

Publications and Reports

“Study of the Distribution and Characterization of Forms of Fe in Particle-Size Fractions of an Entic Haplustoll by Selective Dissolution Techniques, X-Ray Diffraction and Mössbauer Spectroscopy”

S.G. Acebal, M.E. Aguirre, R.M. Santamaría, A. Mijovilovich, S. Petrick, C. Saragovi
Hyperfine Interactions 148/149 (2003) 3-12

Aggregate stability depends on soil properties such as organic matter content, type and quantity of clay and poorly crystalline Fe and Al oxide and oxy-hydroxides. Then, the quantification and characterization of forms of Fe and Al are of major importance for understanding soil structure. Particle-size fractions (5-2 m, 2-1 m, and 1 m) from the Ap horizon of an Entic Haplustoll from Argentina, treated with the selective-dissolution techniques ammonium oxalate (OX), dithionite-citrate-bicarbonate (DCB), NaOH, and Napyrophosphate (PY), are studied by X-ray powder diffraction (XRD) and ^{57}Fe Mössbauer spectroscopy (MS). Quartz, feldspar, smectite, illite and interstratified illite-smectite are predominant whereas Fe and Al oxides and oxy-hydroxides are present in low concentration. Al-substituted hematite and poorly crystallized hematite and goethite are present in similar proportions.

“Temperature Evolution of Crystal Field Interactions Across the Jahn-Teller Transition in a $\text{La}_{7/8}\text{Sr}_{1/8}\text{MnO}_3$ Single Crystal”

G. Alejandro, M.C.G. Passeggi, D. Vega, C.A. Ramos, M. T. Causa, M. Tovar, R. Senis
Physical Review B68 (2003) 214429

We present ESR, x-ray diffraction and dilatometry studies in a $\text{La}_{7/8}\text{Sr}_{1/8}\text{MnO}_3$ single crystal. ESR experiments were performed in the paramagnetic regime ($T_C \sim 180$ K), from 220 K to 570 K at a microwave frequency of 9.4 GHz. We measured the ESR linewidth as a function of temperature with the static magnetic field (H) parallel to the crystallographic directions [100] and [001], referred to the orthorhombic (Pbnm) axes. Detailed angular variations at constant temperature for H rotating in the (001), (010) and (-110) planes were also performed. The temperature dependence of the linewidth for fixed directions clearly reflects the changes in the symmetry of the crystal. At the Jahn Teller (JT) transition, a very noticeable decrease of the linewidth is observed. The angular dependence of the linewidth reveals an anisotropy that is temperature dependent. The amplitude of the variations decreases with T and almost disappears above $T_{JT} \sim 280$ K. However, there is a small remnant anisotropy present up to 400 K. We have carefully investigated the temperature dependence of this anisotropy across the Jahn-Teller transition. We showed that it is related with the evolution of the crystal field interactions. The symmetry of the ESR spectra is explained in terms of a spin Hamiltonian that includes isotropic Heisenberg superexchange, single ion-crystal field, and Dzyaloshinsky-Moriya antisymmetric exchange. The experimental angular variation of the ESR linewidth and its temperature dependence were fitted using the calculated expression for the linewidth as obtained from a perturbative Kubo-Tomita approach. From the ESR data we have obtained a ratio $E/D = -0.4$ for the spin Hamiltonian coefficients associated with the orthorhombic (E) and tetragonal (D) Jahn-Teller distortions of the MnO_6 octahedra. The temperature dependence of the parameters of the model are presented, and the correlation with the dilatometry results are discussed.

“High Temperature Susceptibility in Electron Doped $\text{Ca}_{1-x}\text{Y}_x\text{MnO}_3$: Double Exchange versus Superexchange”

H. Aliaga, M. T. Causa, M. Tovar, A. Butera, B. Alascio, D. Vega, A.G. Leyva, G. Polla, P. König
J. Phys.: Condens. Matter **15** (2003) 249-258

We present a study of the magnetic properties of the electron doped manganites $\text{Ca}_{1-x}\text{Y}_x\text{MnO}_3$ (for $0 \leq x \leq 0.25$) in the paramagnetic regime. For the less doped samples ($x \leq 0.1$) the magnetic susceptibility, $\chi(T)$, follows a Curie-Weiss (CW) law only for $T > 450$ K and, below this temperature, $\chi(T)$ shows a ferrimagnetic-like curvature. We approached the discussion of these results in terms of a simple mean-field model where double exchange, approximated by a ferromagnetic Heisenberg-like interaction between Mn^{3+} and Mn^{4+} ions, competes with classical superexchange. For higher levels of doping ($x \leq 0.15$), the CW behaviour is observed down to the magnetic ordering temperature (T_{mo}) and a better description of $\chi(T)$ was obtained by assuming full delocalization of the e_g electrons. In order to explore the degree of delocalization as a function of T and x , we analysed the problem through Monte Carlo

simulations. Within this picture we found that at high T the electrons doped are completely delocalized but, when T_{mo} is approached, they form magnetic polarons of large spin that cause the observed curvature in $X^{-1}(T)$ for $x \leq 0.1$.

“[Cu(2-Me-imidH)4Cl].Cl: A Conflict between High Symmetry vs. Packing efficiency”

A.M. Atria, P. Cortés, M.T. Garland, R.F. Baggio

Acta Cryst. **E59** (2003) m1075-m1077

The crystal and molecular structure of monomeric Cu(2-Me-imidH)₄Cl.Cl (1) is presented, and compared with that of other two quite related monomeric structures. The monomers are similar, but the supramolecular structures building up are very different. The influence that eventual steric effects might have in determining crystal properties as space group symmetry or packing efficiency is analyzed.

“Redetermination of Catena-Poly-(Bis(μ₂-Pyridine N-Oxyde-O,O)-Dichloro-di-Copper(II))”

A.M. Atria, P. Cortés, M.T. Garland, R.F. Baggio

Acta Cryst. **59** (2003) m967-m969

{[CuCl₂(C₅H₅NO)]₂}_n (1) is a 1D polymer in which the [CuCl₂(C₅H₅NO)]₂ dimers are the elemental constitutive units, joined by a rather long Cl-Cu interaction. The sequence of copper cations is alternatively bridged by two oxygens (Cu...Cu: 3.213(1)Å) and two chlorines (Cu...Cu: 3.706(1)Å). The metallic centers display a very distorted coordination geometry, with the four stronger bonds defining an elemental CuCl₂O₂ polyhedron midway square planar and tetrahedral, which serves as the base of a pyramid, while the loosely bound chlorine occupies the apex. The simultaneous presence of an eager H-bond acceptor as well as a well provided C-H donor leads to a very complex stabilizing network of weak C-H...Cl interactions.

“Three Yttrium Crotonato Complexes with Diimines”

A.M. Atria, R.F. Baggio, M.T. Garland, J.C. Muñoz, A. Soto

Acta Cryst. **C59** (2003) m416-m420

We present herein the synthesis and crystal structure of three new yttrium-crotonato (crot) compounds, associated to three different nitrogenated bases, viz.: phenanthroline (phen), methyl-phenanthroline (mphen) and bipyridylamine (bpa). All three compounds organize as dimers, and will accordingly be formulated as such: [Y(crot)₃(phen)]₂.2(H₂O) (1); [Y(crot)₃(mphen)]₂.2(H₂O) (2) and [Y(crot)₃(aq)₂]₂.4(bpa) (3). Complexes (1) and (2) are isostructural, with the bases acting as chelating ligands, while in complex (3) the coordination sphere is built up by carboxylate and aqua groups, the non coordinated diimine acting as a solvent.

“Two Isomorphous Imidazole (Him) Complexes: M Cl₂ (Him)₂ (H₂O)₂, M = Co, Ni”

A.M. Atria, P. Cortés, M.T. Garland, R.F. Baggio

Acta Cryst. **C59** (2003) m396-m398

The structures of Co(Him)₂Cl₂(H₂O)₂ (1) and Ni(Him)₂Cl₂(H₂O)₂ (2), (Him: imidazole) are isomorphous and constituted by monomers built up around a center of symmetry. The three monodentate ligands (imidazole, chlorine and aqua) define almost perfect octahedra. H-bonding interactions via de imidazole and aqua hydrogen atoms determine a complex 3D superstructure.

“A New Polymeric Phase of Zinc(II) Oxydiacetate: [{Zn(oda)(H₂O)₂.H₂O}]_n”

R. Baggio, M.T. Garland, M. Perec

Acta Cryst. **C58** (2003) m30-m32

A new polymeric phase of zinc(II) oxydiacetate, catena-poly[[[diaquazinc(II)]-oxydiacetato] hydrate], {[Zn(C₄H₄O₅)(H₂O)₂] _H₂O]_n, isomorphous with the Co homologue [Hatfield, Helms, Rohrs, Singh, Wasson & Weller (1987). Proc. Indian Acad. Sci. Chem. Sci. 98, 23-31], is reported. It presents a chain-like structure, generated by

ZnO₆ cores which are bridged by carboxylate groups in an anti-anti conformation along the unique crystallographic b axis. The chains are held together through hydrogen-bonding interactions with the three water molecules.

“Di- μ -trans-2-butenoato- κ^3 -O,O,O’)-di- μ .trans-2-butenoato- κ^2 -O,O’)- bis(trans-2-butenoato-- κ^2 -O,O’) -(1,10-phenanthroline-- κ^2 -N,N’)-dysprosium(III)] dihydrate”

R. Baggio, M. Perec, M.T. Garland
Acta Cryst. **E59** (2003) m1121-1123

The title compound, [Dy(C₄H₅O₂)₃(C₁₂H₈N₂)₂·2H₂O], crystallizes as dimeric units with an inversion centre. Each Dy atom is nine-coordinate to seven oxygen atoms from trans-2-butenoate groups and two nitrogens from a phenanthroline molecule. The dimer is quadruply bridged by trans-2-butenoates bridges). The intradimer Dy...Dy separation is equal to 3.9003(5)Å.

“Cu_xM_{1-x}(HCOO)₂(H₂O)_{1.33} (M = Mg, Co, x = 0.74): Crystal Structure and Hydrogen Bonding System”

R. Baggio, D. Stoilova, M.T. Garland
J.Mol.Struct. **659** (2003) 35-42

The crystal and molecular structure of two isomorphous mixed formates (Cu_xM_{1-x}(HCOO)₂(H₂O)_{1.33}, M = Mg (1), Co (2), x = 0.74) are presented. Crystal data for (1): Monoclinic, P21/c, a = 12.3280(14) Å, b = 7.2262(8) Å, c = 8.7217(10) Å, β = 103.083(2)°, V = 756.80(15) Å³; Z = 4, R1 = 0.0392; (2): Monoclinic, P21/c, a = 12.3202(13) Å, b = 7.2316(8) Å, c = 8.7255(9) Å, β = 103.121(2)°, V = 757.10(14) Å³, Z = 4, R1 = 0.0361. The cationic sites are occupied by a mixture of divalent cations (Cu,M) and the structural motive is composed of double layers of aqualess, Cu rich polyhedra separated by single layers of M rich ones containing both formate ions and coordinated water molecules. The infrared spectra of isotopically dilute (matrix-isolated HDO molecules) formates are analyzed in the region of the OD stretching modes. A discussion of the different strength of hydrogen bonds present in the structure is made at the light of the influence that the metal ions exert both onto the hydrogen bond donors, through direct coordination (synergetic effect) as well as onto hydrogen bond acceptor strength of the formate oxygens through the M–OCHO interactions.

“Polymeric Hexaaquaahexakis(μ_3 -2,2’-Oxydiacetato)-Trizinc(II)-Digadolinium(III)Dodecahydrate”

R. Baggio, M. Perec, M.T. Garland
Acta Cryst. **C59** (2003) m171-m1743

A polymeric heterometallic compound, {[Gd₂Zn₃(C₄H₄O₅)₆(H₂O)₆]₁₂H₂O}_n, comprising zinc(II) and gadolinium(III) cations bridged by carboxylate groups from oxydiacetate ligands, is presented. The Gd III cations lie at sites with crystallographic 32 symmetry and display a tricapped trigonal-prism arrangement, which is defined by six carboxyl and three ether O atoms. The Zn II cations lie at sites with imposed 2/m symmetry and are octahedrally coordinated by four carboxyl O atoms and two apical water ligands, which form strong intramolecular hydrogen bonds. Comparison is made with the previously reported isostructural homologous copper-gadolinium complex

“Tris(Hydrogen Oxydiacetate)-Dysprosium(III) Oxydiacetic Acid Monohydrate”

R.F. Baggio, M. Perec, M.T. Garland
Acta Cryst. **E59** (2003) m994-m996

The title compound Dy(Hoda)₃·H₂Oda·H₂O (H₂Oda: oxydiacetic acid) crystallizes in the monoclinic space group, P21/n and is isostructural with the homologous Y, Gd, and Tb compounds. The structure is described in terms of Dy(Hoda)₃ layers connected by H₂Oda molecules and intermolecular H-bonds.

“Europium(III) and Terbium(III) trans-2-butenoates: synthesis, crystal structure and properties”

B. Barja, P.F. Aramendia, R.F. Baggio, M.T. Garland, O. Peña, M. Perec

Europium(III) and terbium(III) *trans*-2-butenoate polymers, chemical formulas $[\{\text{Eu}_3(\text{MeCH}=\text{CHCO}_2)_9(\text{H}_2\text{O})_4\} \cdot \text{H}_2\text{O} \cdot \text{EtOH}]_n$ **1** and $[\{\text{Tb}(\text{MeCH}=\text{CHCO}_2)_3(\text{H}_2\text{O})\} \cdot \text{MeCH}=\text{CHCO}_2\text{H}]_n$ **2** and their dimeric 1,10-phenanthroline derivatives $[\text{Ln}_2(\text{MeCH}=\text{CHCO}_2)_6(\text{phen})_2] \cdot 2\text{H}_2\text{O}$, with Ln = Eu **3** and Tb **4**, were prepared and characterized by single-crystal X-ray diffraction. The coordination polymers **1** and **2** adopt different carboxylate-bridged infinite chain structures. While **1** shows three independent europium centers linked to each other by three different types and number of carboxylate bridges, the terbium polymer shows one independent metal center bridged by the same type of doubly carboxylates along the chains. Compounds **3** and **4** are isomorphous and isostructural (obvious!!) dinuclear structures with quadruply bridged carboxylato groups, two in the $\eta^1:\eta^1:\mu_2$ and two in the $\eta^2:\eta^1:\mu_2$ modes. Crystal data: **1**, monoclinic, space group *Pc*, $a = 10.097(1) \text{ \AA}$, $b = 10.384(1) \text{ \AA}$, $c = 24.773(2) \text{ \AA}$, $\beta = 96.35(1)^\circ$, and $Z = 2$. **2**, triclinic, space group *P-1*, $a = 7.895(1) \text{ \AA}$, $b = 10.780(1) \text{ \AA}$, $c = 13.575(1) \text{ \AA}$, $\alpha = 97.00(1)^\circ$, $\beta = 93.52(1)^\circ$, $\gamma = 107.34(1)^\circ$, and $Z = 2$. **3**: triclinic, space group *P-1*, $a = 10.557(2) \text{ \AA}$, $b = 11.032(2) \text{ \AA}$, $c = 11.473(2) \text{ \AA}$, $\alpha = 79.11(1)^\circ$, $\beta = 71.54(1)^\circ$, $\gamma = 77.34(1)^\circ$, and $Z = 2$. **4**: triclinic, space group *P-1*, $a = 10.538(1) \text{ \AA}$, $b = 11.010(1) \text{ \AA}$, $c = 11.429(1) \text{ \AA}$, $\alpha = 78.89(1)^\circ$, $\beta = 71.51(1)^\circ$, $\gamma = 77.25(1)^\circ$, and $Z = 2$. Magnetic and photophysical properties for the four compounds are reported.

“Crystal Structure and Luminescence Properties of Terbium(III) Carboxylates”

B. Barja, R. Baggio, M.T. Garland, P.F. Aramendia, O. Peña, M. Perec

Inorganica Chimica Acta **346** (2003) 187/ 196

Single crystals of three terbium(III) carboxylates of formulae $[\text{Tb}_2(\text{CH}_3\text{COO})_6(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$ (**1**), $[\text{Tb}_2(\text{CF}_3\text{COO})_6(\text{H}_2\text{O})_6]$ (**2**) and $[\text{Tb}(\text{Hoda})_3] \cdot \text{H}_2\text{O}$ (**3**) ($\text{H}_2\text{O} = 2,2'$ -oxydiacetic acid) were obtained and their structures determined by X-ray crystallography. Compounds **1** and **2** are dimeric, in the former the terbium atoms are bound by two tridentate carboxylates in the μ_2 -bridging mode, whereas in the latter the bridging is fourfold with all carboxylates in the *syn / syn* coordination mode. Compound **3** is mononuclear containing three tridentate Hoda anions, and consecutive units are linked by a network of H-bonds involving the interstitial molecules. The luminescence spectra of the carboxylates were analyzed in the solid state and in aqueous solution. Comparison of the emission lifetimes in H_2O and D_2O allowed the determination of the average value for q , the number of coordinated water molecules, being 9.2 for **1** and **2** and 3.6 for **3**, respectively. The quenching effect of Cu(II) on the luminescence of the terbium(III) carboxylates was evaluated through the emission decay constants. From the addition of Cu(II) to an aqueous solution of **3**, single crystals of polymeric $[\{\text{Cu}_3\text{Tb}_2(\text{oda})_6(\text{H}_2\text{O})_6\} \cdot 12\text{H}_2\text{O}]_n$ (**4**) were isolated with completely quenched luminescence. Compound **4** exhibits an overall antiferromagnetic interaction.

“From Nonwetting to Prewetting: The Asymptotic Behavior of ^4He Drops on Alkali Substrates”

M. Barranco, M. Guilleumas, E.S. Hernández, R. Mayol, M. Pi, L. Szybisz

Physical Review B68 (2003) 024515-1/7

We investigate the spreading of ^4He droplets on alkali-metal surfaces at zero temperature, within the frame of finite range density-functional theory. The equilibrium configurations of several $^4\text{He}_N$ clusters and their asymptotic trend with increasing particle number N , which can be traced to the wetting behavior of the quantum fluid, are examined for nanoscopic droplets. We discuss the size effects inferring the asymptotic properties of large droplets correspond to those of the prewetting film.

“Películas Dieléctricas Antirreflectantes-Pasivantes en Celdas Solares de Silicio Cristalino para Uso Espacial”

M. Barrera, J. Plá

Avances en Energías Renovables y Medio Ambiente **7** (2003) 09.07

La reflectividad es un parámetro que influye sobre la eficiencia de las celdas solares de Si cristalino. Para reducir la reflectividad, una de las técnicas que se utilizan habitualmente es la deposición de películas dieléctricas de índice y espesor apropiados, siendo el TiO_2 un material de características adecuadas. Consecuentemente se propusieron, optimizaron y fabricaron bicapas de $\text{TiO}_2/\text{SiO}_2$ sobre Si cristalino, donde el SiO_2 posee características pasivantes. La

optimización numérica fue realizada considerando el sistema MgF_2 -vidrio- TiO_2 - SiO_2 -Si, el espectro solar AM0 y una respuesta espectral típica de celdas solares de Si cristalino, teniendo como objetivo la aplicación en ambiente espacial. La fabricación de las bicapas de TiO_2/SiO_2 se realizó mediante un proceso térmico en ambiente oxidante luego de depositar una película de Ti sobre la oblea de Si por evaporación en cámara de vacío. Se presentan resultados de la caracterización óptica de las bicapas obtenidas.

“Simulación del Sistema Eléctrico de la Misión Satelital SAOCOM”

G. Berbeglia, D. Fernández Slezak, E.M. Godfrin, J.C. Durán

Avances en Energías Renovables y Medio Ambiente **7** (2003) 09.07

Se desarrolló un programa de simulación del funcionamiento de sistemas de potencia para satélites cuyo objetivo es predecir la evolución temporal del estado de carga de la batería, la corriente y la tensión del sistema a lo largo de la vida del satélite. Para ello, se estudió el comportamiento de los distintos componentes del sistema (panel solar, batería y regulador) y el requerimiento de potencia. Se explica brevemente el mecanismo para simular el sistema, los modelos de los distintos componentes del satélite involucrados y se presentan algunos resultados con datos correspondientes a la misión satelital SAOCOM. El programa, escrito en FORTRAN90, está diseñado de manera general; los parámetros de entrada son las curvas de tensión vs. carga de la batería, la curva corriente vs. tensión del panel solar, la duración del eclipse, un perfil del ángulo del satélite y otro del consumo energético del mismo.

“Yukawa Fluids: A New Solution of the 1 Component Case”

L. Blum, J.A. Hernando

Cond. Matter Phys. Vol. **6** (2003) 447

In recent work a general solution of the Ornstein Zernike equation for a general Yukawa closure for a single component fluid was found. Because of the complexity of the equations a simplifying assumption was made, namely that the main scaling matrix $b\Gamma$ had to be diagonal. While in principle this is mathematically correct, it is not physical because it will violate symmetry conditions when different Yukawas are assigned to different components. In this work we show that by using the symmetry conditions the off diagonal elements of $b\Gamma$ can be computed explicitly for the case of two Yukawas solving a quadratic equation: There are two branches of the solution of this equation, and the physical one has the correct behavior at zero density. The non physical branch corresponds to the solution of the diagonal approximation. Although the solution is different than in the diagonal case, the excess entropy is formally the same as in the diagonal case.

“Study of Particulate Matter in the Atmosphere of Buenos Aires City”

H. Bogo, M. Otero, P. Castro, M. Ozafrán, A.J. Kreiner, E.J. Calvo, R. Martín Negri

Atmospheric Environment **37** (2003) 1135-1147

The results of the first long-period campaign on particulate matter performed in the city of Buenos Aires are reported. Twenty four hour averages of atmospheric concentrations of PM10, PM2.5 and total suspended particles (TSP) were measured at a site near downtown Buenos Aires from December 1998 to September 1999. The values of PM2.5 concentrations correlate well to the concentrations of carbon monoxide (CO) during the winter period, indicating that direct traffic emissions have an important contribution to PM2.5. The data are less correlated for the case of PM10, indicating that the coarse fraction has a different source, probably resuspended dust. Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) images of atmospheric particles on nucleopore filters are shown. Information about the ion and metal content of the particles is reported.

“Desarrollo, Fabricación y Ensayo de Paneles Solares para Misiones Satelitales Argentinas - Primer Módulo para Ensayos”

C.G. Bolzi, C.J. Bruno, P. Cabot, E. Carella, J.C. Durán, J. Fernández Vázquez, C.D. Franciulli, E.M. Godfrin, V. Goldbeck, M.G. Martínez Bogado, A. Moglioni, J. Plá, S.E. Rodríguez, M.J.L. Tamasi, M. Alurralde, F. Antonuccio, A. Filevich, A. Iglesias, E. Mezzabolta, S.L. Nigro

Avances en Energías Renovables y Medio Ambiente **7** (2003), 04.07

Se presentan los logros alcanzados durante el último año en el desarrollo de paneles solares para misiones satelitales argentinas, en el marco del convenio de cooperación vigente entre la Comisión Nacional de Actividades Espaciales y la CNEA. Se analizan las actividades desarrolladas en los temas más relevantes: caracterización de celdas solares, puesta a punto de los procesos de soldadura y pegado, y desarrollo de diversas técnicas y dispositivos para ensayos. En particular, se describe la elaboración y el ensayo del primer módulo fabricado para la calificación de procesos según requerimientos de la tecnología espacial.

Comment on “Self Segregation vs. Clustering Evolutionary Minority Game”

E. Burgos, H. Ceva, R.P.J. Perazzo
Phys. Rev. Letters **91** (2003) 189801

“Minority Game: A Mean-Field-Like Approach”

I. Caridi, H. Ceva
Physica **A317** (2003) 247-258

We calculate the standard deviation of ($N_1 - N_0$), the difference of the number of agents choosing between the two alternatives of the minority game. Our approach is based on two approximations: we use the whole set of possible strategies, rather than only those distributed between the agents involved in a game; moreover, we assume that a period-two dynamics discussed by previous authors is appropriate within the range of validity of our work. With these approximations we introduce a set of states of the system, and are able to replace time averages by ensemble averages over these states. Our results show a very good agreement with simulations results for most part of the informationally efficient phase.

“Cross Sections for the Excitation of Isovector Charge-Exchange Resonances in ^{208}Tl ”

G. Colò, S.M. Lenzi, E.E. Maqueda, A. Vitturi
Physical Review **C67** (2003) 044306

The Glauber approximation for the treatment of heavy-ion scattering has already been shown to give reliable predictions for the reaction cross section in the particular case of intermediate energy charge-exchange processes. In the present work, we couple a Glauber-type model to microscopic random phase approximation calculations of the charge-exchange excitations of ^{208}Pb . The aim is to solve the long-standing question whether the very elusive charge-exchange isovector monopole has been really identified in the past experiments, or other multipoles were prevalent in the observed spectra.

“PhI=NSes Mediated Aziridination of 11-Pregnane Derivatives: Synthesis of an 11,12-Aziridino Analogue of Neuroactive Steroids”

P.H. Di Chenna, P. Dauban, A. Ghini, R. Baggio, M.T. Garland, G. Burton, R.H. Dodd
Tetrahedron **59** (2003) 1009-1014

Reaction of 11-pregnene-3,20-dione (6) or 3-acetoxy-11-pregnen-20-one (12) with trimethylsilylethanesulfonyl (‘Ses’) iminoiodinane 5 in the presence of copper (I) triflate gave the corresponding a,a-11,12-aziridino steroids 7 and 13 in 53 and 45% yields, respectively. The Ses group of each compound was removed using the TASF reagent and the resulting free aziridine NH was methylated to afford the 11a,12a-N-methyl aziridinosteroids 9 and 15, respectively. The latter is a conformationally constrained analogue of the endogenous neurosteroid pregnanolone (1).

“Pseudo-Random Unitary Operators for Quantum Information Processing”

J. Emerson, Y.S. Weinstein, M. Saraceno, S. Lloyd, D.G. Cory
Science **302** (2003) 2098

In close analogy to the fundamental role of random numbers in classical information theory, random operators are a basic component of quantum information theory. Unfortunately the implementation of random unitary operators on a quantum processor is exponentially hard. Here we introduce a method for generating pseudo-random unitary operators that can reproduce those statistical properties of random unitary operators most relevant to quantum information tasks. This method requires exponentially fewer resources, and hence enables the practical application of random unitary operators in quantum communication and information processing protocols. Using a nuclear magnetic resonance quantum processor we demonstrate the realization of pseudo-random unitary operators that reproduce the expected random distribution of matrix elements.

“Efficient Pseudo-Random Circuits for Quantum Information Science”

J. Emerson, Y. Weinstein, M. Saraceno, S. Lloyd, D.G. Cory
Science 302 (2003) 2098

In close analogy to the fundamental role of random numbers in classical information theory, random operators are a basic component of quantum information theory. Unfortunately the implementation of random unitary operators on a quantum processor is exponentially hard. Here we introduce a method for generating pseudo-random unitary operators that can reproduce those statistical properties of random unitary operators most relevant to quantum information tasks. This method requires exponentially fewer resources, and hence enables the practical application of random unitary operators in quantum communication and information processing protocols. Using a nuclear magnetic resonance quantum processor we demonstrate the realization of pseudo-random unitary operators that reproduce the expected random distribution of matrix elements.

“Head-to-Head Dimers in the Zwitterion of 1-hydroxy-1-phosphono-3-(1-piper-idino)propylidene-1-phosphonate (PHPBP)”

D. Fernández, D. Vega
Acta Cryst. **C59** (2003) o661–o663

The title compound, C₈H₁₉NO₇P₂, is a member of the bisphosphonate family of therapeutic compounds. PHPBP has inner-salt character, consisting of a negatively charged PO₃ group and a positively charged N atom. The six-membered piperidine ring adopts an almost-perfect chair conformation. The hydroxyl group and the N atom have gauche and trans conformations in relation to the O–C–C–N backbone, respectively. Hydrogen bonding is the main contributor to the packing in the crystal, which consists of head-to-head dimers formed through phosphonyl⋯phosphonyl hydrogen bonds, while O–H...O and N–H...O interactions join the dimers into a plane parallel to crystallographic b and c axes.

“Head-to-Head Dimers in the Zwitterion of 1-Hydroxy-3-(Pyrrolidin-1-l)Propylidene-1,1-Bisphosphonic Acid (EB1053)”

D. Fernández, D.R. Vega
Acta Cryst. **C59** (2003) o228–o230

The title compound, 1-hydroxy-1-phosphono-3-(1-pyrrolidinio) propylidene-1-phosphonate, C₇H₁₇NO₇P₂, is a member of the bisphosphonate class of drugs. As a zwitterion, it possesses a negative charge on one of the PO₃ groups and a positive charge on the pyrrolidine N atom. A zwitterion makes a contact with a neighbouring ion through the hydroxyl O atom and two phosphonyl O atoms, one each from two different PO₃ groups. Hydrogen bonding involves O–H...O and N–H...O interactions; the former are involved in the formation of head-to-head dimers, while the latter join the dimers into a chain running along the crystallographic b axis.

“17 α ,21-Dihydroxy-16 β -Methyl-Pregna-1,4-Diene-3,11,20-Trione (Meprednisone)”

D. Fernández, D.R. Vega, J.A. Ellena
Acta Cryst. **C59** (2003) o1–o4

The title compound, C₂₂H₂₈O₅, is a commercial therapeutic agent of the steroid class. Both independent molecules in the asymmetric unit have six-membered A rings that are planar, while the B and C rings adopt normal chair conformations. The five-membered D ring is in a ¹³₁₄-half-chair conformation, and the B/C and C/D ring junctions are in trans positions. Cohesion in the crystal is provided by O–H...O hydrogen bonds, which generate chains of molecules that are organized in a plane that lies along the crystallographic b axis.

“Alendronate Zwitterions Bind to Calcium Cations Arranged in Columns”

D Fernández, D.R. Vega, A. Goeta
Acta Cryst. C59 (2003) m543-m545

Alendronate is a clinically used compound in the treatment of skeletal disorders, the mode of action of which depends on the adsorption to calcium hydroxyapatite crystals of the bone. In the title compound, calcium 4-ammonium-1-hydroxybutylidene-1,1-bisphosphonate, Ca₂·2(C₄H₁₂N₂O₇P₂), alendronate is a zwitterion possessing one negative charge on each PO₃ group, and a protonated nitrogen atom. The zwitterion is disposed with its negative end facing Ca²⁺, while its positive end is stretched far away. The geometry of the carbon chain is all-trans, while the hydroxyl group is twisted. Ca²⁺ lies on a twofold axis parallel to b. The coordination sphere around the metal cation is octahedral, and is determined by monodentate and bidentate coordinated alendronate zwitterions. The bite O...O distance is 3.080(2) Å. Coordinated Ca²⁺ metal cations are arranged at the centre of a column running along c.

“An Alternative Method for the Measurement of Stellar Nuclear-Reaction Rates”

J.O. Fernández Niello, A. Arazi, T. Faestermann, K. Knie, G. Korschinek, E. Richter, G. Rugel, A. Wallner
Brazilian Journal of Physics 33 (2003) 218

For charged-particle induced reactions occurring in astrophysical scenarios, projectile energies are usually well below the Coulomb barrier of the reacting system. Hence, extremely small cross section reaction pose a difficult task for laboratory measurements. Most commonly, these energy-dependent cross sections are studied by detecting the emitted prompt gamma rays following the de-excitation of the produced compound nucleus. In this work we propose an alternative way for the measurement of the extremely small cross sections of the ²⁵Mg (p, γ)²⁶Al resonant reaction, namely the use of the Accelerator Mass Spectrometry (AMS) technique.

“2,6-Bis(2-Benzimidazolyl) Pyridine: Crystal Structure of Two Different Hydrates”

E. Freire, S. Baggio, J.C. Muñoz, R. Baggio
Acta Cryst. C59 (2003) o259-o262

The structures of the mono- and sesquihydrates of 2,6-bis(1H-benzimidazol-2-yl)pyridine (bbip) are reported. Phase (I), C₁₉H₁₃N₅·H₂O, has one water and one bbip molecule in the asymmetric unit, while phase (II), C₁₉H₁₃N₅·1.5H₂O, has three water molecules and two bbip molecules in the asymmetric unit. The compounds exhibit very similar molecular geometries but different packing organizations, which result from intricate hydrogen-bonding schemes.

“2,6-Bis(1H-benzimidazol-2-yl-(N₃)pyridine-κN] (dimethylformamide-(O))(thiosulfato-κ₂O,S) nickel(II) monohydrate”

E. Freire, S. Baggio, J.C. Muñoz, R.F. Baggio
Acta Cryst. C59 (2003) m299-m301

The structure of Ni(bbip)(ths)(dmf)·H₂O, bbip: 2,6-bis(2-benzimidazolyl)pyridine (C₂₁H₁₅N₅), ths: thiosulfate (S₂O₃); dmf: dimethylformamide (C₃H₇NO) is monomeric, with the nickel ion octahedrally surrounded by a tridentate (N,N',N'') bbip, a bidentate (S,O) ths and a monodentate (O) dmf. The hydrogen atoms corresponding to the hydration water molecule and the amino groups in bbip are involved in H-bonding, and determine a spatial organization of broad layers parallel to (001), connected by weak interactions.

“Classical Decays in Decoherent Quantum Maps”

I. García Mata, M. Saraceno, M.E. Spina
Physical Review Letters **91**, N° 6 (2003) 064101-1

The linear entropy and the Loschmidt echo have proved to be of interest recently in the context of quantum information and of the quantum to classical transitions. We study the asymptotic long-time behavior of these quantities for open quantum maps and relate the decays to the eigenvalues of a coarse-grained superoperator. In specific ranges of coarse graining, and for chaotic maps, these decay rates are given by the Ruelle-Pollicott resonances of the classical map.

“Heat Capacity of Helium in Cylindrical Environments”

S.M. Gatica, E.S. Hernández, L. Szybisz
Physical Review **B68** (2003) 144501-7

We perform a systematic investigation of the structure, elementary, and phonon excitations of quantum fluid ^4He adsorbed in the interior of carbon nanotubes. We show that the helium fluid inside the cylinder behaves exactly as in planar films on a graphite substrate, presenting the same kind of layering transition. This tendency is confirmed by the behavior of a single ^3He impurity diluted into adsorbed ^4He . We also present a simple description of the lowest excitation modes of the adsorbed fluid and compute the low-temperature contribution of the phonon spectrum to the specific heat, which displays the dimensionality characteristics reported in previous works.

“Analysis of the $[56, 2^+]$ Baryon Masses in the $1/N_c$ Expansion”

J.L. Goity, C. Schat, N.N. Scoccola
Phys. Lett. **B564** (2003) 83

The mass spectrum of the positive parity $[56, 2^+]$ baryons is studied in the $1/N_c$ expansion up to and including $O(1/N_c)$ effects with $SU(3)$ symmetry breaking implemented to first order. A total of eighteen mass relations result, several of which are tested with the available data. The breaking of spin-flavor symmetry is dominated by the hyperfine interactions, while spin-orbit effects are found to be small.

“Nonlocal Chiral Quark Models at Finite T and μ ”

D. Gómez Dumm, N.N. Scoccola
Proceedings of the “Hadrons Physics 2002”, Bento Gonçalves, Brasil. Ed. C.Vasconcellos, World Scientific
Singapore (2003) 315-318

Chiral quark models with nonlocal covariant separable interactions at finite temperature and chemical potential are investigated. In particular we study the chiral phase transition for some definite nonlocal regulators. We find that in all cases the transition is of first order for low values of T , turning into a smooth crossover at a certain “end point”. Predictions for the position of this point are given.

“Magnetism of Small Mn Clusters”

J.A. Guevara, A.M. Llois, F. Aguilera-Granja, J.M. Montejano-Carrizales
Physica Status Solidi **B279** (2003) 456

The role of structure on the magnetic properties of Mn clusters is investigated by performing calculations for different *bcc* families. In the very small cluster region calculations are also done for icosahedral structures. The spin polarized electronic properties of these geometries are calculated by solving a *spd* tight binding Hubbard-like Hamiltonian in the unrestricted Hartree-Fock approximation by using a bulk-like parametrization and adding extra orbital of *s*-like character to taking into account spillover effects. Conclusions about the structure of these clusters as a function of size are drawn by comparing with recent experimental results. We find that the preferred structure is always *bcc*. The magnetic coupling within the clusters is non ferromagnetic.

“Bis[2,6-bis(1H-Benzimidazol-2-yl-κN³)pyridinato-κN]Zinc(II)”

M.A. Harvey, S. Baggio, J.C. Muñoz, R. Baggio
Acta Cryst. **C59** (2003) m283-m285

The structure of Zn(C₁₉H₁₂N₅)₂ is monomeric and formed by neutral Zn(bbip-H)₂ entities (bbip-H: the anionic form of bisbenzimidazolepyridine, after having lost one of its hydrogen atoms). It was solved from a racemic twin, and the ligand presents its unique N-H imidazolyl hydrogen atom disordered into two symmetry related positions, thus rising the molecular symmetry as required by the space group. The planar ligands bind at 84.6(3)° from one another defining a distorted octahedral environment around the metal.

“Two New Dimeric Cadmium(II) and Zinc(II) Sulfate Complexes with 2,4,6-Tris(2-Pyridyl)-1,3,5-Triazine and 2,2':6',2''-Terpyridine”

M. Harvey, S. Baggio, S. Russi, R. Baggio
Acta Cryst. **C59** (2003) m175-m177

The structures of two new sulfate complexes are reported, namely di-μ-sulfato-κ³O,O:O''-bis{aqua[2,4,6-tris(2-pyridyl)-1,3,5-triazine-κ³N¹,N²,N⁶]cadmium(II)} tetrahydrate, [Cd₂(SO₄)₂(C₁₆H₁₂N₆)₂(H₂O)₂]_n·4H₂O, and di-μ-sulfato-κ²O:O''-bis[(2,2':6',2''-terpyridine-κ³N¹,N^{1'},N^{1''})zinc(II)] dihydrate, [Zn₂(SO₄)₂(C₁₅H₁₁N₃)₂]_n·2H₂O, the former being the first report of a Cd(tpt) complex [tpt is 2,4,6-tris(2-pyridyl)-1,3,5-triazine]. Both compounds crystallize in the space group P1 and form centrosymmetric dimeric structures. In the cadmium complex, the metal center is heptacoordinated in the form of a pentagonal bipyramid, while in the zinc complex, the metal ion is in a fivefold environment, the coordination geometry being intermediate between square pyramidal and trigonal bipyramidal. Packing of the dimers leads to the formation of planar structures strongly linked by hydrogen bonding.

“Weak C-H...O Interactions Leading to Measurable Effects in Polymeric Sulfates of General Formula [MM(SO₄)NN(H₂O)₂]_n, MM: Cd, Zn; NN: 2,2'-bipyridyne, 1,10-phenanthroline, 2,9-dimethyl-1,10-phenanthroline”

M.A. Harvey, S. Baggio, M.T. Garland, R.F. Baggio
Aust.J.Chem. **56** (2003) 1161-1165

The structure of two sulfate complexes, namely [Zn(SO₄)phen(H₂O)₂]_n (**Zn-phen**) and [Cd(SO₄)bpy(H₂O)₂]_n (**Cd-bpy**), **bpy**: 2,2'-bipyridyne, **phen**: 1,10-phenanthroline, are presented. They are polymeric and isomorphous to an homologous series already reported, viz.: [Zn(SO₄)bpy(H₂O)₂]_n^[1] (**Zn-bpy**), [Cd(SO₄)dmph(H₂O)₂]_n^[2] (**Cd-dmph**), [Cu(SO₄)bpy(H₂O)₂]_n^[3] (**Cu-bpy**) and [Cu(SO₄)phen(H₂O)₂]_n^[4] (**Cu-phen**), **dmph**: 2,9-dimethyl-1,10-phenanthroline). The compounds organize into double polymeric chains internally linked through strong (O-H)_{water}...O_{sulfate} bonds. The interaction between these “strips” is governed by weak (C-H)_{ligand}...O_{sulfate} bonds, which explain a seemingly abnormal expansion/contraction of some cell parameters in the homologous series. Both compounds are monoclinic, C2/c. (**Zn-phen**): a 15.156(3), b 14.152(3), c 6.7010(13) Å, β 103.43(3)°, V 1398.0(5)Å³, Z = 4, conventional R (on F) being 0.028 for 1615 No observed reflections (I>2σ(I)). (**Cd-bpy**): a 15.705(3), b 13.049(3), c 6.8912(14) Å, β 104.59(3)°, V 1366.7(5)Å³, Z 4, R 0.052, N_o 1516.

“Signature Inversion and Deformation Driving Effects in ¹⁷⁸Ir”

D. Hojman, M. A. Cardona, D. R. Napoli, S. M. Lenzi, J. Davidson, M. Davidson, C. A. Ur, G. Lo Bianco, C. M. Petrache, M. Axiotis, D. Bazzacco, M. De Poli, G. de Angelis, E. Farnea, T. Kroell, S. Lunardi, N. Marginean, T. Martínez, R. Menegazzo, B. Quintana, and C. Rossi Alvarez
Phys. Rev. C **67** (2003) 024308

High spin states in ¹⁷⁸Ir were investigated by means of in-beam γ-ray spectroscopy techniques using the multidetector array GASP. Excited states of ¹⁷⁸Ir were populated through the ¹⁵⁹Tb(²⁴Mg, 5n) fusion - evaporation reaction at E(²⁴Mg) = 131-141 MeV. Fourteen rotational bands have been observed and their configurations discussed. Alignments, band crossing frequencies, dynamical and kinematical moments of inertia, and electromagnetic

properties have been analyzed in the framework of the cranking model. Signature inversion in the $\pi i_{13/2} \otimes v i_{13/2}$ and $\pi h_{9/2} \otimes v i_{13/2}$ structures has been identified and interpreted in the framework of the particle rotor model with residual p-n interaction and variational moment of inertia (VMI). In bands involving the $\pi i_{13/2}$ orbital an increase in the deformation, relative to the other bands, has been found.

“Microstructural Analysis of Carbon Films obtained from C₆₀ Fullerene Ion Beams”

H. Huck, E.B. Halac, M. Reinoso, A.G. Dall'Asén, A. Somoza, W. Deng, R. S. Brusa, G. P. Karwasz, A. Zecca
Applied Surface Science **211/1-4** (2003) 379

Carbon films have been produced by accelerating C₆₀⁺ ions on silicon substrates with energies between 100 eV and 800 eV. The resulting films have been characterized by Raman and Positron Annihilation spectroscopies. Different deposition regimes have been distinguished depending on the energy of the incident fullerenes. At low energies intermolecular covalent bonds begin to insinuate, while at higher energies there is a coexistence of polymeric and amorphous carbon islands. Furthermore the samples have been annealed in order to study their thermal behavior. The results of Raman and positron annihilation spectroscopies are explained in terms of the structure obtained at different deposition energies.

“Comparison of the Performance of Two Different E-Noses in Hops Classification”

A. Lamagna, D. Rodriguez, S. Reich, N. Scoccola, A. Boselli, M. Cerdan
Proceedings of the “9th International Symposium on Olfaction and Electronic Nose (ISOEN02)”, Roma, Italia, 2002.
Eds. Arnaldo D'Amico, C. Di Natale. ISBN 88-7999-450-6. Aracne Editrice S.R.L., Roma (2003)

Hops, the female inflorescences of the hop plant (*Humulus lupulus* L.), are used in the brewing industry to add bitterness and aroma to the beer. It suffers a continuous process of deterioration after the crop due to oxidative processes when exposed to ambient air. Thus an early alarm of oxidative processes is an important parameters for the brewing industry. Due to requirements of local beer industries which demand rigorous and yet not very expensive quality control techniques to successfully compete within the beer market, we have studied the feasibility of electronic noses, to perform some of the tasks currently undertaken by conventional gas chromatography. The two aspects we address in this work are the quick discrimination of various types of pellets through their aroma and the detection of departures from the desired aroma due to aging processes or lousy storage.

“Nanotubes of Rare Earth Manganese Oxide”

P. Levy, A.G. Leyva, H.E. Troiani, R.D. Sánchez
Applied Physics Letters **83** (2003) 5247

We report the synthesis of rare earth manganese oxide based nanotubes. The pore wetting technique was used to obtain structures of nominal composition La_{0.325}Pr_{0.300}Ca_{0.375}MnO₃ with 800 nm external diameter, 4000 nm length and wall thickness below 100 nm exhibiting magnetic and magnetoresistive behaviour below 200 K, including non volatile memory. Walls are found to be formed by small crystals of approximately 20 nm. Structures obtained using different diameter of pores, as small as 100 nm, have a similar aspect ratio. Results show for the first time the realization of nanotubes of manganites exhibiting intrinsic phase separation.

“Persistent Magnetoresistive Memory in Phase Separated Manganites”

P. Levy, F. Parisi, J. Sacanell, L. Granja, M. Quintero, J. Curiale, G. Polla, A.G. Leyva, R.S. Freitas, L. Ghivelder, C. Acha, T. Y. Koo, S.-W. Cheong
Journal of Magnetism and Magnetic Materials **258** (2003) 293-295

We have studied magnetic and transport properties on different manganese - oxide - based compounds exhibiting phase separation: polycrystalline La_{5/8-y}PryCa_{3/8}MnO₃ (y=0.3) and La_{1/2}Ca_{1/2}Mn_{1-z}FezO₃ (z = 0.05), and single crystals of La_{5/8-y}PryCa_{3/8}MnO₃ (y~0.35). Time dependent effects indicate that the fractions of the coexisting phases are dynamically changing in a definite temperature range. We found that in this range the ferromagnetic fraction “f” can be easily tuned by application of low magnetic fields (< 1 T). The effect is persistent after the field is

turned off, thus the field remains imprinted in the actual value of “ f ” and can be recovered through transport measurements. This effect is due both to the existence of a true phase separated equilibrium state with definite equilibrium fraction “ f_0 ”, and to the slow growth dynamics. The fact that the same global features were found on different compounds and in polycrystalline and single crystalline samples, suggests that the effect is a general feature of some phase separated media.

“Casimir Interaction Between Two Concentric Cylinders: Exact versus Semiclassical Results”

F.D. Mazzitelli, M.J. Sánchez, N.N. Scoccola, J. von Stecher
Phys.Rev. **A67** (2003) 013807

We compute the Casimir energy for two perfectly conducting, infinite, concentric cylinders. We first obtain the zero point electromagnetic energy using a semiclassical approximation that takes into account families of classical periodic orbits that reflect off both cylinders. Then we compute the exact energy using the mode-by-mode summation technique based on Cauchy's theorem. We analyze the validity of the semiclassical approximation and show that it improves the results obtained through the proximity theorem.

“Cantilever's Behavior in the Ac Mode of an AFM”

V.B. Nunes, S.I. Zanette, A.O. Caride, R. Prioli, A.M.F. Rivas
Material Characterization 50 (2003) 173

In this paper a model with a small number of unknown parameters is used to simulate the motion of a cantilever in the ac mode of an atomic force microscope (AFM). The results allow determining the dependence of the transition from non-contact to tapping operating mode on the height of the contamination layer and on the stiffness of the sample.

“A Two-step Method for the Preparation of Chiral Cathinones”

M. Osorio-Olivares, M. Caroli Rezende, S. Sepúlveda-Boza, B.K. Cassels, R.F. Baggio, J.C. Muñoz Acevedo
Tetrahedron Asymmetry **14** (2003) 1473–1477

A simple method for the preparation of homochiral ring-substituted 1-aryl-2-aminopropanones **2** (‘cathinones’) is described, involving initial Friedel–Crafts acylation of aromatics with (S)- or (R)-N-trifluoroacetylalanyl chloride, followed by acid hydrolysis of the intermediate trifluoroacetamido intermediates **1**, for which X-ray diffraction analysis confirmed the structures.

“K X-Ray Production Induced by ^{12}C on Several Elements”

M.J. Ozafrán, M.E. Debray, R. Eusebi, A.J. Kreiner, M.E. Vázquez, A.A. Burlón, P. Stoliar
Nuclear Instruments and Methods in Physics Research **B201** (2003) 317-324

K X-ray production cross sections, photopeak energy shifts and $I(K\beta)/I(K\alpha)$ intensity ratios are measured for ^{12}C projectiles, in the 14 to 50 MeV bombarding energy range, on several elements (Al, Si, S, Cl, K, Ca, Ti, Cr, Fe, and Cu), using high resolution Si(Li) X-ray spectroscopy. A comparison is made with calculated ECPSSR cross-section values corrected by multiple ionization of K, L and M target subshells and electron capture into the partially empty K-shell of the projectile. The main application for these measurements is multielement trace analysis through PIXE (Particle Induced X-ray Emission).

“Free Energy Calculations of Elemental Sulfur Crystals via Molecular Dynamics Simulations”

C. Pastorino, Z. Gamba
J. Chem. Phys. Vol. **119** (2003) 2147

Free energy calculations of two crystalline phases of the molecular compound S8 were performed via molecular dynamics simulations of these crystals. The elemental sulphur S8 molecule model used in our MD calculations

consists of a semi-flexible closed chain, with fixed bond lengths and intra-molecular potentials for its bending and torsional angles. The intermolecular potential is of the atom-atom Lennard-Jones type. Two free energy calculation methods were implemented: the accurate thermodynamic integration method and an estimation that takes into account the contribution of the zero point energy and the entropy of the crystalline vibrational modes to the free energy of the crystal. The last estimation has the enormous advantage of being easily obtained from a single MD simulation. Here we compare both free energy calculation methods and analyze the reliability of the fast estimation via the vibrational density of states obtained from constrained MD simulations. New results on α - and α' -S8 crystals are discussed.

“Diffusion of Ta in α - Ti”

R.A. Pérez, F. Dymont, G. García Bermúdez, D. Abriola, M. Behar
Applied Physics **A76** (2003) 247

The diffusion of Ta in the hcp (α) phase of high purity Ti (99.99 %) was studied at different temperatures from 911 up to 1123 °K. To obtain the penetration profiles were used the Rutherford Backscattering Spectrometry (RBS) and Heavy Ion RBS (HIRBS) techniques. The evolution of the diffusion coefficient, D, as a function of temperature follows the prediction of the Arrhenius law. The activation energy of the diffusion process is (318 ± 7) kJ/mol, similar to that corresponding to self-diffusion in α -Ti. On the other hand, the measured values of D are systematically lower than those corresponding to self-diffusion by a factor of approximately 5. This reduction could be explained taking into account the mass difference between Ta and Ti. An increase of the diffusion coefficient was measured when the diffusion proceeds on a less pure Ti (99.9%) matrix. This increment is higher at lower temperatures.

“Optimization of ITO Layers for Heterojunction a-Si/c-Si Solar cell Applications”

J. Plá, M.J.L. Tamasi, R. Rizzoli, M. Losurdo, E. Centurioni, C. Summonte, F. Rubinelli
Thin Solid Films **425** (2003) 185

A detailed study of the antireflecting properties of Indium Tin Oxide (ITO) thin films used as front electrodes in a-Si/c-Si heterojunction (HJ) solar cells is presented. Radiofrequency magnetron sputtering deposition conditions of ITO layers were optimised for HJ solar cells applications. An XPS analysis was performed on the deposited films and a correlation between the film composition and the experimental parameters used in the sputtering process was established. The ITO layer thickness was optimised considering the a-Si layer thickness, its optical characteristics and the HJ solar cell spectral response. In our devices, the optimal ITO film thickness was established to be in the range 80 - 90 nm depending on the solar cell spectral response. A thickness tolerance of ± 10 nm was found to be suitable by accepting a minor degradation of the device performance. Finally, device simulation results obtained by the AMPS code are reported.

“Influence of Velocity in Nanoscale Friction Processes”

R. Prioli, A.M.F. Rivas, F.L. Freire Jr., Y.A.O. Caride
Applied Physics **A76** (2003) 565-569

Force microscopy images of boric acid crystals were obtained experimentally and simulated with the use of a two dimensional mechanical model. An analysis of the stick and slip movement of the microscope tip shows that the energy dissipation mechanism is strongly influenced by the non-linear dynamics of the sliding system. The contributions of stick and viscous forces on the energy dissipation (or friction forces) are studied as a function of the relative scanning velocity. At low relative velocities, the stick forces are shown to be responsible for the energy dissipation. This energy is velocity dependent, due to the coupling between the two degrees of freedom of the sliding system. As the scanning velocity increases the stick forces are damped, then the viscous force is predominant in the energy dissipation process.

“Effects of Nb Content on the Zr_2Fe Intermetallic Stability”

C. Ramos, C. Saragovi, M. Granovsky, D. Arias

With the aim of studying the stability range of the Zr_2Fe intermetallic when adding Nb, the range of existence of the cubic ternary phase (λ_1) and the corresponding two-phase field between them, four samples were analyzed, each one containing 35 at.% Fe and different at.% Nb: 0.5, 4, 10 and 15. Optical and scanning electron metallographies, X-ray diffraction, microprobe analysis and Mössbauer Spectroscopy were performed to determine and characterize the phases present in the samples. Results show that the Zr_2Fe compound accepts up to nearly 0.5 at.% Nb in solution, since the $Zr_2Fe + \lambda_1$ region is stable in the (0.5-3.5) at. % Nb range. To summarize these results an 800°C section of the ternary Zr-Nb-Fe diagram, in the studied zone, was proposed.

“Lateral Force Microscopy Profiles for Amorphous Potentials”

A.M.F. Rivas, R.R.M. Zamora, R. Prioli
Ultramicroscopy **97** (2003) 315-320

In this work the lateral force profiles of the scanning force microscope tip, on an amorphous surface, were simulated with the use of an independent oscillator model. The correlation between the lateral force profiles and the surface potential were studied as a function of the tip-surface normal force and relative scanning velocity. It is shown that, the microscope resolution is governed by the quotient between the average potential interaction energy and the average elastic energy stored before the jumps. We show that there is an optimal velocity with which the scanning tip better senses the surface potential and we present its scaling laws.

“New Homobinuclear Carboxylate-Bridged Gadolinium(III) Complexes”

A. Rizzi, R. Baggio, M.T. Garland, O. Peña, M.Perec
Inorg. Chim. Acta **353** (2003) 315- 319

Two novel gadolinium(III) trans-2-butenolate dimeric compounds [$Gd_2(O_2CCH=CHCH_3)_6(H_2O)_4 \cdot 2H_2O$] (**1**) and [$Gd_2(O_2CCH=CHCH_3)_6(phen)_2 \cdot 2H_2O$] (**2**) have been synthesized via hydrothermal routes. Compound **1** consists of two independent dimers in the unit cell, one is doubly bridged ($\eta^2 : \eta^1 : \mu^2$) and the other quadruply bridged (two $\eta^1 : \eta^1 : \mu^2$ and two $\eta^2 : \eta^1 : \mu^2$). Compound **2** is dimeric with a quadruply bridged core (two $\eta^1 : \eta^1 : \mu^2$ and two $\eta^1 : \eta^2 : \mu^2$). Crystal data: $C_{24}H_{42}Gd_2O_{18}$ (**1**), triclinic P-1, $a = 10.505(2)$ Å, $b = 10.545(2)$ Å, $c = 15.943(4)$ Å, $\alpha = 89.74(2)^\circ$, $\beta = 81.83(2)^\circ$, $\gamma = 86.18(2)^\circ$, $Z = 2$. $C_{24}H_{27}GdN_2O_8$ (**2**), triclinic P-1, $a = 10.564(3)$ Å, $b = 11.030(4)$ Å, $c = 11.492(5)$ Å, $\alpha = 79.17(3)^\circ$, $\beta = 71.58(3)^\circ$, $\gamma = 77.35(3)^\circ$, $Z = 2$. Magnetic susceptibility measurements in the range 2-300 K and EPR data in powder samples are presented.

“Structure and Magnetic Properties of Layered High Spin Co(II)(L-Threonine) $_2(H_2O)_2$ ”

A.C. Rizzi, C.D. Brondino, R. Calvo, R.F. Baggio, M.T. Garland, R.E. Rapp
Inorg.Chem. **42** (2003) 4409-4416

We report the structure and the magnetic properties of a cobalt(II) compound with the amino acid L-threonine, $Co(C_4H_8NO_3)_2(H_2O)_2$. It crystallizes in the orthorhombic chiral space group C2221, with a : 5.843(5) Å, b : 10.120(10) Å, c : 22.36(3) Å, and Z : 4. The Co(II) ion is in a deformed octahedral environment on a 2-fold symmetry axis parallel to the crystallographic axis b . It is bonded to two threonine molecules in a bidentate fashion, via one oxygen from the carboxylate end and the R-amino nitrogen. A water molecule occupies the third independent site. The Co(II) ions are arranged in layers with intralayer and interlayer distances of 5.84 and 11.18 Å, respectively. Magnetic measurements data reflect the molecular character of a compound with weak exchange interactions. EPR measurements in polycrystalline and single-crystal samples indicate a distorted axial symmetry around the Co(II) ion, as expected from the structural results. Eigenvalues and eigenvectors of the g tensor are determined. The measured principal g values (5.81, 4.56, and 2.23) reflect a high-spin Co(II) ion, as suggested by the type of ligands and the molecular symmetry. From the incomplete collapse of the hyperfine structure we estimate $0.25 < |J| < 1.2$ cm⁻¹ between neighboring Co(II) ions within a layer, transmitted through H-bonds. A higher limit $|J| < 0.07$ cm⁻¹ is estimated for the exchange interactions between Co(II) ions in neighboring layers. From a global fit of a spin Hamiltonian with spin 3/2 to magnetization and EPR data we obtain a zero field splitting $\delta \sim 231$ cm⁻¹ between the

two lowest doublet states. The results are discussed in terms of the molecular and electronic structure of the compound.

“Multisensor Array and Pattern Recognition Techniques for Characterization of Different Mate Brands”

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Proceedings of The 7th International Conference on Sensors and Microsystems, Editors, C. Di Natale, A. D’Amico, L. Dori, G.C. Cardinali y S. Nicoletti, World Scientific Publishing Co. ISBN 981-238-181-3 (2003) 208-210

We report preliminary results of our first prototype of electronic nose (e-nose) for discrimination between different mate brands. This work shows advances along the three main lines of our e-nose system: i) development and characterization of each of the six sensors in the array, ii) electronic interface for control of the sensor array and for data acquisition and iii) design and optimization of the pattern recognition algorithm.

“70-Baryons $1/N_c$ Expansion”

C.L. Schat, J. Goity, N.N. Scoccola

Proceedings of the “Hadrons Physics 2002”, Bento Gonçalves, Brazil, 2002. Ed. C.Vasconcellos, World Scientific Singapore (2003) 311-314

The discussion of the 70-plet of negative parity baryons illustrates the large N_c QCD approach to orbitally excited baryons. In the case of the $L=1$ baryons the existing data allows to make numerous predictions to first order in the $SU(3)$ symmetry breaking. New relations between splittings are found that follow from the spin-flavor symmetry breaking. The $\Lambda(1405)$ is well described as a three-quark state and a spin-orbit partner of the $\Lambda(1520)$.

“El Exótico Pentaquark. ¿Una Nueva Clase de Partícula Subnuclear ?”

N.N. Scoccola

Ciencia Hoy (Argentina), Vol. 13 N° 77 (2003) 64-66

En un artículo publicado en *Physical Review Letters* el 4 de julio último, un grupo de más de 50 físicos experimentales anunció haber dado con la primera evidencia de lo que podría ser un nuevo tipo de partícula subatómica, el pentaquark.

“Excited Baryon Spectroscopy in the $1/N_c$ Expansion”

N.N. Scoccola

Proceedings of the AIP Conf. “II International Workshop on Hadron Physics Effective Theories of Low Energy QCD”, Coimbra, Portugal, 2002.

AIP Conference Proceedings **660** (2003) 48-61

We analyze the masses of the negative parity $SU(6)$ 70-plet baryons using the $1/N_c$ expansion to order $1/N_c$ and to first order in $SU(3)$ breaking. At this level of precision there are twenty predictions which include the well known Gell-Mann Okubo and equal spacing relations together with four new relations involving $SU(3)$ breaking splittings in different $SU(3)$ multiplets. Although the breaking of $SU(6)$ symmetry occurs at zeroth order in $1/N_c$, it turns out to be small. The dominant source of the breaking is the hyperfine interaction which is of order $1/N_c$. The spin-orbit interaction, of zeroth order in $1/N_c$, is entirely fixed by the splitting between the singlet states $\Lambda(1405)$ and $\Lambda(1520)$, and the spin-orbit puzzle is solved by the presence of other zeroth order operators involving flavor exchange.

“Trace Elements Content in Size Classified Volcanic Ashes as Determined by Inductively Coupled Plasma–Mass Spectrometry”

P. Smichowski, D. Gómez, S. Rosa, G.I. Polla

Microchemical Journal **75** (2003) 109-117

At present there is an increasing concern as regards the release of potentially toxic metals into the environment. Volcanic eruptions are a natural source of metals and metalloids in the atmosphere. Toxic trace elements ejected during an eruptive episode may produce hazardous effects for people and the environment in areas close to the volcano. In this context, a study was undertaken to investigate the concentration of metal and metalloids in ashes ejected from Copahue volcano, Neuquén, Argentina. Two samples (A and B) of deposited particles were collected one day after the first eruption and size-fractionated in four sub-samples (S1, S2, S3, S4). Analysis was performed by inductively coupled plasma-mass spectrometry (ICP-MS) and the accuracy for the entire analytical procedure was performed by means of the certified reference material CRM GBW 07105 Rocks (NRCCRM, China). The elements considered were: As, Cd, Cr, Cu, Hg, Ni, Pb, Sb, U, V and Zn. The adverse effect of potentially interfering species on the mass-spectrometric determination of these elements was also taken into account. The concentration intervals found in the four fractions are as follows (in $\mu\text{g g}^{-1}$): As, 6.0-2.6; Cd, 0.71-0.36; Cr, 29.5-54.0; Cu, 132-49.0; Hg, 0.020-0.007; Ni, 36.0-26.0; Pb, 15.5-2.55; Sb, 1.07-0.30; U, 2.57-1.94; V, 152-106; Zn, 85.5-55.0. The elements with the highest concentrations were: Cu, V and Zn. All fractions, in both samples, were found to be enriched in some toxic trace elements in the following order $\text{Sb} > \text{Cd} > \text{As}$. On the contrary, samples were depleted in Ni, Cr and Hg. Lead was the element that exhibits a noticeable difference in concentration between the finer and coarser fractions.

“Curvature effects on the surface tension and thickness at the free interface of ^4He systems”

L. Szybisz, I. Urrutia

Physical Review **B68** (2003) 054518/1-13

The thickness W and the surface energy σ_A at the free surface of superfluid ^4He are studied. Results of calculations carried out using density functionals for cylindrical and spherical systems are presented in a unified way, including a comparison with planar slabs. It is found that for large species W are compared with prior theoretical results and experimental data. Experimental data favor results evaluated by adopting finite range approaches. The behavior of σ_A and $W\sigma_A$ exhibits overshoots similar to that found previously for the central density, and the trend of these observables towards their asymptotic values is examined.

“Comparación del Daño por Radiación producido por Protones y Electrones en Celdas Solares para Uso Espacial”

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Avances en Energías Renovables y Medio Ambiente **7** (2003) 04.01

Continuando con los estudios de daño por radiación en celdas solares para usos espaciales se presentan los resultados de la irradiación con electrones de 2,6 MeV realizada en un acelerador LINAC del Centro Atómico Bariloche de la Comisión Nacional de Energía Atómica (CNEA). Se estudió la degradación de los parámetros eléctricos y electrónicos de celdas solares de Si cristalino elaboradas en el Grupo Energía Solar de la CNEA y de doble juntura de $\text{GaInP}_2/\text{GaAs}/\text{Ge}$, bajo los efectos de la irradiación con electrones. Estos resultados se comparan con los obtenidos anteriormente en irradiaciones con protones, obteniéndose un coeficiente de daño equivalente entre protones de 10 MeV y electrones de 2,6 MeV.

“Low Energy Proton Irradiation Effects on Alveolar Macrophages from Young and Aged Rats”

D.R. Tasat, R. Mancuso, B.L. Molinari, G. Saint-Martin, A. Pérez de la Hoz, O.A. Bernaola, A.J. Kreiner, J.A. Schuff, Palmieri M, Mazal A, Stoliar P, Burlón A, Davidson M, Davidson J, M.E. Debray, J.M. Kesque, H. Somacal, A. Valda, F. Naab, M.J. Ozafrán, M.E. Vázquez

Cellular and Molecular Biology **V49** (2003)

A prospective study was undertaken to assess the radiotoxicity of accelerated particles, in pulmonary alveolar macrophages (AM). We evaluated the effects of a single dose (10-75 Gy) of an external low-energy (20 MeV) proton beam on cultured AM oxidative metabolism and phagocytic function. Macrophages are the first line of defense against invading pathogens and are known to generate superoxide anion (O_2^-), nitric oxide (NO), and mediators of antimicrobial and antitumoral defense mechanisms. We obtained AM by bronchoalveolar lavage from young (1-2 mo. old) and aged (9-12 mo. old) male Wistar rats. Cell viability, phagocytosis, O_2^- and NO production in control and proton-irradiated cultured AM were evaluated. The effect of proton irradiation on cell

viability was dose-dependent. The higher doses induced a dramatic decrease in viability in the aged population. Phagocytosis increased 1.3-1.4 fold in both populations irrespective of the dose delivered. Generation of O_2 was always higher in the aged population for all the doses assayed and showed no significant variation from the control values. In the young population a clear increase was observed with doses of 25 and 50 Gy. NO production in AM from young animals rose in a dose-dependent manner. Conversely, proton irradiation did not affect NO production in macrophages from aged animals. The results of this study demonstrate that AM isolated from young and aged rats are functionally different and show a distinct behavior when exposed to proton irradiation. These findings suggest that age may condition response and must be taken into account when accelerated particle-radiotherapy protocols are considered as a valid therapeutic option for the treatment of cancer. To the best of our knowledge, this is the first report comparing sham-irradiated and proton-irradiated young and aged AM.

“Different Time Scales in Wave Functions Intensity Statistics”

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Phys. Rev. **E67** (2003) 066212

Unstable periodic orbits scar wave functions in chaotic systems. The local short term dynamics also influences the associated spectra that follow the otherwise universal Porter-Thomas intensity distribution. We show here how this deviation extends to other longer periodic orbits sharing some common dynamical characteristics. This indicates that the quantum mechanics of the system can be described quite simply with few orbits, up to the resolution associated with the corresponding lengths.

“Mössbauer Studies of Corrosion Products Developed in Prohesion Test over Galvanized Steel Sheets”

M. Zapponi, T. Pérez, C. Ramos, C. Saragovi

Hyperfine Interactions 148 (1) (2003) 145-151

Precoated galvanized steel sheets were submitted to Prohesion test (PT) and to outdoor exposure test (OT). The corrosion products were different in both cases: surprisingly greigite was detected in samples of Prohesion test. Goethite, lepidocrocite, pyrite and magnetite were also found in these samples and the presence of akaganeite cannot be discarded. On the other hand, goethite, lepidocrocite, magnetite, akaganeite and silicates were found in outdoor exposure samples. This study allows concluding that in the Prohesion G-85 test the corrosion mechanism is different from that in the marine atmosphere for the analyzed samples and could not be used to predict the performance of this type of outdoor exposed materials.