

[Chem. Pharm. Bull., 42, 768-773 (1994)]

[Lab. of Pharm. Physical Chemistry]

Mechanochemical Solid-State Polymerization. VI. Quantum Chemical Considerations for Structural Criteria of Mechanically Polymerizable Vinyl Monomers.

SHIN-ICHI KONDO, KATSUYUKI MURASE, MASAYUKI KUZUYA*

To provide the structural criteria for mechanically polymerizable vinyl monomers in metallic vessels, we carried out the MO calculations (AM1 method) of several acrylamide, acrylate and styrene derivatives as model compounds for such reactions. It was found that the nature of LUMO of vinyl monomers is closely related to the capability for initiation of mechanochemical polymerization. The following requisite concerning the nature of LUMO was shown to be a necessary condition for the activity of such reactions: Even if the LUMO energy is lower than 0.166eV in the AM1 scheme, the LUMO coefficient must be highly localized in the vinyl group.

[Bull. Chem. Soc. Jpn., 67, 641-647 (1994)]

[Lab. of Pharm. Physical Chemistry]

Quantum Chemical Rationale on Free-Radical Formation of Irradiated Acrylic Polymers.

AKIHIRO NOGUCHI, SHIN-ICHI KONDO, MASAYUKI KUZUYA*

The bond cleavage of poly (acrylic acid) (PAA) and poly (methacrylic acid) (PMAA) in their excited states was investigated by means of molecular orbital calculations (AM1 and IND O/S-CI methods) using model molecules. The calculated reaction potentials for the bond cleavages in the excited states showed that the most dissociative bonds are the α -C-H bond for PAA and the C-C bond associated with the decarboxylation for PMAA. β -C-C bond cleavage following the above-mentioned side-bond cleavages seems to be feasible in the higher excited states. The formation of free radicals in the plasma- and γ -irradiations of PAA, PMAA, and their esters could be well explained as reactions in the excited states.

[Chem. Pharm. Bull., 42, 1896-1901 (1994)]

[Lab. of Pharm. Physical Chemistry]

Nature of Protein Adsorption in Artificial Tear Solution on Plasma-Irradiated Polymethylmethacrylate Surface.

KAORU KAMIYA, YASUKICHI YANAGIHARA, TOMOKAZU TAKAI, MASAYUKI KUZUYA*

To evaluate the effect of plasma treatment on protein adsorption onto a polymer surface, we examined the adsorption behavior of protein after immersion of Ar plasma treated polymethylmethacrylate (PMMA) plate in the artificial tear solution containing lysozyme, albumin and γ -globulin. It was found that the total adsorption of protein in the artificial tear solution to PMMA is suppressed by the Ar plasma treatment. But the adsorption of each component protein differs according to the surface condition of polymers and obviously corresponds to the change with time in the surface wettability. It is concluded that introduction of a hydrophilic group into the PMMA surface by plasma treatment and coming off of it are associated with the adsorption behavior of proteins.