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## Molecular Geometry in Polymerization Formation



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### ABSTRACT

The crosslinking agent used to obtain a MIP (Molecularly Printed Polymer) performs the following three main functions: control of the morphology of the polymeric matrix (gel-like polymer, macroporous polymer or microgel powder); stabilization of binding sites capable of molecular recognition; mechanical stabilization of the polymeric matrix. Proposal: Molecular modeling observing a polymerizable scale factor in  $k$  set of functional monomers using the cross-linking agent tetra-methylene-dimethacrylate. Where the equation is:  $k \cdot (K-n) = Rt^1 - Rt^2 / Rr$  It is explained that  $k$  is the subset of parameters obtained in distribution of probability density between the AB interval, with the total number of events possible being equal to the solvent ratio that occurs in T1 initial time and T2 time interval to be measured divided by the ratio crosslinking. Diffusion coefficient of chemical species:  $k^1 \cdot (Kn - plim^\infty) = DX + DY + DZ$  where  $k^1$  which is the initial coefficient of molar ratio / kinetic ratio multiplied by  $kn$  which is the exponential critical exponent of renormalized reactivity decreased by progression critical kinetic limit equal to the correlation to the three-dimensional chemical crossing matrix determinants in X, Y and Z.

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### 1. Introduction

The crosslinking agent used to obtain a MIP (Molecularly Printed Polymer) performs the following three main functions: control of the morphology of the polymeric matrix (gel-like polymer, macroporous polymer or microgel powder); stabilization of binding sites capable of molecular recognition; mechanical stabilization of the polymeric matrix.

**Proposal:** Molecular modeling observing a polymerizable scale factor in  $k$  set of functional monomers using the cross-linking agent tetra-methylene-dimethacrylate. Where the equation is:  $k \cdot (K-n) = Rt^1 - Rt^2 / Rr$

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Diffusion coefficient of chemical species:  $k^1 \cdot (Kn - plim^\infty) = DX + DY + DZ$  where  $k^1$  which is the initial coefficient of molar ratio/kinetic ratio multiplied by  $kn$  which is the exponential critical exponent of renormalized reactivity decreased by progression critical kinetic limit equal to the correlation to the three-dimensional chemical crossing matrix determinants in X, Y and Z.

Homogeneous or heterogeneous catalysis of single atom organic metals, covalence, kinetics, complex burger system, coupling of aromatic azo-aromatic compounds, organometallic compounds, nucleophilic attack to spatial structure, possibility of efficient catalyst that integrates homogeneous and heterogeneous processes by transition metals coupled to spatial chains, selectivity of catalysis by Pt platinum which is a transition metal, the oxygen waves act as Lewis acids - possibility: A Lewis acid is a chemical species in which one of its constituent atoms has electron deficiency. This column makes it susceptible to accept an electron pair, and therefore to create a coordinated covalent bond with a Lewis base. In which isolated and positively charged metal centers can successfully suppress the adsorption of C = C bonds, which would easily occur in their nanoparticle counterparts.

Reaction distribution of acid and solvents  $Dtma/Dtre = Dtms/Dtcs$  which means acid molar ratio determinant divided by Lewis acid electron exchange determinant equal to the solvent molar ratio determinant divided by the solvent kinetic ratio determinant.

For the creation of Molecularly Printed Polymers in the improvement of high performance catalytic agents, the following solution is adopted:

First of calculating through the Graph Theory the stability index of most graphs, looking at vertices and edges together, for synthesis of nucleophilic attack, then we have:

The stability index of almost every graph is surprisingly low compared to the number of vertices in the graph:

However small the positive number  $\epsilon$ , we have  $\alpha(G) < (2 + \epsilon) \log_2 n$

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for almost every graph  $G$  in  $G(n)$ . PROOF: Let  $k$  be the number  $d(2 + \varepsilon) \log_2 ne$  and denote by  $Q(n, k)$  the set of  $k$  graphs in  $G(n)$  for which  $\alpha \geq k$ . It remains to show that  $\lim_{n \rightarrow \infty} |Q(n, k)| / |G(n)| = 0$ . (2.1) Let  $X$  be a subset of  $V$  with  $k$  elements. There is a one-to-one correspondence between the graphs in  $G(n)$  in which  $X$  is stable and the subsets of  $V(2) \times X(2)$ . Therefore,  $X$  is stable at  $2N - K$  of the graphs, where  $K = k2$ . Since  $V$  has  $k \leq nk$  subsets of cardinality  $k$ , we have  $|Q(n, k)| \leq nk 2N - K$ , and therefore  $|Q(n, k)| / |G(n)| \leq nk 2^{-k} - k(k-1)/2$ . It follows that  $2 \log_2 (|Q(n, k)| / |G(n)|) \leq 2k \log_2 n - k(k-1) = k(1 + 2 \log_2 n - k) \leq d(2 + \varepsilon) \log_2 ne (1 + 2 \log_2 n - (2 + \varepsilon) \log_2 n) = d(2 + \varepsilon) \log_2 ne (1 - \varepsilon \log_2 n)$ . (2.2)

Since  $\lim_{n \rightarrow \infty} (1 - \varepsilon \log_2 n) = -\infty$ , we have  $\lim_{n \rightarrow \infty} |Q(n, k)| / |G(n)| = 0$ .

$\log_2 |Q(n, k)| / |G(n)| = -\infty$ , and that proves (2.1). For example, if  $\varepsilon = 0.2$  then, by virtue of (2.2), we have  $|Q(1024, 22)| \leq 2 \cdot 220 - 231 |G(1024)|$  and therefore a fraction of at least  $1 - 2^{-11}$  (more than 99.9%) of the graphs in  $G(1024)$  have  $\alpha < 22$ , mainly in the occurrence of spatial determination of exchange of electron pairs.

In addition, we need to worry about the rotation part of an integral.  $\int \Psi_{ij} \Psi_{ij} - K e_{ij} = R_{12}$ .

Note that  $1 / r_{ij}$  does not depend on any rotation coordinates. This means that all elements of the  $1 / r_{ij}$  matrix must be diagonal in the rotation ( $\alpha / \beta$ ) of the electrons  $i$  and  $j$ . For 2 electrons  $2 \cdot 2 \cdot 2$  and  $1s = J_1s, K e_{1s} = 0 e_j, 1s\alpha, 2s\alpha = J_1s, 2s, K_1s\alpha, 2s\alpha = K_1s, 2s e e, J_1s\alpha, 2s\beta = J_1s, 2s, K_1s\alpha, 2s\beta = 0$ . If, instead, we look explicitly at the  $\alpha\beta + \beta\alpha$  and  $\alpha\beta - \beta\alpha$  generate their own states, we want  $2^{-1/2} [s_1s\alpha, 2s\beta \pm \Psi_1s\beta, 2s\alpha] \cdot 1 [\Psi_1s\alpha, 2s\beta \pm \Psi_1s\beta, 2s\alpha] r_{12}$  from which we obtain  $1 \cdot 1 (J_1s2s + J_1s2s) (K_1s2s + K_1s2s) = J_1s2s K_1s2s$ . 2 of the diagonal of the transverse terms 6 terms note that this inversion of the signal comes from the permutation of 1-2 electrons. The upper signal corresponds to the triplet  $E_{3s} = J_1s, 2s - K_1s, 2s E_{1s} = J_1s, 2s + K_1s, 2s$ .

Calculate the probability density of Bayesian electron statistics: Probability Density In statistics, the probability density distribution is a function used to represent the probability distribution of a continuous random variable. Uses the calculation:  $f(x) = \int_{-\infty}^{\infty} \delta(x - x') f(x') dx$

Then the systems calculation described by a Hamiltonian is made, calculating the scale factor that reduces the freedom of the atom's dimensional system.

The trajectory integral must be calculated, which consists of a superposition of local harmonic oscillator trajectory integrals centered on average positions ( $x_0$ ), each with its own frequency  $\Omega(x_0)$ .

Finally, the Slater determinants are used to calculate the energies. In addition to calculating for the spin connection of the paired electrons in opposite directions, the electron rotation orbitals and the determination of space orbitals, so to speak the esterification reactions are accelerated by the presence of  $H^+$  ions, so one can establish the formation of diagrams and computational modeling of a Molecularly Printed Polymer through the creation of a spatial modeling algorithm, in view of the library of polymers and chemical affinities, creating a complex system of graphic determinants of vertices and edges for molecular geometry. There was a discovery that the stability index of almost all graphs is low compared to the number of vertices in the graph.

#### Conflict Of Interest

None

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None

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