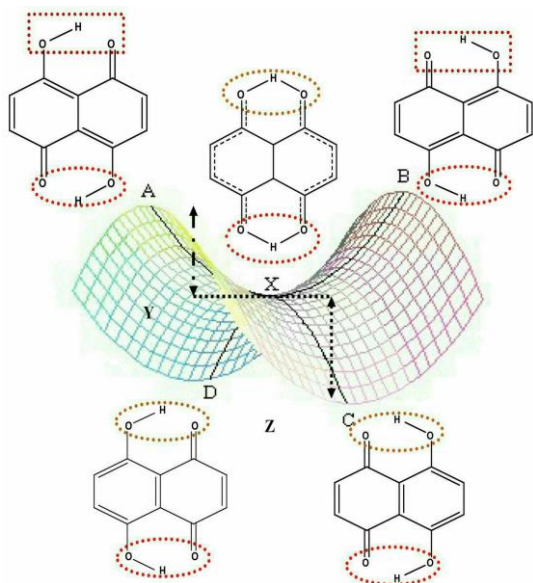
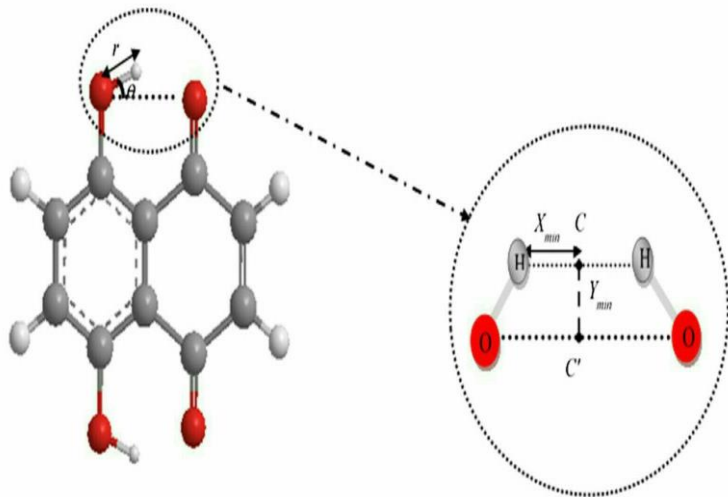


# P5158: THE EFFECT OF THE SADDLE POINT POSITION AND THE OH-BONDING FORCE CONSTANT ON THE TRANSITION FREQUENCIES OF H-BOND OF NAPHTHAZARIN

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**AXC OR DXC**



**DFT**

$$2V = K_s X^2 + K_{ss} X^4 + K_b Y^2 + K_{ssb} X^2 Y$$

Effect of  $k_b$  &  $Y_{\min}$

$$\left(\frac{\partial V}{\partial Y}\right)_X = 0$$

$$K_b Y_{\min} + \frac{1}{2} K_{ssb} X_{\min}^2 = 0$$

