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Quantum-Chemical StudyFor Some Coumarin Compounds by using semi-empirical methods

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Abstract: In the present research, we studiedthe properties of some coumarin derivatives by using semi – empirical methods (ZINDO/1, ZINDO/S and PM3),We carried out to determine the binding energy ΔEb , heat of formation $\Delta H^{o}F$, and dipole moment for some coumarin derivatives. Also the electronic transitions and vibration frequencies were calculated for these compounds. Electrostatic potential , HOMO and LUMO energies were calculated to determine the reactive sites of these compounds.
Keywords : Coumarin, Semi – empirical methods,Dipole moment , Binding energy.

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