

Subject Index

- Ab initio**
Theoretical studies of cooperativity effects in the ternary complexes of nitrous acid with ammonia and water 193
- Absorption coefficient**
Analytical calculation of far infrared spectra of ice in terms of a molecular model 117
- Ag**
Tautomerism of thymine on gold and silver nanoparticle surfaces: surface-enhanced Raman scattering and density functional theory calculation study 9
- AM1d calculations**
Potentiometric and AM1d studies of silicon podands—silver(I) complexes 227
- Ammonia**
Theoretical studies of cooperativity effects in the ternary complexes of nitrous acid with ammonia and water 193
- Arene ligand**
X-ray crystallographic study of two dinuclear triply-bridged *p*-cymene osmium complexes 161
- Artificial neural networks**
Using artificial neural networks to develop molecular mechanics parameters for the modelling of metalloporphyrins. III. Five coordinate Zn(II) porphyrins and the metalloporphyrins of the early 3d metals 67
- Arylsulfonates**
Coordination network: synthesis, characterization, crystal structure and packing of thallium *m*-nitrobenzenesulfonate, Tl(*m*-NO₂C₆H₄SO₃) 247
- Au**
Tautomerism of thymine on gold and silver nanoparticle surfaces: surface-enhanced Raman scattering and density functional theory calculation study 9
- Autocorrelation function**
Analytical calculation of far infrared spectra of ice in terms of a molecular model 117
- Azo dye**
Theoretical and NMR structural characterisation of a polymorphic azo dye 239
- B3LYP**
Theoretical and NMR structural characterisation of a polymorphic azo dye 239
- Benzoyltrifluoroacetone**
The novel one-dimensional chain of europium(III) complex [Eu₂(BTA)₆(4,4'-bpdo)]_n containing dimers bridged by terminal oxygen atoms of 4,4'-bpdo molecules 99
- Biological activities**
Spectroscopic study, antimicrobial activity and crystal structures of *N*-(2-hydroxy-5-nitrobenzalidene)4-aminomorpholine and *N*-(2-hydroxy-1-naphthylidene)4-aminomorpholine 253
- 4,4'-Bipyridine dioxide**
The novel one-dimensional chain of europium(III) complex [Eu₂(BTA)₆(4,4'-bpdo)]_n containing dimers bridged by terminal oxygen atoms of 4,4'-bpdo molecules 99
- Boron trifluoride**
Matrix isolation FTIR and DFT studies of methyl isocyanide-boron trifluoride complex 165
- Bovine serum albumin**
Studies on the interaction between 1-hexylcarbamoyl-5-fluorouracil and bovine serum albumin 143
- Bridging ligand**
X-ray crystallographic study of two dinuclear triply-bridged *p*-cymene osmium complexes 161
- ¹³C CP-MAS NMR**
Theoretical and NMR structural characterisation of a polymorphic azo dye 239
- ¹³C NMR**
ESI MS, NMR and PM5 semiempirical studies of oligomycin A and its complexes with Li⁺ and Na⁺ cations 261
- Carboxylate**
Layered zinc (II) and cadmium (II) dicarboxylates with aromatic chelate ligand-syntheses, crystal structures and luminescent properties 91
- Cd(II) complex**
Hydrothermal syntheses of a series of novel *cis*- and *trans*-pydc complexes with three-dimensional supramolecular architectures (pydc=pyridine-2,5-dicarboxylic acid) 105
- Chemical shift calculation**
¹H and ¹³C chemical shift calculations for 12-oxa-pentacyclo[6.2.1.1^{6,9}.0^{2,7}.0^{2,10}]dodeca-4-eno systems using GIAO method at different levels of theory 281
- Chromium**
Photochemical reactions of group 6 metal carbonyls with *N*-salicylidene-2-hydroxyaniline and bis-(salicylaldehyde)-phenylenediimine 171
- Circular dichroism**
Studies on the interaction between 1-hexylcarbamoyl-5-fluorouracil and bovine serum albumin 143
- Cobalt**
Keggin polyoxometalate with pendant tricyclic, aromatic entity 1
- Combinatorial chemistry**
Vibrational spectroscopic encoding of polystyrene resin bead: a combined FT-IR and computational study 155
- Complex dielectric permittivity**
Analytical calculation of far infrared spectra of ice in terms of a molecular model 117

Complexes with Zn(II) or H⁺

Synthesis, crystal structure, IR and Raman properties of 1,2-diacetamidocyclohexane and its complexes with ZnBr₂ and HBr₃ 39

Conformation

Intramolecular forces: the molecular structure and conformation of 2-cyclopropylpyridine and 4-cyclopropylpyridine 25

Synthesis and crystal structure of 2-debenzoyl and 4-deacetyl 1-deoxybaccatin VI derivatives 59

Design of peptides with α , β -dehydro-residues: synthesis and crystal structure of a tripeptide *N*-benzyloxycarbonyl- Δ Val- Δ Phe-I-Ala-OCH₃ 189

Conformational analysis

Structural characterization of *N*-phosphoryl branched peptides 179

Cooperativity

Theoretical studies of cooperativity effects in the ternary complexes of nitrous acid with ammonia and water 193

Coordination

An N₈O₆ cryptand: the host for Ag⁺ guests and H₂O molecules 137

Coordination chemistry

Layered solids based on second-sphere coordination interactions: synthesis, spectroscopic characterization, crystal structure and packing of two copper(II) naphthalene-2-sulfonates 291

Coordination network

Coordination network: synthesis, characterization, crystal structure and packing of thallium *m*-nitrobenzenesulfonate, Tl(*m*-NO₂C₆H₄SO₃) 247

Coordination polymer

Layered zinc (II) and cadmium (II) dicarboxylates with aromatic chelate ligand-syntheses, crystal structures and luminescent properties 91

Copper(II)

Layered solids based on second-sphere coordination interactions: synthesis, spectroscopic characterization, crystal structure and packing of two copper(II) naphthalene-2-sulfonates 291

Crystal packing

X-ray crystallographic study of two dinuclear triply-bridged *p*-cymene osmium complexes 161

Crystal structure

Design and syntheses of two novel supermolecular frameworks through weak interactions 51

Synthesis and crystal structure of 2-debenzoyl and 4-deacetyl 1-deoxybaccatin VI derivatives 59

Two-dimensional structural topology involving Pt...K and K...S weak interactions: complex of *cis-anti-cis*-dicyclohexyl-18-crown-6 with K₂mnt and K₂PtCl₄ 79

The novel one-dimensional chain of europium(III) complex [Eu₂(BTA)₆(4,4'-bpdo)]_n containing dimers bridged by terminal oxygen atoms of 4,4'-bpdo molecules 99

Hydrothermal syntheses of a series of novel *cis*- and *trans*-pydc complexes with three-dimensional supramolecular architectures (pydc = pyridine-2,5-dicarboxylic acid) 105

Oscillation of spontaneously generated optical activity in (\pm)-1-(*p*-nitrobenzoyloxy)indane solutions: 'serial S_N2 reactions' in aggregates supported by the crystal structure. Frozen S_N2 transition states and enantioselective distortions 113

An N₈O₆ cryptand: the host for Ag⁺ guests and H₂O molecules 137

Design of peptides with α , β -dehydro-residues: synthesis and crystal structure of a tripeptide *N*-benzyloxycarbonyl- Δ Val- Δ Phe-I-Ala-OCH₃ 189

Spectroscopic study, antimicrobial activity and crystal structures of *N*-(2-hydroxy-5-nitrobenzalidene)4-aminomorpholine and *N*-(2-hydroxy-1-naphthylidene)4-aminomorpholine 253

Crystal chemistry of protonated 1,2-bis(di-*R*-aminomethyl)-benzenes. Part VII: 1,2-bis(dipropylaminomethyl)benzene perchlorate 271

Cu(II) complexes

Synthesis, characterization and crystal structures of two discrete Cu(II) complexes with mixed-ligands: [Cu(mal)(L)(H₂O)]·H₂O and [Cu(Phmal)(L)₂] (mal = malonate dianion, phmal = phenylmalonate dianion and L = 5,5'-dimethyl-2,2'-bipyridine) 183

Cyclopropane

¹H and ¹³C chemical shift calculations for 12-oxa-pentacyclo[6.2.1.1^{6,9}.0^{2,7}.0^{2,10}]dodeca-4-eno systems using GIAO method at different levels of theory 281

Cyclopropyl groups

Intramolecular forces: the molecular structure and conformation of 2-cyclopropylpyridine and 4-cyclopropylpyridine 25

1D and 0D H-bonded adducts

The 1D and 0D weakly hydrogen-bonded adducts 18-crown-6/4-phenylthiosemicarbazide (1/2) and *cis-anti-cis*-dicyclohexyl-18-crown-6/*N,N'*-diphenylthiourea (1/2) 85

DAACH

Synthesis, crystal structure, IR and Raman properties of 1,2-diacetamidocyclohexane and its complexes with ZnBr₂ and HBr₃ 39

 α , β -dehydro-residue

Design of peptides with α , β -dehydro-residues: synthesis and crystal structure of a tripeptide *N*-benzyloxycarbonyl- Δ Val- Δ Phe-I-Ala-OCH₃ 189

1-Deoxybaccatin VI derivatives

Synthesis and crystal structure of 2-debenzoyl and 4-deacetyl 1-deoxybaccatin VI derivatives 59

DFT

Theoretical studies of cooperativity effects in the ternary complexes of nitrous acid with ammonia and water 193

DFT calculation

Tautomerism of thymine on gold and silver nanoparticle surfaces: surface-enhanced Raman scattering and density functional theory calculation study 9

Matrix isolation FTIR and DFT studies of methyl isocyanide-boron trifluoride complex 165

Dicyclohexyl-18-crown-6

Two-dimensional structural topology involving Pt...K and K...S weak interactions: complex of *cis-anti-cis*-dicyclohexyl-18-crown-6 with K₂mnt and K₂PtCl₄ 79

Dielectric response

Analytical calculation of far infrared spectra of ice in terms of a molecular model 117

Distortion

The influence of *ortho*-substitution within the ligand on the geometry of the tris(2,2'-bipyridine)ruthenium(II) and tris(1,10-phenanthroline)ruthenium(II) ions 129

Distortion of CrO₄²⁻ guest ions

Infrared study of the vibrational behavior of CrO₄²⁻ guest ions matrix-isolated in metal (II) sulfates (Me = Ca, Sr, Ba, Pb) 211

2D-QSAR

MIA-QSAR: a simple 2D image-based approach for quantitative structure-activity relationship analysis 149

Download English Version:

<https://daneshyari.com/en/article/9770345>

Download Persian Version:

<https://daneshyari.com/article/9770345>

[Daneshyari.com](https://daneshyari.com)