Maximizing the Solar Energy Storage of the Four Substituted Norbornadiene-Quadricyclane System: DFT Calculations[1]

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Abstract—The purpose of this research is to study the solar energy storage in norbornadiene (**1**)/quadricyclane (**2**) system by four direct attachments of substituents at two carbon atoms on both sides of the double bonds C_2=C_3 and C_5=C_6 in $\mathbf{1_X}$ and $\mathbf{2_X}$; calculating the relative energies at B3LYP/6-311++G** level of theory. The solar energy storage of four electron donating substituents, (push-push effect), X (X = $-NH_2$, $-OH$) and four electron withdrawing substituents, (pull-pull effect) X (X = $-CO_2H$, $-CONH_2$, $-NO_2$ and CN) were examined. The solar absorption bands were calculated for $\mathbf{1_X}$. The DFT calculations reveal that the bands were shifted to the visible spectrum region when the electron withdrawing substituents were used rather than the electron donating substituents.

Keywords: solar energy, norbornadiene, quadricyclane, electronic effects, light absorption, substitution effects.

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