IMPROVING THE EFFICIENCY OF DIPHENYLDISULFIDE AS A DEVULCANIZING AGENT

Pumza Mente, Chris Woolard and Cedric McCleland

Department of Chemistry, Nelson Mandela Metropolitan University, Summerstrand, Port Elizabeth
E-mail: s211163872@live.nmmu.ac.za

ABSTRACT

Rubber recycling has been an interesting aspect in the rubber industry for quite some time. This interest has been raised by the difficulty of rubber materials to decompose and also the complications involved in its recycling process. Rubber devulcanization is a potential method for recycling of rubber waste materials. Diphenyldisulfide is one of the compounds used to increase the rates of this process by affecting the carbon-sulfur bond breakage. Devulcanization by diphenyldisulfide is said to follow a three step radical mechanism. In this research these three radical steps have been investigated using Spartan molecular modelling software with Density functional theory B3LYP hybrid and the basis set 6-31G** to optimize the relative reaction enthalpies involved in the process.

The first step involves the breakage of the sulfur-sulfur bond by Diphenyldisulfide. This step has been optimized by investigating the effects, on BDE's of the S-S bond in DPDS, introduced by adding different substituents on the phenyl rings. The efficient substituents were those lowering BDE's for the S-S bond when substituted in the para position in XPhS - SPhX. These efficient substituents were then used to investigate effects of substituting at different positions in the phenyl rings as well as the effect of adding multiple substituents in one ring. Hydroxy and the amine groups were observed to be the most efficient substituents, the decrease in DBE of S-S was greatly signified by substituting these groups at ortho position and the effect was further enhanced by substituting three of these groups in one ring.

The second step involves reaction of RSSR with $XPhS^{\cdot}$. This step has been optimized by investigating the enthalpy of the above reaction.

The third step is the reaction of XPhS – R with $XPhS^{\cdot}$. This step has been optimized by investigating the reaction enthalpies of the above reaction. The optimal devulcanizing agent was found to be Bis(2,4,6-Trihydroxy-Phenyl)Disulfide and it was applied to model the breaking of crosslinks in vulcanized natural rubber monomer [Di(2-MethylButene)Disulfide]. The results obtained on application of this model agreed with hypothesis - Bis(2,4,6-Trihydroxy-Phenyl)Disulfide lowers the BDE of the S-S bond in natural rubber.

Acknowledgement: Nelson Mandela Metropolitan University and Recycling and Economic Development Initiative of South Africa (REDISA) for financial assistance.