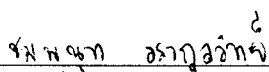
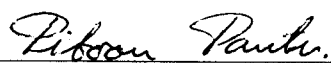


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Diels-Alder reactions of [60]fullerene, C_{60} , have been studied using the B3LYP/LANL2DZ//AM1 approach. The low computational method, B3LYP/LANL2DZ//AM1, appears to be acceptable in obtaining reasonable estimates of reaction energies and energy barriers. The calculations reveal that the electron deficiency character and the stabilized LUMO orbital cause the C_{60} to be much more reactive for the Diels-Alder reaction than ethylene molecule. In addition, the strain relief during product formation also helps decreasing the energy barrier for the Diels-Alder reaction. The presence of Na^+ metal ion in the cavity of C_{60} , though decreases product stability, increases kinetically reactivity of Diels-Alder reaction due to the pronounced electron deficiency of the central double bond of C_{60} caused by the metal cation. Among the Diels-Alder reactions of C_{60} -1,3-butadiene, C_{60} -2,3-dimethylbutadiene, C_{60} -o-quinodimethane, the electron donating ability of diene leads to the more reactive and more exothermic reactions. In the case of o-quinodimethane, the aromatic stabilization of the adjacent ring causes the reaction to be kinetically and thermodynamically much more favorable than the reaction with butadiene and 2,3-dimethylbutadiene.



Student's signature



Thesis Advisor's signature

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