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Density functional theory investigation of electrophilic addition reaction of chlorine to tricyclo[4.2.2.$2^{2,5}$]dodeca-1,5-diene

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Abstract: Potential energy surface (PES) of the tricyclo[4.2.2.$2^{2,5}$]dodeca- 1,5-diene (TCDD)-Cl_2 system was studied by B3LYP/6-311+G(d,p) method and the configurations [reactants, molecular charge-transfer (CT) complex, transition states (TS1 and TS2), intermediate (INT), and product (P)] corresponding to the stationary points (minima or saddle points) were determined. Initially, a molecular CT-complex forms between Cl_2 and TCDD. With a barrier of 22.362 kcal mol^{-1} the CT-complex can be activated to an intermediate (INT) with energy 14.682 kcal mol^{-1} higher than that of the CT-complex. The intermediate (INT) then transforms easily (barrier 5.102 kcal mol^{-1}) into the