

## CONTENTS

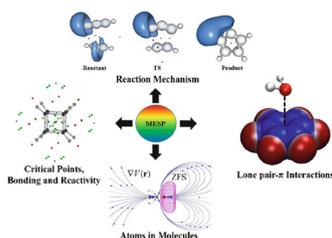
### Special Issue on CHEMICAL BONDING

Guest Editors: Eluvathingal D. Jemmis, Elangannan Arunan and V. Subramanian

### One hundred years of Lewis Chemical Bond!

E Arunan, E D Jemmis and V Subramanian . . . . . 1517–1518

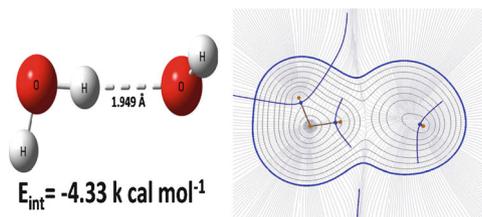
### Perspective Articles



### Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules

Shridhar R Gadre and Anmol Kumar . . . . . 1519–1526

This perspective highlights the topographical analysis of molecular electrostatic potential (MESP) as a tool for understanding the bonding and reactivity patterns of molecules. It shows how the phenomena/concepts such as lone pairs,  $\pi$ -delocalization, arrows in reaction mechanism and atoms in molecules, etc., are brought out in a transparent way through the MESP topography mapping.

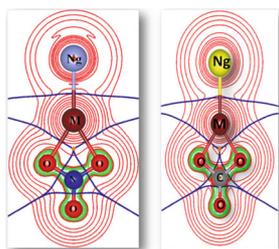


### Bader's Theory of Atoms in Molecules (AIM) and its Applications to Chemical Bonding

P Shyam Vinod Kumar, V Raghavendra and V Subramanian . . . . . 1527–1536

In this perspective article, the basic theory and applications of the “Quantum Theory of Atoms in Molecules” have been presented with examples from different categories of weak and hydrogen bonded molecular systems.

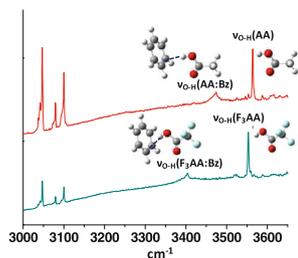
### Regular Articles



### A computational study on structure, stability and bonding in Noble Gas bound metal Nitrates, Sulfates and Carbonates (Metal = Cu, Ag, Au)

Manas Ghara, Sudip Pan, Jyotirmoy Deb, Anand Kumara, Utpal Sarkar and Pratim Kumar Chattaraj . . . . . 1537–1548

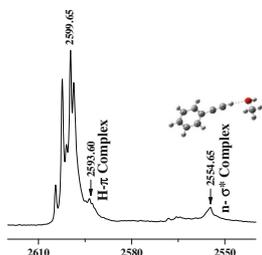
Different nitrates, sulfates and carbonates of noble metals (M = Cu, Ag, Au) can bind noble gas (Ng) atoms quite effectively. The M-Ng bonds in these compounds are found to be partially covalent in nature.



### Matrix isolation infrared spectra of O-H ··· $\pi$ Hydrogen bonded complexes of Acetic acid and Trifluoroacetic acid with Benzene

Pujarini Banerjee, Indrani Bhattacharya and Tapas Chakraborty . . . . . 1549–1555

The spectral red-shifts of the probe  $\nu_{\text{O-H}}$  bands of carboxylic acid-benzene  $\pi$ -hydrogen bonded complexes in an argon matrix were found to correlate with their respective aqueous phase acidities ( $\text{p}K_{\text{a}}$ ), and are explained in terms of local charge transfer effects.

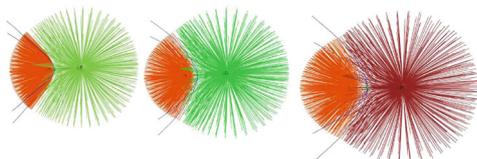


### The elusive $\equiv\text{C-H}\cdots\text{O}$ complex in the hydrogen bonded systems of Phenylacetylene: A Matrix Isolation Infrared and *Ab Initio* Study

Ginny Karir, Mariyam Fatima and K S Viswanathan . . . . 1557–1569

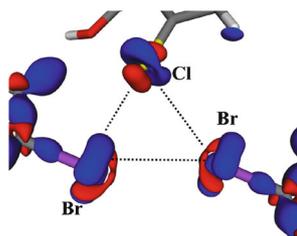
The  $\equiv\text{C-H}\cdots\text{O}$  hydrogen bonded complex in phenylacetylene-methanol system, which is a  $n\text{-}\sigma^*$  interaction and a local minimum was observed in a cryogenic inert gas solid. This  $n\text{-}\sigma^*$  local minima had eluded observation in gas phase studies.

### Why are Hydrogen Bonds Directional?



Abhishek Shahi and Elangannan Arunan . . . . . 1571–1577

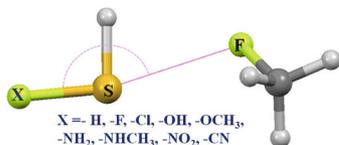
Atomic basins, calculated using AIM theory, of HF/HCl/HBr show that an acceptor atom A has to approach at  $\text{A-H-X} > 110$  for forming a hydrogen bond with HX. This provides a rationale for setting a limit on the hydrogen bond angle, which has been an empirical practice so far.



### Analysis of an unusual hetero-halogen bonded trimer using charge density analysis: A case of concerted type I $\text{Br}\cdots\text{Br}$ and type II $\text{Br}\cdots\text{Cl}$ interactions

Mysore S Pavan and Tayur N Guru Row . . . . . 1579–1587

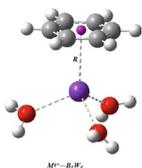
An unusual triangular motif consisting of a hitherto uncharacterized Type I  $\text{Br}\cdots\text{Br}$  contact along with two Type II  $\text{Br}\cdots\text{Cl}$  interactions as edges of the triangle is seen in the crystal structure of 4-bromo-2-chlorobenzoic acid. The nature of such bonding is analyzed based on both experimental and theoretical charge density followed by topological analysis.



### Understanding the effect of substitution on the formation of $\text{S}\cdots\text{F}$ chalcogen bond

Rahul Shukla and Deepak Chopra . . . . . 1589–1596

The aim of this study is to understand the effect of substitution on the nature and characteristics of  $\text{S}\cdots\text{F}$  chalcogen bonds.



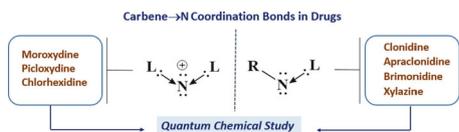
### The Effect of Hydration on the Cation- $\pi$ Interaction Between Benzene and Various Cations

Vikash Dhindhwal and N Sathyamurthy . . . . . 1597–1606

The effect of hydration on cation- $\pi$  interaction in  $\text{M}^q + \text{B}_m \text{W}_n$  ( $\text{B}$  = benzene;  $\text{W}$  = water;  $\text{M}^q = \text{Na}^+, \text{K}^+, \text{Mg}^{2+}, \text{Ca}^{2+}, \text{Al}^{3+}$ ,  $0 \leq n$ ;  $m \leq 4$ ,  $1 \leq m + n \leq 4$ ) complexes has been investigated using *ab initio* quantum chemical methods. Interaction energy values computed at the MP2 level of theory using the 6-31G(d,p) basis set reveal a qualitative trend in the relative affinity of different cations for benzene and water in these complexes. The  $\pi$ -cloud thickness values for benzene have also been estimated for these systems.

**Carbene→N<sup>+</sup> Coordination Bonds in Drugs: A Quantum Chemical Study**

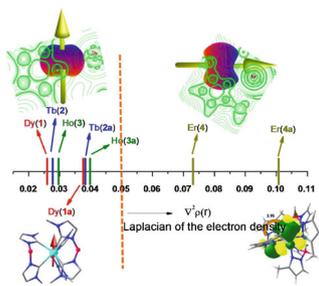
Deepika Kathuria, Minhajul Arfeen, Apoorva A Bankar and Prasad V Bharatam. . . . . 1607–1614



Evaluation of electron localization function (ELF), molecular orbitals, charge density, nucleophilicity, proton affinity and complexation energy estimation confirm the presence of coordination bonds (L→N←L)<sup>⊕</sup> in the drug molecules like picloxydine, chlorhexidine and moroxydine in their cationic state. Further, electronic structure analysis of drugs like clonidine, apraclonidine, brimonidine and xylazine indicated the presence of electronic structure similar to L→N-R systems.

**Role of Lanthanide-Ligand bonding in the magnetization relaxation of mononuclear single-ion magnets: A case study on Pyrazole and Carbene ligated Ln<sup>III</sup> (Ln=Tb, Dy, Ho, Er) complexes**

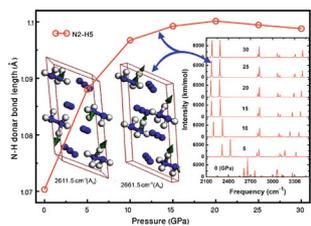
Tulika Gupta, Gunasekaran Velmurugan, Thayalan Rajeshkumar and Gopalan Rajaraman . . . . . 1615–1630



Calculations were carried out on a series on Ln(Bc<sup>Me</sup>)<sub>3</sub> and Ln(Bp<sup>Me</sup>)<sub>3</sub> (Ln = Tb, Dy, Ho, Er) complexes to ascertain the anisotropic variations of two ligand field environments and the influence of Lanthanide-ligand bonding on the magnetic anisotropy. Using the Laplacian density, we are able to quantify the prolate and oblate nature of the electron clouds in lanthanides.

**Structural, vibrational and bonding properties of hydro-nitrogen solids under high pressure: An *ab-initio* study**

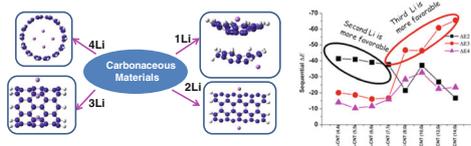
G Vaitheeswaran, N Yedukondalu and B Moses Abraham . . . . . 1631–1639



Structural, equation of state, and vibrational properties of Tetramethyl Ammonium Azide and HydroZonium Azide were calculated using van der Waals density functional theory calculations and their implications are discussed to explore the stability and hydrogen bonding.

**Anomalous Lithium Adsorption Propensity of Monolayer Carbonaceous Materials: A Density Functional Study**

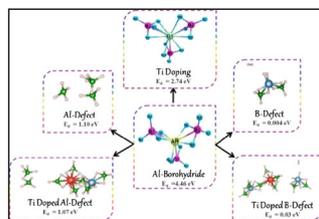
Swati Panigrahi, Deivasigamani Umadevi and G Narahari Sastry. . . . . 1641–1649



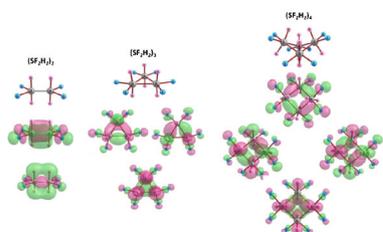
An exhaustive analysis has been carried out to study the lithium adsorption on the carbonaceous materials such as corannulene, sumanene and CNT. Our study provides in depth understanding on the adsorption of Li on buckybowls and carbon nanotubes with various size, dimension and chirality.

**Role of Ti doping and Al and B vacancies in the dehydrogenation of Al(BH<sub>4</sub>)<sub>3</sub>**

Indrani Choudhuri, Arup Mahata, Kuber Singh Rawat and Biswarup Pathak . . . . . 1651–1662



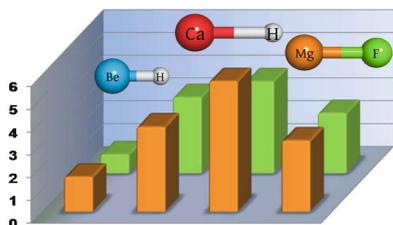
The H<sub>2</sub> molecular dehydrogenation (E<sub>d</sub>) energies are presented for Ti-doped Al(BH<sub>4</sub>)<sub>3</sub>, and systems with Al/B-defects in Ti-doped and Al(BH<sub>4</sub>)<sub>3</sub>.



### Computational design of Oligo-sulfuranes

Chakkingal P Priyakumari and Eluvathingal D Jemmis . . . 1663–1669

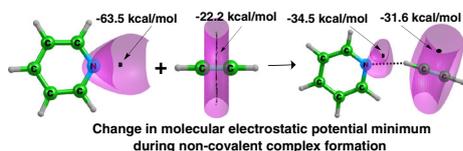
$\text{SF}_2\text{H}_2$  with equatorial F atoms is isolobal to  $\text{CH}_2$  and forms the oligomers  $(\text{SF}_2\text{H}_2)_2$ ,  $(\text{SF}_2\text{H}_2)_3$ , and  $(\text{SF}_2\text{H}_2)_4$  analogous to ethylene, cyclopropane and cyclobutane, respectively. The skeletal S-S bonds are formed by the overlap of antibonding fragment orbitals of  $\text{SF}_2\text{H}_2$ .



### Calculation of hyperfine structure constants of small molecules using Z-vector method in the relativistic coupled-cluster framework

Sudip Sasmal, Kaushik Talukdar, Malaya K Nayak, Nayana Vaval and Sourav Pal. . . . . 1671–1675

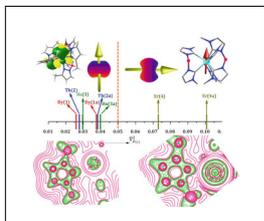
Magnetic hyperfine structure constants of some small molecules are calculated using Z-vector method in the relativistic coupled-cluster framework. The comparison with the reported extended coupled-cluster results reveals that Z-vector method can produce more accurate wavefunction in the near nuclear region than the extended coupled-cluster method.



### Molecular electrostatic potential analysis of non-covalent complexes

Padinjare Veetil Bijina and Cherumuttathu H Suresh. . . . . 1677–1686

The change in electron distribution during the formation of non-covalent complexes by hydrogen, dihydrogen, lithium, tetrel, chalcogen, pnicogen and halogen bonding has been analyzed on the basis molecular electrostatic potential (MESP) features of the complex and monomers; a strong linear correlation between MESP parameter and interaction energy is obtained.



Cover picture: Controlling Magnetic-Anisotropy in Lanthanides using Agostic interactions. For details, see the paper by Tulika Gupta *et al.* (1615–1630)