposium, 7-9, December 2017.

A Weak Bond Route to Shorten the Ultrashort Sextuple Bond in Cr_2 and Mo_2, in Modern Trends in Inorganic Chemistry (MTIC)-XVII, Pune, 11-14, December 2017.

R. P. Mitra Memorial Lecture, Univerity of Delhi, Boranes, Borophenes, Brospherenes, and Boron, New Delhi, 12, January 2018.

Generalizations Across the Periodic Table: Chemistry of [L]M(μ-CCR)$_2$M[L] and [L]M(μ-RC$_4$R)M[L] - Similarity of Main Group Compounds with Lanthanides, and Transition Metals with Actinides, Current Trends in Chemistry (CTric2018) Cochin University of Science and Technology, 16-17, Feb 2018.

Hückel 4n+2, Wade's n+1 and mno Rules, Emerging Trends in Chemical Science, Dibrugarh University, Assam, 26-28, Feb 2018.

H-Bond and other Weak Interactions Across the Periodic Table of Elements, National Seminar on Chemistry, Kerala University, 11-12, October 2018.

Boron Plays Hide and Seek: Inevitability of Uncertainties, International Conference on Main-group Molecules to Materials (MMM-2018), IISc, Bangalore, 28-31, October 2018.

Nature Plays Dice with Boron: Inevitability of Uncertainties, HarishChandra Research Institute Colloquium, Allahabad, 5 November 2018.

Boron Plays Hide and Seek: Inevitability of Uncertainties, Department of Chemistry, Cotton University,19 Nov 2018.

Understanding numbers from Quantum Chemistry Computations, Three Lectures in the workshop on Quantum Chemistry, Department of Chemistry, Dibrugarh University, 20-21 November 2018.

Nature Plays Dice with Boron: Inevitability of Uncertainties, Workshop on Computational Science, Bangalore University, Bangalore, 30 November 2018.

Nature Plays Dice with Boron: Inevitability of Uncertainties, Symposium on New Frontiers in Chemical Science, IIT Bombay, Mumbai, 13-14 Dec 2018.

Beta-C-H Bond Activation Across the Transition Metals, International Conference on Organometallics and Catalysis, ICOC2018, Goa, 14-16, Dec 2018.

Hueckel 4n+2, Wade's n+1 and mno Rules in borophenes, beta- and tau-boron, International Conference on the Chemistry and Physics of Materials, St. Thomas College, Trichur, 19-21, Dec 2018.

Hückel 4n+2, Wade's n+1 and mno Rules in borophenes, beta- and tau-boron in the symposium Recent Trends in Chemical And Environmental Sciences, Punjabi University Patiala, 7-8 Feb 2019, also at Guru Nanak Dev University, Amritsar, 11 Feb 2019.

Nature Plays Dice with Boron: Inevitability of Uncertainties, Theoretical Chemistry Symposium-TCS 2019, Department of Chemistry, BITS PILANI,13-14 Feb 2019.

Novel Chemistry Inspired by the Periodic Table of Elements, DAE-BRNS Theme Meeting Commemorating "150 Glorious Years of Periodic Table" IYPT2019, BARC, 16, Feb 2019.

Nature Plays Dice with Boron: Inevitability of Uncertainties, International Conference on Advanced Chemical and Structural Biology, ICACSB-2019, PRIST University, 19-21 Feb 2019, Chennai.

Nature Plays Dice with Boron: Inevitability of Uncertainties, Invited Lecture at the symposium: Frontiers of Sciences (Past, Present & Future) – Physical, Chemical and Earth Sciences" Banaras Hindu University, 11th March, 2019, Varanasi.

Nature Plays Dice with Boron: Inevitability of Uncertainties, Seminar as Visiting Professor at Department of Chemistry, IIT Bombay, Mumbai, 11th April 2019.

Importance of Early Questions, Kerala State Higher Education Council-Faculty Development Program for Science Teachers – Philosophy of Science, M G University, Kottayam, 31 August 2019.

Borophenes: A new Material on the Block, DAE-CCS-2019 Computational Chemistry Symposium, 7-9, Nov 2019. Continuum in H-bond and other Weak Interactions (X-Z…Y):
Shift in X-Z stretch from Blue through Zero to Red.

Structural Chemistry of Polyhedral Boranes, BRICS WORKSHOP 2020 Frontiers in Inorganic Chemistry, Catalytical and Biomedical Applications, IISER Kolkata, 3 Jan 2020.

Continuum in H-bond and other Weak Interactions (X-Z…Y): Shift in X-Z stretch from Blue through Zero to Red, Conference on 100 years of Hydrogen Bonding, Indian Institute of Science, Bangalore, 9-10 January 2020.

Importance of Early Questions, Frontier Lecture Series, Dept. of Chemistry, University of Calicut, 13 Jan 2020.

Continuum in H-bond and other Weak Interactions (X-Z…Y): Shift in X-Z stretch from Blue through Zero to Red, "Functional Smart & Supramolecular Materials (FSSM-2020)", SPARC (MHRD) sponsored symposium, IIT Kharagpur, 29-30 Jan 2020.