

Abstracta

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Trabalhos Aceitos para Publicação

A023-97 à A025-97

Trabalhos Aceitos para Apresentação em Conferências

C001-97 à C006-97

[A023.97] "Determination of Electron Paramagnetic Resonance Parameters for Osmium(III) Low-Spin Systems Using Graphical Solutions"

A. N. Medina, F. G. Gandra, M. L. Baesso, J. B. Lima, B. R. McGarvey, D. W. Franco

Optical absorption and electron paramagnetic resonance (EPR) results for the low-spin compounds $[\text{Os}(\text{NH}_3)_5\text{L}]\text{O}_3\text{SCF}_3\text{N}]$ $\text{L} = 4,4'$ -dithiodipyridene (dtdp) or H_2O , $n = 3$; $\text{L} = \text{O}_3\text{SCF}_3$, $n = 2$] are reported. The EPR powder spectrum is analysed and from the three experimental g-values the crystal-field parameters and the energy levels are determined. The negative sign obtained for the axial splitting in $[\text{Os}(\text{NH}_3)_5(\text{dtdp})][\text{O}_3\text{SCF}_3]$ has been interpreted to be the result of an OsIII L back-bonding interaction. The IR optical spectrum shows a broad band at 2080 nm that is compared to the estimate obtained from the EPR results. Analytical expressions for the crystal-field parameters and energy levels of the system are derived. In addition, an alternative graphical method which simplifies the estimation of ligand-field parameters from the EPR parameters is presented.

Journal of the Chemical Society-Faraday Transactions 93 (11), 2105-2111, 1997

[A024.97] "A Critical Analysis of Helmholtz's Argument Against Weber's Electrodynamics"

J. J. Caluzi e K. T. Assis

We present Helmholtz's argument against Weber's electrodynamics. It is related with a fixed charged non-conducting spherical shell and a charged particle moving inside it. Then we utilize Weber's electrodynamics plus Schrödinger's expression for gravitational interactions in order to obtain the equation of motion and to study this situation. We show that this approach avoids the problems pointed out by Helmholtz. Moreover, it indicates that the effective inertial mass of the charged particle will depend not only on the electrostatic potential of the shell but also on its velocity. This is a relevant aspect of Weber's theory.

Foundations of Physics 27 (10), 1445-1452, 1997

[A025.97] "The Formation of Nanostructures on Silicon Surfaces in the Presence of Hydrogen"

O. Teschke, D. M. Soares, L. A. O. Nunes

The presence of hydrogen in HF solutions at a silicon substrate surface is shown to be sufficient to produce a photoluminescent porous silicon layer. The photoluminescence measurements of bubbled and anodized samples show similar spectra when illuminated with UV radiation. This is strong evidence that the hydrogen produced by the anodic silicon dissolution reaction is also responsible for the formation of nanostructures. Highly efficient photoluminescent layers are formed when the hydrogen etching contribution is comparable to that induced by the anodic current. Hydrogen etching takes place as follows: hydrogen reacts by exchanging electrons with the nonpolar H-covered sites thereby fixing the difference of potential between them and the solution. This electron transfer also charges the semiconductor space charge region resulting in a difference of potential between the semiconductor and the solution. Therefore the regions that do not exchange electrons with the hydrogen-silicon bonds become positively polarized relative to the solution, which results in the breaking of the silicon-hydrogen bonds, the subsequent covering of these silicon atoms by F ions followed by silicon dissolution.

Applied Physics Letters 70 (21), 2840-2842, 1997

[C001.97] "Converting an Emergency Generator to a Cogeneration System: case study in a hospital"

J. L. Silveira, M. J. L. Cavalcanti, F. E. A. dos Santos, C. A. Luengo

Nowadays, the situation is delicate for industrial and service sectors. Electric power suppliers, with concession from the government, cannot produce appropriately to supply the increasing energy demand. Based in this reality, these private sectors are looking for more efficient and alternative technologies. They intend to solve the big electric energy deficit which puts in jeopardy the regional and national economic development. Cogeneration is one of the alternatives with increasing number of followers. It is a way to use primary energy to supply electric (or mechanic) and thermal energy at the same time to an user. In this paper, we present an study of the possible conversion of an emergency generator into a cogeneration system. The aim is complementary hot water production in a hospital to save energy. This system upgrading will produce electricity and recover the residual heat from exhaust gases to produce useful heat, increasing the operational efficiency of the system. Initially, the heat recovery system is calculated based in real from tests in a emergency generator. Such equipment is a Caterpillar (550 kW), installed at the Hospital with 400 beds located next to University of Campinas (UNICAMP), São Paulo, Brazil. The water will be heated to 600 C in accordance with Thermodynamics and Heat Transfer Laws. Finally, we show the economic feasibility of this conversion terms of capital amortisation time and utilisation equivalent period.

In: Fourth Asian-Pacific International Symposium on Combustion and Energy Utilization - 4th APISCEU, Bangkok, Thailand, 8-12 dezembro, 1997

[C002.97] "Activation of Mesophase by Oxygen Plasma"

A. R. Coutinho, C. Otani, M. Massi, S. Otani, H. S. Maciel, C. A. Luengo

Active carbons (AC) are characterized by large specific surface areas and high porous volumes, their main property is to adsorb gases and liquids [1]. Due to their microporous structure. AC are applied for several adsorption processes such as water treatment, gas mixture separation, chemical products purification and others. The conventional process of AC production utilizes coal and biomass, which are carbonized at high temperature and activated by steam, air or CO_2 . Recently, AC are obtained from new raw materials, cellulose, carbon fibers, mesocarbon microbeads [2-4]. Moreover, new techniques like chemical processes and plasma corrosion were also employed [5-8].

In: Twenty-Third Biennial Conference on Carbon, Pennsylvania, USA, 13-18 julho, v. II, 28-29, 1997

[C003.97] "The Study of QI Extraction from Coal Tar Pitch Using Coal-Tar-Derived Oils as Solvent in a Centrifugation Process"

A.T. Gontijo, C. Otani, S. Otani, C. A. Luengo

Quinoline Insoluble (QI) fraction is a very complex important component of pitches, which remains as one of the subjects intensively investigated even in this decade. While the optimization of mechanical properties of synthetic graphite can be ascribed to the adequate choice of binder pitch with specific range of QI contents, the development of special form of carbon, such as carbon fibers, depends on the pitches from which the natural QI has been completely removed [1-2]. Many physical and/or chemical methods can be applied to the pitch QI extraction process. The dilution of pitch by coal-tar-derived organic oils followed by physical separation has been noticed to be efficient [3-5]. The aim of the present

work is to recognize the basic chemical components of several organic oils produced at a metallurgical coke production plant, as well as their efficiency as QI extraction agent.

In: **Twenty-Third Biennial Conference on Carbon Pennsylvania, USA, 13-18 julho. A Centrifugation Process, v. II, 198-199, 1997**

[C004.97] "Production of Mesophase from a Coal Tar Pitch in a Semi-Pilot Polymerization Reactor"

A. T. Gontijo, C. Otani, S. Otani, C. A. Luengo

Anisotropic phase formation and growth, in an isotropic pitch media, are associated with complex physico-chemical processes which are intermediate steps of the pyrolytic transformation towards carbon materials [1-2]. These reactions are strongly dependent on process parameters and also on the chemical characteristics of pitches used as raw materials [2-3]. An experimental device was designed and constructed to establish better conditions for mesophase formation in a coal tar soft pitch, produced by the USIMINAS metallurgical coke plant.

In: **Twenty-Third Biennial Conference on Carbon Pennsylvania, USA, 13-18 julho, v. II, 30-31, 1997**

[C005.97] "High Yield Carbons from Eucalyptus Wood at Elevated Pressures"

G. Bezzon, C. A. Luengo, X. Daí, M. J. Antal Jr.

The controlled pyrolysis of biomass at elevated pressures results in high yields of a good quality charcoal with a cycle of two hours or less and a reduced energy consumption. Due to the high yields, this process minimizes gases and liquids production, diminishing the pollutants generated by the conventional biomass pyrolysis [1-3]. Further oxidation under controlled conditions, can activate the charcoal obtained in the pyrolysis step, increasing its internal surface area and pore volume. Depending on the burn-off and the reaction time, high yields of activated carbon in a short period can be achieved. For a good pore development the oxygen diffusion and the reaction must have compatible rates otherwise, only the external surface is consumed and the pores are not formed.

In: **Twenty-Third Biennial Conference on Carbon Pennsylvania, USA, 13-18 julho, v. II, 258-261, 1997**

[C006.97] "Influence of Naphthalene Based Coal Tar Derived Oils on Mesophase Characteristics"

A. T. Gontijo, C. Otani, S. Otani, C. A. Luengo

There are several proposals of materials and methods useful in conversion of isotropic pitches to anisotropic mesophase [1-2]. Some emphasize heat treatment equipment and processing parameters[1]. Others report on the effects on

mesophase yield and quality of physico-chemical treatments of pitches[2]. A great deal of research shows a definite interest in primary quinoline insolubles fraction (QI) effects over mesophase nucleation, growth and coalescence. The main purpose of this work is to study the solvent effectiveness of coal tar derived oils on the soft coal tar pitch, to remove the QI fraction for improving mesophase production yield[3,4].

In: **Twenty-Third Biennial Conference on Carbon Pennsylvania, USA, 13-18 julho, v. II-2: Carbonization, Mesophase and Graphitization, 1997**

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