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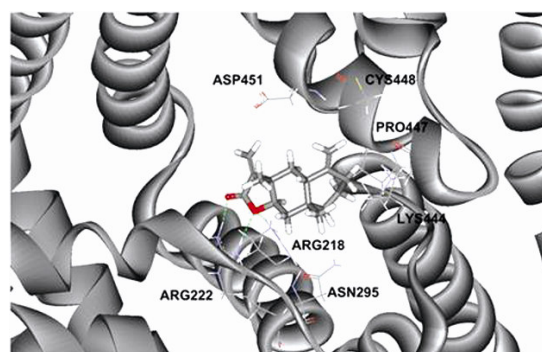
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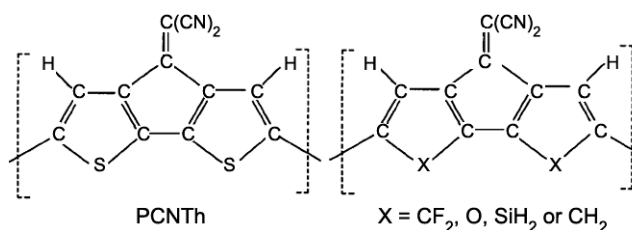
CONTENTS

- 1547 Studies on the binding of isosalantolactone to human serum albumin by molecular spectroscopy and modeling** Molecular modeling shows that hydrophobic interactions and hydrogen bonds play a major role in binding of isosalantolactone to human serum albumin.



Yang Sun, Chun-Mei Hu, Guo-Bo Li,
Sheng-Yong Yang, Lu-Sha Liu, Chun-Lei Tan,
Song Wei, Xiao-Yun Hu, Ying-Yong Zhao*
& Jun Fan*

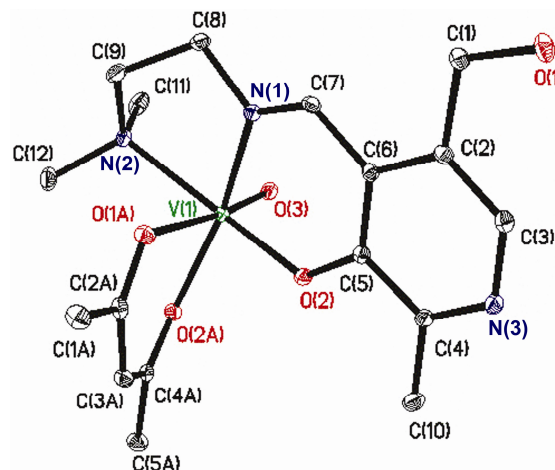
- 1555 Designing novel donor-acceptor copolymers using genetic algorithm** Genetic algorithm has been used for designing novel binary copolymers based on donor and acceptor polymers, with a common thiophene-based copolymer. Copolymers containing lower concentration of the thiophene copolymer have better intrinsic as well as extrinsic conductivity.



Vinita Arora & A K Bakhshi*

- 1562** Synthesis, characterisation and catalytic activities of vanadium complexes containing ONN donor ligand (E)-4-[(2-(dimethylamino)ethylimino) methyl-5-(hydroxymethyl)-2-methylpyridin-3-ol

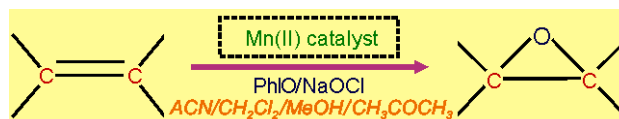
Dioxidovanadium(V) complex encapsulated in the cavity of zeolite-Y is an effective catalyst for the oxidation of styrene, cyclohexene, methyl phenyl sulfide and diphenyl sulfide.



Mannar R Maurya*, Manisha Bisht & Fernando Avecilla

- 1574** Epoxidation of olefins catalyzed by manganese(II) complexes of Schiff base ligand having N_2O coordination sphere

The catalytic efficiency of mononuclear manganese(II) complexes having two N_2O coordination spheres for epoxidation of (*E*)-stilbene and styrene using PhIO and NaOCl as terminal oxidants are influenced not only by their structural features, but also by the nature of terminal oxidant, substrate as well as the solvents. Epoxidation proceeds with the formation of two different intermediates, $O=Mn(IV)(L)(X)$ and $Cl-O-Mn(II)(L)(X)$ [$X=NO_3/SCN/N(CN)_2$], in the presence of PhIO and NaOCl respectively.

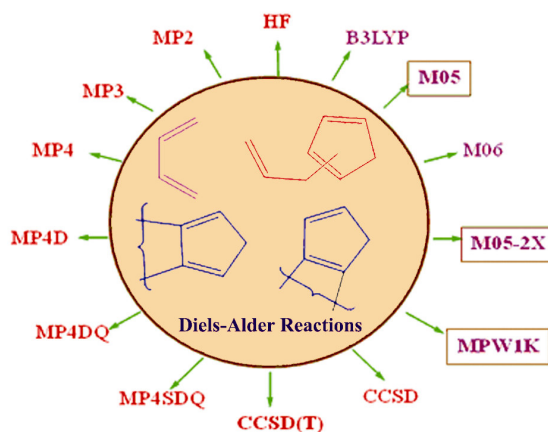


Averi Guha & Debasis Das*

Notes

1579 Performance of *ab initio* and DFT methods in modeling Diels-Alder reactions

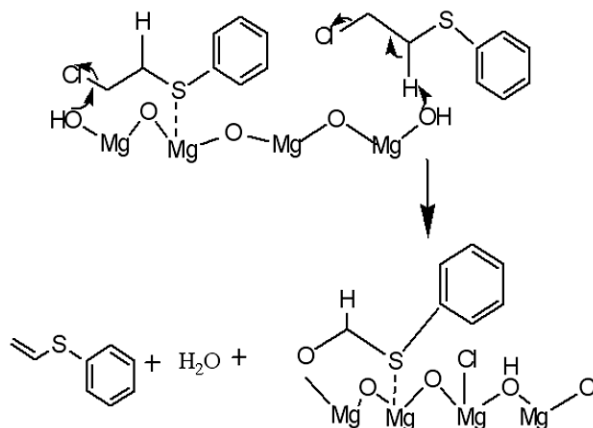
The new DFT functionals, viz., M05, M05-2X and MPW1K appear to be well suited to model Diels-Alder reactions for acyclic, cyclic and annelated dienes respectively.



Gaddamanugu Gayatri

1587 Synthesis of nano-MgO and identification of the destructive product of its reaction with 2-chloroethyl phenyl sulfide

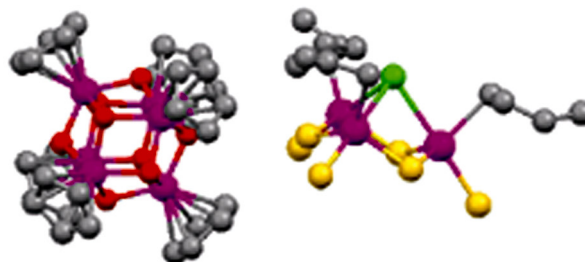
Nanocrystalline magnesium oxide prepared by the sol-gel method shows the formation of nano-MgO materials with crystallite size in the range of 5-20 nm and surface area of 336-556 m²/g. It can be used effectively for decontaminating (2-chloroethyl) phenyl sulfide, a mimic of bis(2-chloroethyl) sulfide. Nonpolar media aids material transfer to the reactive surface sites without blocking these sites.



Bozorgmehr Maddah*, Amir Aminifar &
Hossein Chalabi

1592 A structural study on the cubic crystalline modification of $[\text{Cp}_6\text{Ti}_6\text{O}_8][\text{Bu}_3\text{Sn}_3\text{S}_3(\text{SH})_3\text{Cl}]_2$

Crystal and molecular structures of a cubic crystalline form of $[\text{Cp}_6\text{Ti}_6\text{O}_8][\text{Bu}_3\text{Sn}_3\text{S}_3(\text{SH})_3\text{Cl}]_2$ is reported. The cation, $[\text{Cp}_6\text{Ti}_6\text{O}_8]^{2+}$, is a cluster comprising an octahedron with six Ti(IV) atoms at the vertices, while the anion is a six membered ring (with alternate Sn and S atoms) having a chair conformation. The crystal undergoes phase transition on cooling.



Neetu Singh & Subrato Bhattacharya*

1597 Guide to Authors

Authors for correspondence are indicated by (*)