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A DFT study of the ring opening mechanism of tetraethyl-2-aryl-1,2-epoxygembisphosphonates

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A DFT investigation of the ring opening mechanism of tetraethyl 2-aryl-1,2-epoxygembisphosphonates on the C-O bonds of the oxirane ring using ammonia as the nucleophile were carried out. Thermodynamic data obtained in both the gas phase and solvent simulations showed that the ring opening is favoured at the less hindered carbon (C2) of the oxirane ring. Varia-tion of the substituent on C2 to lower the activation energy revealed electron-donating methoxybenzene to be the best sub-stituent in this study.

HPC content

I am not sure what to insert here.

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