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Analytic Summary

Boyd, Russell J. (Dalhousie University. Department of Chemistry. Halifax, Nova Scotia - Canada B3H 4J3): Molecular Electron Densities and Density Funcional Theory (Orig en)

In: *Formula*. 4, 5-28

Abstract: Recent progresses in the calculation of electronic properties by means of density functional methods will be reviewed. Particular attention will be paid to the comparison of the electron densities of small molecules calculated by use of various exchange and correlation functionals with the results of quadratic configuration interaction method. The prospects for the development and parametrization of new functionals for use in density functional methods from high-level ab initio electron densities will be summarized.

Key words: Electron density. Density Funcional Theory.

Sarasola, Cecilia; López, Xabier; Ugalde, Jesus M. (Euskal Herriko Unibertsitatea. Kimika Fakultatea. 1072 posta kutxa - 20080 - Donostia): Screeening Effects on the Electronic Structure of Atoms and Molecules (Orig en)

In: *Formula*. 4, 29-44

Abstract: The variational self consistent field molecular orbital method is used to compute both atomic and molecular energies for the Yukawa potential. Both, closed-shell and open-shell Slater determinant type of configuration wave functions are expanded as linear combinations of Gaussian basis functions, for which a complete analytical solution for all the required basic integrals is obtained. The energies obtained by this method for the hydrogen atom compare satisfactorilly with more accurate calculations, even for short expansions of the orbitals. For the groung states of the H_2^+ and H_2 molecules our model predicts that the bond length increases and the dissociation decreases as the screening parameter increases.

Key words: Screening effects. Electronic Structure.

Eriksson, Leif A. (University of Stockholm. Department of Physics. Box 6730 - 113 85 Stockholm): Understanding Radicals; Recent Results from Theoretical Studies of Radical-Matrix Interatcions and Biophysical Systems (Orig en)

In: *Formula*. 4, 45-71

Abstract: A number of examples are presented, in which a recent gradient correscted density functional theory (DFT) approach is employed for the study of radicals and radical hyperfine structures. The examples included cover both neutral and charged radicals. Of particular interest are the effects on the radical geometries and hyperfine properties due to the surrounding matrix, as well as modelling explicit effects of hydrogen bonding on the spin density distributions and hfcc of amino acid radicals. Throughout we compare with available data from electron paramagnetic resonance (EPR) experiments, and, where available, with previous theoretical work.

Key words: Radicals. Hyperfine structure.

García, Alberto (Universidad del Paìs Vasco. Departamento de Física Aplicada II. Apartado 644. 48080 - Bilbao); **Vanderbilt, David** (Rutgers University. Department of Physics and Astronomy. Piscataway - NJ 08855-0849 USA): Structural Instabilities in Perovskites: Ab-initio Calculation of the Dynamical Properties of Ferroelectric $PbTiO_3$ (Orig en)

In: *Formula*. 4, 73-90

Abstract: A first-principles study of the vibrational modes of $PbTiO_3$ in the ferroelectric tetragonal phase has been performed at all the main symmetry points of the Brillouin zone (BZ). The calculations use the local-density approximation and ultrasoft pseudopotentials with a plane-wave basis, and reproduce well the available experimental information on the modes at the T point, including the LO-TO splittings. The work was motivated in part by a previously reported transition to an orthorhombic phase at low temperatures [J. Kobayashi, Y. Uesu, and Y. Sakemi, Phys. Rev., B **28**, 3866 (1983).] We show that a linear coupling of orthorhombic strain to one of the modes a T plays a role in the discussion of the possibility of this phase transition. However, no mechanical instabilities (soft modes) are found, either at T or at any of the other high-symmetry points of the BZ.

Key words: Perovskites. Change's phase.

Lecea, Begoña (Universidad del País Vasco. Farmazi Fakultatea. Apartado de correos 450. 01008 - Gasteiz); **Arrieta, Ana**; **Roa, Guillermo**; **Cossio, Fernando P.** (Universidad del País Vasco. Facultad de Química. Apartado 1072. 20080 - Donostia): Periselectivity in Electrocyclic Processes: [2+2] vs. [4+2] Selectivity in the Cycloaddition Reaction between Ketenes and ab-Unsaturated Imines (Orig en)

In: *Formula*. 4, 91-109

Abstract: The aim of the present work is to explore computationally the behaviour of several model ketenes and 1-azadienes in order to develop a general model which could eventually explain the variables governing the formation of [2+2] an [4+2] cycloadducts. Since the electrocyclic step determines the outcome of the reaction, we well focus on the transition states compatible with the electrocyclic process. Solvent effect has been taken into account using the Onsager model.

Key words: Electrocyclic Processes. Solvent effect.

Largo, Antonio (Universidad de Valladolid. Facultad de Ciencias. Departamento de Químicas Física. 47005 - Valladolid)**; Río, Emma del**; **Barrientos, Carmen** (Universidad de Valladolid. Facultad de Ciencias. Departamento de Químicas Física. 47005 - Valladolid): Interstellar Chemistry of Binary Phosphorus-Carbon Compounds (Orig en)

In: *Formula*. 4, 111-150

Abstract: The structure and energetics of various C_nP (n = 2 – 4) molecules is addressed with the aim to shed light on the gas phase chemistry of these interesting molecular radicals. Also, we present a detailed study of the C_3P^+ under conditions compatible with those of the interstellar space is discussed.

Key words: Ion -molecule reactions. Interstellar Chemistry.

Elejabarrieta Olabarri, Mª Jesús (Eusko Ikaskuntza. Mª Díaz de Haro, 11 - 1. - 48013 - Bilbao): El análisis modal: aplicación a la acústica musical (The modal analysis: application to the musical acustic) (Orig.es)

In: *Formula*. 4, 153-165

Abstract: The modal analysis applied to the musical acoustic is based on the vibrational mechanics, acoustic and music. After the beginning of the modal analysis with the vibrational study on the strings it has been applied experimentally to the two-dimensional systems and finally its mathematical formulation has been obtained. the importance of this analysis has been fundamental to improve the quality of the musical instruments, specially in the case of picked and rubbed string instruments.

Key words: Modal analysis. Acoustic. Music.

Escobal, Ana; Iriondo, Carmen; Laborra, Concepción (Univ. del País Vasco. Fac. de Ciencias. Dpto. de Química Orgánica. Apdo.644. 48080 Bilbao): Determinación cromatográfica de componentes orgánicos volátiles en txakoli blanco de Bizkaia (Determination of volatile organic compounds in white Txakoli from Bizkaia by gas chromatography) (Orig.es)

In: *Formula*. 4, 167-176

Abstract: The aim of this work is the determination of organic volatile compounds in white Txakoli wine. This work is part of a project whose object is the chemical characterization of Txakoli from Biscay. We have used the gas chromatography methods for the determination of some volatile compounds in this fresh wine obtained from different varieties of grapes.

Key words: Txakoli. Volatile organic compounds.

Fernández Rico, Jaime (Univ. Autónoma de Madrid. Dpto. de Química Física Aplicada. Cantoblanco. 28049 Madrid): El papel de la Química Cuántica en la Química Moderna (The role of quantic chemistry in Modern Chemistry) (Orig. es)

In: *Formula*. 4, 177-182

Abstract: It is stressed that Chemistry is the science with the most favourable incidency in our daily life and our welfare. A short summary of the historical evolution of concepts and techniques leading to chemistry as a science in the last years of the eighteenth century is presented. From then, two periods separated by the birth of Quantum Mechanics can be distinguished. In the first one, concepts and models are established on pure empirical basis. In the second one, there exists a theory potentially able to explain them. Finally, it is remarkable the insufficiency of the efforts invested in the interpretation of the concepts and relations of the empirical Chemistry in the framework of this theory.

Key Words: Chemical concepts. Historical evolution. empirical estructural chemistry. Theorical Chemistry.

González, León; Marín, Angel (Univ. Pública de Navarra. Dpto. de Matemática e Informática. Campus Arrosadía. 31006 Iruñea): Pseudoigualdades de segundo orden (Second order false equalities) (Orig.es)

In: *Formula*. 4, 183-197

Abstract: In this paper methods of extension for the equality relation are introduced. These methods allow to give in an homogeneous frame matching or similarity measures among fuzzy subsets, most of which have arisen in various forms both in mathematical analysis and fuzzy logic applications.

Key words: Blurry logic. Equality. Operating implication.

Meyer, Yves (Eusko Ikaskuntza. Mª Díaz de Haro, 11-1º. 48013 Bilbao): Comprensión de datos y restauración de imágenes con ruido según David Donoho (Data compression and restoration of images with noise according to David Donoho) (Orig.es)

In: *Formula*. 4, 199-210

Abstract: The wavelet offers some interesting possibilities for the elimination treatment of the noise of signals and images and it creates an unconditional and universal base that is useful to all the Besov spaces. These spaces give a detailed and precise description of certain types of signals and images, permitting an evaluation of the quality of the image that was reconstructed after nonlinear compression. The algorithms of optimum compression are in the centre of the problems that the non linear noise supression has. A description of the findings that were made by Donoho on images of the geometric type is presented. The challenge consists in finding a priviliged orthonormal base of the space of finite energy signals.

Key words: Small waves. Signal noise. Geometric pintures. Besov spaces.

Molinero de Miguel, Mª Eugenia; Ruiz Parrado, Virtudes; Valle Cuezva del, Angel (Laboratorio Municipal de Bilbao. Luis Briñas, 16 - 48013 Bilbao): Estudio de los niveles de Estroncio 89 y 90 en leche (Study of 89 Sr and 90 Sr Levels in milk) (Orig.es)

In: *Formula*. 4, 211-218

Abstract: Most artificial radionuclids enter our organism basically through water and food. Since milk is the main vehicle of 89Sr and 90Sr, and because of its high consumption in our country, it seems very interesting and necessary to have a periodic control. After extraction with trichloroacetic acid, milk is purified by ion exchange cromatography, concentration and detection in a Geiger-Muller Counter. 23 samples were tested. The levels obtained were very low and similar enough. All of them were under maximum levels recommended by EEC.

Key words: Radioactive. Control. Milk.

Molinero de Miguel, Mª Eugenia; Ruiz Parrado, Virtudes; Valle Cuezva del, Angel (Laboratorio Municipal de Bilbao. Luis Briñas, 16 - 48013 Bilbao): Niveles de radioactividad gamma total en leche y aguas envasadas (Total Gamma-Ray levels in milk and bottled water) (Orig.es)

In: *Formula*. 4, 219-225

Abstract: The most important Gamma-emmitting redionuclids are 131Y, 137Cs and 140Ba. They are dangerous and related with cancer, leukaemia, etc. Gamma-Ray represents the most dangerous and harmful radiations. So a systematic control is very important to detect futur accidents. We have used the Becquerel LB-200 scintillation counter with a Nal detector. No previous treatment is required. 47 samples of milk and 11 of bottled water were tested. All levels were under maximum recommended by EEC.

Key words: Total Gamma-Ray. Milk. Bottled water.

Molinero de Miguel, Mª Eugenia; Ruiz Parrado, Virtudes; Valle Cuezva del, Angel (Laboratorio Municipal de Bilbao. Luis Briñas, 16 - 48013 Bilbao): Radioactividad beta total medio-ambiental en Bilbao (Environment total beta radioactivity in Bilbao) (Orig.es)

In: *Formula*. 4, 227-233

Abstract: The development of human activities leads to the increase of environment irradiation. Radioactive contamination due to nuclear tests has gone down since 1962, but other sources maintain the risk of contamination. Due to this, a permanent control is necessary in order to get a faster reaction in nuclear incidents. The sample is obtained by filtration and introduced in a Geiger-Muller Counter. Background radiation levels and air filtration flow has to be considered to calculate the Total Beta Radioactivity concentration. 149 samples were tested. The data were very low, lower than registeres in 1988.

Key words: Total Beta Radioactivity. Aire.

Pérez Sebastián, Miguel A. (Univ. del País Vasco. Dpto. Física Teórica e Historia de la Ciencia. Apdo. 644. 48080 Bilbao): Historia de la gravedad cuántica (History of Quantum Gravity) (Orig.es)

In: *Formula*. 4, 235-252

Abstract: In this work we propose a historical view of the different attempts to describe gravity by means of a quantum theory, that have taken place during the last 60 years. Although none of those proposals succeeded completely in achieving that aim, physicists today still keep on working in some of the research lines we are about to examine. We shall refer briefly to those early attemps from the 30's, to continue with the so-called semiclassical theory, the canonical theory and the path integral method. We shall deal with some aspects of quantum cosmology and other theories recently proposed with the aim of completing the description of gravity.

Key words: History of the Science. Gravity. Quantum theory. General relativity.

Sáenz Agirre, Jon (Instituto Vasco de Estudios e Investigación, S.A. IKEI. Rodríguez Arias, 5-6. 48008 Bilbao): Cronología de la meteorología dinámica (Chronology of dynamic meteorology) (Orig.es)

In: *Formula*. 4, 253-281

Abstract: In this work we propose a historical view of the different attempts to describe gravity by means of a quantum theory, that have taken place during the last 60 years. Although none of those proposals succeeded completely in achieving that aim, physicists today still keep on working in some of the research lines we are about to examine. We shall refer briefly to those early attemps from the 30's, to continue with the so-called semiclassical theory, the canonical theory and the path integral method. We shall deal with some aspects of quantum cosmology and other theories recently proposed with the aim of completing the description of gravity.

Key words: History of dynamic meteorology

Tellaeche Celaá, Angel (Eusko Ikaskuntza. Mª Díaz de Haro, 11-1º. 48013 Bilbao): La Física y la Química en la LOGSE (The Physics and the Chemestry in the LOGSE) (Orig.es)

In: *Formula*. 4, 283-300

Abstract: The "LOGSE" is going to be applied the present course year in the educational levels corresponding to the Secondary Education. For this reason, it is convenient that the teaching stall has a clear knowledge about what is wanted with this new Education law and, besides, they have to get used to the new terminology. This work tries to give, some guide lines in this sense, and above all, referred to the subjects of Physics and Chemistry, subjects that in the E.S.O., are included in the field of the Natural Sciences.

Key words: Curricular desing. Logse. Physic. Chemistry.

Analytic Summary

López, Xabier; Ugalde, Jesus M. (Euskal Herriko Unibertsitatea. P.K. 1072. 20080 Donostia): 3. Lerroko elementu ez-alkalinoen cluster-ak. Fosforo katioiaren kimika (Lineal clusters of non-alchalyne elements. Chemistry of the phosphorus cathion) (Orig.eu)

In: *Formula*. 4, 301-319

Abstract: In this work some results on the gas-phase chemistry of P^+ are shown. We have studied the reactivity of the P^+ in its triplet ground state (^3P) with hydrides molecules such as SH_2, *ClH* and *FH*. We have discussed about the possibility of these ion-molecule reactions take place under interstellar conditions. In a second part of the work, we have characterized various ionic clusters of P^+ in both its triplet (^3P) and singlet (^1D) spin states. We have emphasized on properties like, optimum geometries and binding energies. Besides, binding mechanisms are discussed in terms of the topologic analysis of the charge density, **p**. Finally, we have performed a detailed analysis of various dioxides formed by the P^+ cation.

Key words: Radicals. Phosphorus Reactivity.

Varona Fernández, Mª Amparo (Univ. del País Vasco. Dpto. de Electricidad y Electrónica. Apdo. 644. 48080 Bilbao): Antecedentes y desarrollo de los sistemas actuales de reconocimiento automático del habla (Historical evolution in the current Automatic Speech Recognition Systems) (Orig.es)

In: *Formula*. 4, 321-346

Abstract: Historical evolution of Continuous Speech Recognition Systems in shown. These systems have two important steps: synthesis and analysis. A synthesiser reproduces the human voice and the analyser should understand the human voice. Nowadays the voice synthesis is very developed but the voice analysis is a very important open problem in the field of Artificial Intelligence. Finally some research directions for the future are pointed out.

Key Words: The recognition of the speech. Synthesis and analysis.