An Investigation of Interactions in Barakol Complexes

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Barakol has various interactions that contribute to its biological activities. This work presents the first successful crystal structure determination of anhydrobarakol and its analogues. Anhydrobarakol and anhydrobarakol hydrochloride were crystallized in a monoclinic system, space group $P2_1/c$ and $P2_1/n$, $Z = 4$ with unit cell parameters a = 13.2280(7), b= 6.8738(2) , c = 19.7879(9) Å, β = 127.013(2)° and a = 12.2547(2), b = 8.051(2) , c = 12.8133(2) Å, β = 99.514(1)°, respectively. The novel 1:1 molecular complexes of barakol and carboxylic acid (phthalic acid and 3-hydroxybenzoic acid) were synthesized and charactherized by spectroscopic and X-ray crystallographic techniques. Electrostatic effects, electron delocalization, and intermolecular interactions in the barakol ring system were investigated. The X-ray crystallographic studies revealed that the barakol-phthalate complex exists in an ion-pair complex. The formation of barakol-phthalate ion-pair complex is stabilized by the complementary of ion-ion interaction,π-π interaction and hydrogen bonding. The barakol-3-hydroxybenzoic acid complex is a π-π molecular complex. The co-crystallization of barakol- 3-hydroxybenzoic acid complex is solely stabilized by π-π interactions. The spectroscopic studies including IR, ^{1}H-NMR and UV-visible are consistent with the results from the X-ray analysis.

Keywords: barakol, x-ray diffraction, spectroscopic method