

ASSESSMENT STATUS REPORT OF UTD

Name of the School: **School of Chemical Sciences**

Year of Report: **2012-2013**

Part A: The plan of action chalked out by the IQAC in the beginning of the year towards quality enhancement and the outcome achieved by the end of the year.

IQAC conceived of infusing further rigour in execution of all academic programmes so that students are encouraged to face challenges in emerging careers in chemical sciences. To meet this objective, brain storming sessions were held. It was decided to hold the expert lectures from time to time. Sound planning of the course work for Ph.D was undertaken and need based as well as effective syllabi of Research Methodology and Computer Applications were designed.

The outcome was encouraging and one student Ms.Sarabjot Kaur Makkad was able to achieve All India Rank 7th in the CSIR-UGC NET and was offered **Shyama Prasad Mukherjee (SPM) fellowship**. Besides, Ms.Pallavi Gupta has also qualified NET and obtained 13th rank.

Part B:

1.	Activities reflecting the goals and objectives of the institution	To explore new horizons of knowledge in chemical sciences and to blend it effectively in academic curricula for overall educational purpose. To fulfill these goals and objectives, we have undertaken following activities. <ul style="list-style-type: none">• Rigorous teaching with teaching aids.• Strong emphasis on research activities.• Encouragement to the students to undertake challenging assignments.• Seminar presentation by students.
2.	New academic programmes initiated	Ph.D. course work
3.	Innovations in curricular design and transaction	Emphasis on conceptual learning
4.	Inter-disciplinary programmes started	In all M.Sc. programmes interdisciplinary papers such as Mathematics for Chemists, Biology for Chemists, Computer Applications, Bioorganic Chemistry, Bioinorganic Chemistry and Environmental Chemistry have been included.
5.	Examination reforms implemented	Semester system is followed in its true spirit. Answer sheets are shown to the students after evaluation.

6.	Candidates qualified NET/SLET/GATE etc.	No of students selected through NET / GATE : NET = 03 ; GATE: 02 Mr.Pankaj Bariya (NET-2012) Ms.Sarabjot Kaur(NET-2013),AIR 7 th ,Awarded SPM fellowship Ms.Pallavi Gupta(NET-2013), AIR 13 th Mr.Pramod Gavel (GATE-2012) Mr.Kuber Singh Rawat(GATE-2012)
7.	Initiative towards faculty development programme	I) Dr. A. V. Bajaj participated in NME-ICT program (SAKSHAM) in association with Microsoft on June 10, 2013 to June 20, 2013. ii) Dr. Pratibha Sharma attended a Workshop at IIT, Indore on February 22-23, 2013. iii) Faculty members of the School are doing collaborative research with national institutes and various international universities.
8.	Total number of seminars / Lectures/workshops organized	School organized a lecture on March 4, 2013 on the occasion of National Safety Day in the department. Prof. R. M. Choukse delivered his lecture on "Safety Measures".
9.	Research projects a)Newly implemented: b)Completed:	See Annexure I Ongoing : 05 Completed: 06
10.	Patents generated if any	Nil
11.	New collaborative research programmes	See Annexure II
12.	Research grants received from various agencies	See Annexure I
13.	Details of research scholars	Students with fellowships : 04 Students without fellowship : 17
14.	Citation index of faculty members and impact factor	See list of publications of faculty members with impact factor. See Annexure III
15.	Honors/Awards to the faculty	<ul style="list-style-type: none"> Prof. Ashok Kumar (in Faculty category)and Mr. Pankaj Patidar (in Student Category) have been awarded by "Best Science Research Award of MPCST in 2012"
16.	Internal resources generated	Departmental Fees

17.	Details of departments getting SAP, COSIST (ASSIST) / DST.FIST, etc. assistance/recognition	Rs. 30 lakhs as FIST support from DST
18.	Community services	Faculty , students and non teaching staff participated in plantation activities
19.	Teachers and officers newly recruited	One (Contractual)
20.	Teaching-Non-teaching staff ratio	Ratio : 1:2 (11: 19)(as per sanctioned posts)
21.	Improvements in the library services	New books with latest titles have been added in the Library.
22.	New books/journals subscribed and their value	Procurement of various standard books has been done from time to time and facility of various International Journals has been provided for all faculty members and Research scholars through Science Direct.
23.	Courses in which student assessment of teachers is introduced and the action taken on student feedback	Student's feedback was analyzed. Overall rating of the faculty members was very good.
24.	Unit cost of education Unit Cost = Total annual expenditure budget (Actual) divided by the number of students enrolled	About Rs. 1.15 Lakh per student
25.	Computerization of administration and the process of admissions and examination results, issue of certificates	<ul style="list-style-type: none"> • All the results of the semester examination grade sheets are prepared on the computer. • All day to day letters, Dept profiles, data asked from the University are prepared on the computer.
26.	Increase in the infrastructural facilities	FTIR and UV-Vis spectrophotometer were optimally utilized .
27.	Technology up gradation	Networking facility through IT center has been provided to facilitate teaching and research.
28.	Computer and internet access and training to teachers and students	Yes
29.	Financial aid to students	Scholarship to SC/ST students is provided by state Government for M.Sc students.
30.	Activities and support from the Alumni Association	Alumni help the students to find opportunities of research and jobs.

31.	Activities and support from the Parent Teacher Association	Informal meetings with parent of students to help in career path identification.														
32.	Health services	Students are provided health centre facility by the University.														
33.	Performance in sports activities	Students participated in the sports activity organized by UTD sports association.														
34.	Incentives to outstanding Sports persons	None														
35.	Student achievements and awards	<ul style="list-style-type: none"> • Mr. Pankaj Patidar has been awarded by “Best Science Research Award of MPCST in 2012” • Mr. Sunil Patidar and Mr. Dileep Singh Sisodiya won the award in Quiz competition organized by MPCST in 2012. • Ms Sarabjot Kaur awarded prestigious Shyama Prasad Mukherjee (SPM) fellowship owing to her 7th All India Rank in NET Exam.2013 														
36.	Activities of the Guidance and Counseling unit	<p>Faculty members guide the students from time to time on various issues including research opportunities and preparation for NET/ GATE exam.</p> <p>Mentors have been appointed for a group of 20 students. Mentors are appointed to look after the students problems. Faculty members for different courses are as follows:</p> <table border="0"> <thead> <tr> <th>Mentor</th> <th>Course</th> </tr> </thead> <tbody> <tr> <td>Dr. A. V. Bajaj</td> <td>M. Sc. Chemistry (1st sem.)</td> </tr> <tr> <td>Dr. A. Kumar</td> <td>M. Sc. Appl.Chemistry (1st sem.)</td> </tr> <tr> <td>Dr. H.P.S. Chauhan</td> <td>M. Sc. Pharma.Cemistry (1st sem.)</td> </tr> <tr> <td>Dr. Pratibha Sharma</td> <td>M. Sc. Chemistry (3rd sem.)</td> </tr> <tr> <td>Dr. S. Khare</td> <td>M. Sc. Applied Chemistry (3rd sem.)</td> </tr> <tr> <td>Dr. Sheela Joshi</td> <td>M. Sc. Pharma.Chemistry (3rd sem.)</td> </tr> </tbody> </table>	Mentor	Course	Dr. A. V. Bajaj	M. Sc. Chemistry (1st sem.)	Dr. A. Kumar	M. Sc. Appl.Chemistry (1st sem.)	Dr. H.P.S. Chauhan	M. Sc. Pharma.Cemistry (1st sem.)	Dr. Pratibha Sharma	M. Sc. Chemistry (3rd sem.)	Dr. S. Khare	M. Sc. Applied Chemistry (3rd sem.)	Dr. Sheela Joshi	M. Sc. Pharma.Chemistry (3rd sem.)
Mentor	Course															
Dr. A. V. Bajaj	M. Sc. Chemistry (1st sem.)															
Dr. A. Kumar	M. Sc. Appl.Chemistry (1st sem.)															
Dr. H.P.S. Chauhan	M. Sc. Pharma.Cemistry (1st sem.)															
Dr. Pratibha Sharma	M. Sc. Chemistry (3rd sem.)															
Dr. S. Khare	M. Sc. Applied Chemistry (3rd sem.)															
Dr. Sheela Joshi	M. Sc. Pharma.Chemistry (3rd sem.)															
37.	Placement services provided to students	Faculty members guide the students for job opportunities in academic Institutions and Industries.														
38.	Development programmes for non-teaching staff	Informal guidance for upgradation of computer skills.														
39.	Healthy practices of the institution	<ul style="list-style-type: none"> • Regular and quality teaching • Active participation in research activity 														
40.	Linkages developed with National/International, Academic/Research bodies	See Annexure II														
41.	Any other relevant information the institution wishes to add	<p>School’s mission is to provide high quality education and training for high flying careers in Chemical Sciences. Our distinguishing features are:</p> <ul style="list-style-type: none"> • Theoretical and practical knowledge of Instrumental 														

		<p>Techniques.</p> <ul style="list-style-type: none"> • Interpretation of various types of spectra. Nuclear Magnetic Resonance (NMR) Electron Spin Resonance (ESR), Infrared (IR), Ultraviolet-Visible (UV-Visible), Mössbauer, Mass Spectrometry. • The strength of the School has been and continues to be excellence in research and teaching. • The faculty is extremely well qualified and motivated with a strong commitment to research.
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(PART – C)

Detail the plans of the institution for the next year:

Yearly plan: 2013 -2014

Curriculum

- It is planned to increase the diversity in spectral interpretation w.r.t. new examples and relevant patterns.
- It is planned to revise syllabus to meet contemporary requirements. Restructuring of the curriculum will be done with a focus to introduce Physicoorganic Chemistry and Nanomaterial Chemistry in the M.Sc. course and LASER chemistry in Ph.D course work syllabi.
- To develop prudent approach in the students taking NET and similar quality oriented competitive examinations

Strategies of Teaching Learning

- Use of teaching aids to be encouraged and novel methods of learning such as quiz to be adopted as and when applicable.
- Students will be encouraged to develop their soft skills and communication skills.

Student Feedback System Design

Students' feedback about the School, faculty members and the curriculum would be practiced as per IQAC design.

Collection of Feedback and its Analysis: Format of Analysis

Feedback will be collected by Dec 2013 and May 2014 and will be analyzed by faculty members. The overall report will be prepared and necessary improvements will be done for coming year.

Improvement Plan**Infrastructure**

New building for School of Chemical Sciences needs to be constructed on high priority basis.

Research Activities and Promotion

- Faculty members would be encouraged to participate in seminars and conferences
- Collaborative research activities will be promoted.

**Name and Signature of the
Coordinator QAC**

**Name and Signature of the
HEAD**

Annexure I

Details of research grant received from different agencies during the last five years: 2008-2013

Name of the Investigator	Title of the project and duration	Status	Amount sanctioned	Funding agency
Dr. R. Prasad	Surface and catalytic studies of nanocrystalline and nanoporous metal oxides.	Completed	Rs.3,06,000/-	CSR-UGC-DAE
	Studies of few catalytic vapour phase alkylation and cyclization reactions.	Completed	Rs. 7,64,800/-	UGC, New Delhi
Dr. Ashok Kumar	Synergistic extraction and spectrophotometric determination of toxic metal ions and lanthanides at trace level by chromogenic substituted calix(n) arenes.	Completed	Rs. 10,46,000/-	CSIR, New Delhi
	Synergistic extraction and stripping voltammetric determination of toxic metal ions and lanthanides at trace level.	Completed	Rs. 17,00,000/-	DST, New Delhi
Dr.H.P.S. Chauhan	Synthetic, Spectroscopic, Thermal and Biochemical Studies on some Group 14 (Si, Ge and Sn) and Group 15 (As, Sb and Bi) Metal and Organometallic Complexes with some sulphur and/or Oxygen Donor Organic Ligands.	Completed	Rs.4,11,100/-	UGC, New Delhi
Dr.Pratibha Sharma	Design, Synthesis, Electrochemical Studies and Evaluation of Therapeutic Potential of Purines and Benzimidazoles Through Quantitative Structure - Activity Relationship	Completed	Rs.17,20,000/-	DRDO,New Delhi
Dr. R. Prasad	Quantum Mechanical and Molecular Mechanics Computation of few molecules, Reactions and	Ongoing	Rs. 4,94,000/-	MPCST, Bhopal

	Nano materials.			
Dr.H.P.S. Chauhan	Group 15 Metal and Organometallic Derivatives with Mixed Sulphur and/or Oxygen Donor Ligands: Synthesis and Characterization: Thermal and Biochemical Studies	Ongoing	Rs. 8,04,800/-	UGC, New Delhi
Dr.H.P.S. Chauhan	Studies on the synthesis and characterization of some group 15 Metal nano complexes with Sulfur donor ligands.	Ongoing	Rs. 7,83,000/-	MPCST, Bhopal.
Dr. KK Pandey	Structure and bonding analysis of ylidine complexes Ln-M≡E-R (M=Cr, Mo, W; E=Si, Ge, Sn, Pb; R=Cp, MeS): A DFT study	Ongoing	Rs. 5,95,000/-	CSIR, UGC
Dr. Ashok Kumar	Efficient Construction of Novel Triazole as Potential Therapeutics : A Classical Versus Click Chemistry Approach	Ongoing	Rs. 44,84,000/-	DRDO ,New Delhi

International Collaboration of the Professors:

Dr. K.K. Pandey

Collaborative Research work with European and American Scientists

- (1) Prof. G. Frenking
Faculty of Chemistry,
University of Marburg,
Germany
- (2) Prof. Phillip P. Power
Department of Chemistry
University of California Davis
USA
- (3) Prof. Agusti Lledos
Department of Chemistry,
University of Autonomia Barcelona, Spain
- (4) Prof. F. Maserus
Institute of Chemical Research of Catalonia (ICIQ),
Tarragona, Spain
- (5) Dr. D. G. Musaev
Director
Emerson Centre for Scientific Computation,
Emory University, USA
- (6) Prof. D. C. Liotta
Editor: J. Medicine Chem. Letters (American Chemical Society, USA)
Department of Chemistry,
Emory University, USA
- (7) Prof. Simon Aldridge
Department of Chemistry,
Oxford University, UK
- (8) Prof. Holger Braunschweig
Department of Chemistry,
University of Wurzburg, Germany

(9) Prof. Cameron Jones
School of Chemistry
Monash University, Australia

Annexure III

SCHOOL OF CHEMICAL SCIENCES DEVI AHILYA UNIVERSITY INDORE

List of Publications with Impact factors (2008-2013):

No. of Publication during 2008-13 in international journals = 104.

1. Stretched σ -borane complexes of rhodium: A theoretical study
K.K. Pandey
Inorg. Chem. Commun. 11 (2008) 288
Impact Factor: 1.972
2. σ -Borane complexes of nickel, palladium and platinum. A theoretical study
K.K. Pandey
J. Mol. Struct. (THEOCHEM) 855 (2008) 18
Impact Factor: 1.288
3. Mixed-ligand Ru(II) complexes with 2,2'-bipyridine and tetradentate Schiff bases ligands: Synthesis, physico-chemical study, DFT analysis, electrochemical and Na binding properties
L. Mishra, R. Prajapati, K.K. Pandey
Spectrochimica Acta (A): Molecular and Bimolecular Spectroscopy 70 (2008) 79-85.
Impact Factor: 1.952
4. Transition Metal sigma-borane complexes
K.K. Pandey
Coord. Chem. Revs. 253 (2009) 37
Impact Factor: 12.110
5. Linear M \equiv E-Me Versus Bent M-E-Me: Bonding Analysis in Heavier Metal-ylidyne Complexes [(Cp)(CO)₂M \equiv EMe] and Metallo-ylidenes [(Cp)(CO)₃M-EMe] (M = Cr, Mo, W; E = Si, Ge, Sn, Pb)
Krishna K. Pandey and Agustí Lledós
Inorg. Chem. 48 (2009) 2748-2759.
Impact Factor: 4.601
6. The Nature of M-B Versus M=B Bonds in Cationic Terminal Borylene Complexes: Structure and Energy Analysis in the Borylene Complexes [(η^5 -C₅H₅)(CO)₂M{B(η^5 -C₅Me₅)}}]⁺, [(η^5 -C₅H₅)(CO)₂M(BMes)]⁺, and [(η^5 -C₅H₅)(CO)₂M(BNMe₂)]⁺ (M = Fe, Ru, Os)

Krishna K. Pandey, Agusti Lledos and Feliu Maseras
Organometallics 28 (2009) 6442-6449.
Impact Factor: 3.963

7. Structure and Bonding Energy Analysis of Cobalt, Rhodium and Iridium Borylene Complexes $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})\text{M}(\text{BNX}_2)]$ ($\text{X} = \text{Me}, \text{SiH}_3, \text{SiMe}_3$) and $[(\eta^5\text{-C}_5\text{H}_5)(\text{PMe}_3)\text{M}\{\text{BN}(\text{SiH}_3)_2\}]$ ($\text{M} = \text{Co}, \text{Rh}, \text{Ir}$)
Krishna K. Pandey and Djamaladdin G. Musaev
Organometallics 29 (2010) 142-148.
Impact Factor: 3.963
8. Linear versus bent bonding in metal-phosphinidene complexes: Theoretical studies of the electrophilic phosphinidene complexes $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{M}(\text{PMe})]^+$, $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_3\text{M}(\text{PMe})]^+$ ($\text{M} = \text{Cr}, \text{Mo}, \text{W}$)
Krishna K. Pandey and Agusti Lledos
J. Organomet. Chem. 695 (2010) 206-214.
Impact Factor: 2.384
9. Computational Studies of Transition Metal Selectivity of Octapeptide Repeat Region of Prion Protein (PrP)
Krishna K. Pandey, James P. Snyder, Dennis C. Liotta and Djamaladdin G. Musaev
J. Phys. Chem. A 114 (2010) 1127-1135.
Impact Factor: 2.946
10. New ruthenium(II) thiolato complexes: Synthesis, reactivity, spectral, structural and DFT studies
Sudhakar D. Dwivedi, Santosh K. Dubey, Ashish K. Singh, Krishna K. Pandey and Daya S. Pandey
Inorg. Chim. Acta 363 (2010) 2095-2103.
Impact Factor: 1.846
11. Structure and Bonding Energy Analysis of M-Ga Bonds in Dihalogallyl Complexes $\text{Trans-}[\text{X}(\text{PMe}_3)_2\text{M}(\text{GaX}_2)]$ ($\text{M} = \text{Ni}, \text{Pd}, \text{Pt}; \text{X} = \text{Cl}, \text{Br}, \text{I}$)
Krishna K. Pandey, Pankaj Patidar, Holger Braunschweig
Inorg. Chem. 49 (2010) 6994-7000.
Impact Factor: 4.601
12. Nature of M-Ga Bonds in Dihalogallyl Complexes $(\eta^5\text{-C}_5\text{H}_5)(\text{Me}_3\text{P})_2\text{M}(\text{GaX}_2)$ ($\text{M} = \text{Fe}, \text{Ru}, \text{Os}$) and $(\eta^5\text{-C}_5\text{H}_5)(\text{OC})_2\text{M}(\text{GaX}_2)$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}$): A DFT Study
Krishna K. Pandey, Pankaj Patidar, Simon Aldridge
J. Phys. Chem. A 114, 2010, 12099-12105.
Impact Factor: 2.946
13. Nature of Bonding in Terminal Borylene, Alkyene and Gallylene complexes of Vanadium and Niobium $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_3\text{M}(\text{ENR}_2)]$ ($\text{M} = \text{V}, \text{Nb}; \text{E} = \text{B}, \text{Al}, \text{Ga}; \text{R} = \text{CH}_3, \text{SiH}_3, \text{CMe}_3, \text{SiMe}_3$): A DFT Study
Krishna K. Pandey, Holger Braunschweig, Agusti Lledós

Inorg. Chem. 50 (2011) 1402-1410.
Impact Factor: 4.601

14. DFT Study on the Alkylborylene and Haloborylene Complexes of Manganese and Rhenium: Structure and Bonding Energy Analysis in $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{M}(\text{BR})]$ and $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{M}(\text{BX})]$ (M = Mn, Re; R = Me, Et, iPr, tBu; X = F, Cl, Br, I)
Krishna K. Pandey, Holger Braunschweig, Rian D. Dewhurst
Eur. J. Inorg. Chem. 2011, 2045-2056
Impact Factor: 3.049
15. Unexpected Generation of Diastereomers by Double Diboration of a Dialkyne
F. Bauer, H. Braunschweig, K. Groß, Christoph Lambert, Krishna K. Pandey, K. Radacki, D. Reitzenstein
Chem.Eur.J.17(2011)5230-5233.
Impact Factor: 5.925
16. Nature of M-Ga Bonds in Cationic Metal-Gallylene Complexes of Iron, Ruthenium and Osmium $[(\eta^5\text{-C}_5\text{H}_5)(\text{L})_2\text{M}(\text{GaX})]^+$. A Theoretical Study
Krishna K. Pandey, Simon Aldridge
Inorg. Chem. 50 (2011) 1798-1807.
Impact Factor: 4.601
17. Nature of M-Bi bonds in dihalobismuth complexes of nickel, palladium and platinum $\text{trans-}[X(\text{PMe}_3)\text{M}(\text{BiX}_2)]$ (M = Ni, Pd, Pt; X = Cl, Br, I)
Krishna K. Pandey
Comput. Theoret. Chem. 967 (2011) 140-146.
Impact Factor: 1.288
18. Nature of M-E bonds in metallocylenes, germylenes, stannylenes and plumbylens $[(\eta^5\text{-C}_5\text{H}_5)(\text{Me}_3\text{P})(\text{H})_2\text{M}(\text{EPh})]$ (M = Fe, Ru, Os; E = Si, Ge, Sn, Pb)
Krishna K. Pandey, Philip P. Power
Organometallics 30 (2011) 3353-3361
Impact Factor: 3.963
19. Structure and bonding energy analysis of cationic metal-alkyne complexes of molybdenum and tungsten $[(\text{MeCN})(\text{PMe}_3)_4\text{M}\equiv\text{EMes}]^+$ (M = Mo, W; E = Si, Ge, Sn, Pb): A Theoretical Study
Krishna K. Pandey, Pankaj Patidar, Philip P. Power
Inorg. Chem. 50 (2011) 7080-7089. Impact Factor: 4.601
20. Structure and bonding analysis of dimethylgallyl complexes of iron, ruthenium and osmium $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{M}(\text{GaMe}_2)]$ and $[(\eta^5\text{-C}_5\text{H}_5)(\text{Me}_3\text{P})_2\text{M}(\text{GaMe}_2)]$
Krishna K. Pandey
J. Phys. Chem. A 115 (2011) 8578-8585.
Impact Factor: 2.946
21. Structure and bonding in haloarylallyl complexes of iron, ruthenium and osmium

- $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{M}\{\text{Ga}(\text{X})(\text{Ph})\}]$: A theoretical study
Krishna K. Pandey, Pankaj Patidar
J. Organomet. Chem. 696 (2011) 3536-3542.
Impact Factor: 2.384
22. Bis(borylene) Complexes of Cobalt, Rhodium, and Iridium $[(\eta^5\text{-C}_5\text{H}_5)\text{M}(\text{BNX}_2)_2]$
(X = Me, SiH₃, SiMe₃): A Bonding Analysis
Krishna K. Pandey
Organometallics 30 (2011) 5851- 5858
Impact Factor: 3.963
23. Structure and bonding analysis of dihalogallyl and dimethylgallyl complexes of molybdenum and tungsten $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_3\text{M}(\text{GaX}_2)]$ (M = Mo, W; X = Cl, Br, I, Me): A Theoretical Study
Krishna K. Pandey
Comput. Theoret. Chem. 973 (2011) 13-19.
Impact Factor: 1.288
24. The nature of M-Ga in metal(I) gallyl complexes of copper, silver and gold: A Theoretical study
Krishna K. Pandey
J. Organomet. Chem. 701 (2012) 75-79
Impact Factor: 2.384
25. Theoretical investigation of M≡E bonds in transition metaleylidyne complexes trans- $[\text{H}(\text{PMe}_3)_4\text{M}\equiv\text{ER}]$ (M = Mo, W; E = Si, Ge, Sn, Pb; R = Mes, Xylyl)
Krishna K. Pandey, Pankaj Patidar
J. Organomet. Chem. 702 (2012) 59-66
Impact Factor: 2.384
26. Structure and bonding analysis in dihalobismuth complexes of iron, ruthenium and osmium $[(\eta^5\text{-C}_5\text{H}_5)(\text{CO})_2\text{M}(\text{BiX}_2)]$: A theoretical Study
Krishna K. Pandey, Pankaj Patidar, Pradeep Tiwari
Polyhedron 34 (2012) 84-91.
Impact Factor: 2.057
27. What is the best bonding model of the (σ-H-BR) species bound to a transition metal: Bonding analysis in complexes $[(\text{H})_2\text{Cl}(\text{PMe}_3)_2\text{M}(\sigma\text{-H-BR})]$ (M = Fe, Ru, Os)
Krishna K. Pandey
Dalton Trans. 41 (2012) 3278-3286.
Impact Factor: 3.840
28. Structure and bonding analysis of dimethylgallyl complexes of cobalt, rhodium and Iridium $[\text{Me}(\text{PMe}_3)_2(\text{Me}_3\text{GaCl})\text{M}(\text{GaMe}_2)]$ (M = Co, Rh, Ir) and $[\text{Me}(\text{PMe}_3)_2\text{ClIr}(\text{GaMe}_2)]$: A theoretical study
Krishna K. Pandey
J. Organomet. Chem. 710 (2012) 6-11.
Impact Factor: 2.384
29. Theoretical investigation of triple bond in molybdenum complexes trans-

[X(PMe₃)₄Mo≡E(Mes)] (X = F, Cl, Br, I; E = Si, Ge, Sn, Pb): A DFT study
Krishna K. Pandey, Pankaj Patidar
Polyhedron 37 (2012) 85-93.
Impact Factor: 2.057

30. A theoretical study of the bonding and charge distribution in cationic group 8 metal borylene and alkyne complexes: Consequences for complex stability and reactivity
Krishna K. Pandey
Polyhedron, 43 (2012) 131-139.
Impact Factor: 2.057
31. The Nature of Mo≡E Bonds: Structure and Bonding Analysis of the Molybdenum-Ylidyne Complexes Trans-[X(dmpe)₂Mo≡E(η¹-C₅H₅)] (E = Si, Ge, Sn, Pb; X = H, Cl, Br, I, CN)
Krishna K. Pandey, Pankaj Patidar, Alexander C. Filippou
Inorg. Chem. 2012 Accepted.
Impact Factor: 4.601
32. Bonding energy analysis in cationic borylene complexes of palladium and platinum: A theoretical study
Krishna. K. Pandey
Polyhedron 52 (2013) 1431-1439.
Impact Factor: 2.057
33. Nature of M-(η²-H-SiR₂) in chromium, molybdenum and tungsten complexes [(η²-C₅H₅)(dmpe)M(η²-H-SiR₂)] and [(η²-C₅H₅)(CO)₂M(η²-H-SiR₂)]: A theoretical study
Krishna K. Pandey
Polyhedron 55(2013) 241-248
Impact Factor: 2.057
34. Nature of M-Ge Bonds in the Metallogermylene Complexes of Chromium, Molybdenum, and Tungsten [(η⁵-C₅H₅)(CO)₃M{GeN(SiMe₃)R}] and [(η⁵-C₅H₅)(CO)₃M{GeN(Ph)R}] (R = Ph, Mesityl (Mes)): A Theoretical Study
Krishna K. Pandey and Cameron Jones
Organometallics 32 (2013) 3395-3403
Impact Factor: 3.963
35. Bonding analysis of the neutral electrophilic phosphinidene complexes of vanadium and niobium [(η⁵-C₅H₅)(CO)₃M(PNR₂)] (R = Me, ⁱPr, ^tBu): A DFT study
Krishna K. Pandey, Pradeep Tiwari, Pankaj Patidar
J. Organomet. Chem. 740 (2013) 135-140.
Impact Factor: 2.384
36. Accurate theoretical description of the M-PNR₂ bonds in phosphinidene complexes of manganese and rhenium [(CO)₅M-PNR₂]⁺ (R = Me, ⁱPr, ^tBu) and [(PMe₃)(CO)₄M-PNⁱPr₂]⁺: A DFT-D3 study

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