Poster Presentation

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The Effect of the Methanol Molecule in the Stabilization of C18H18O4 Chalcone

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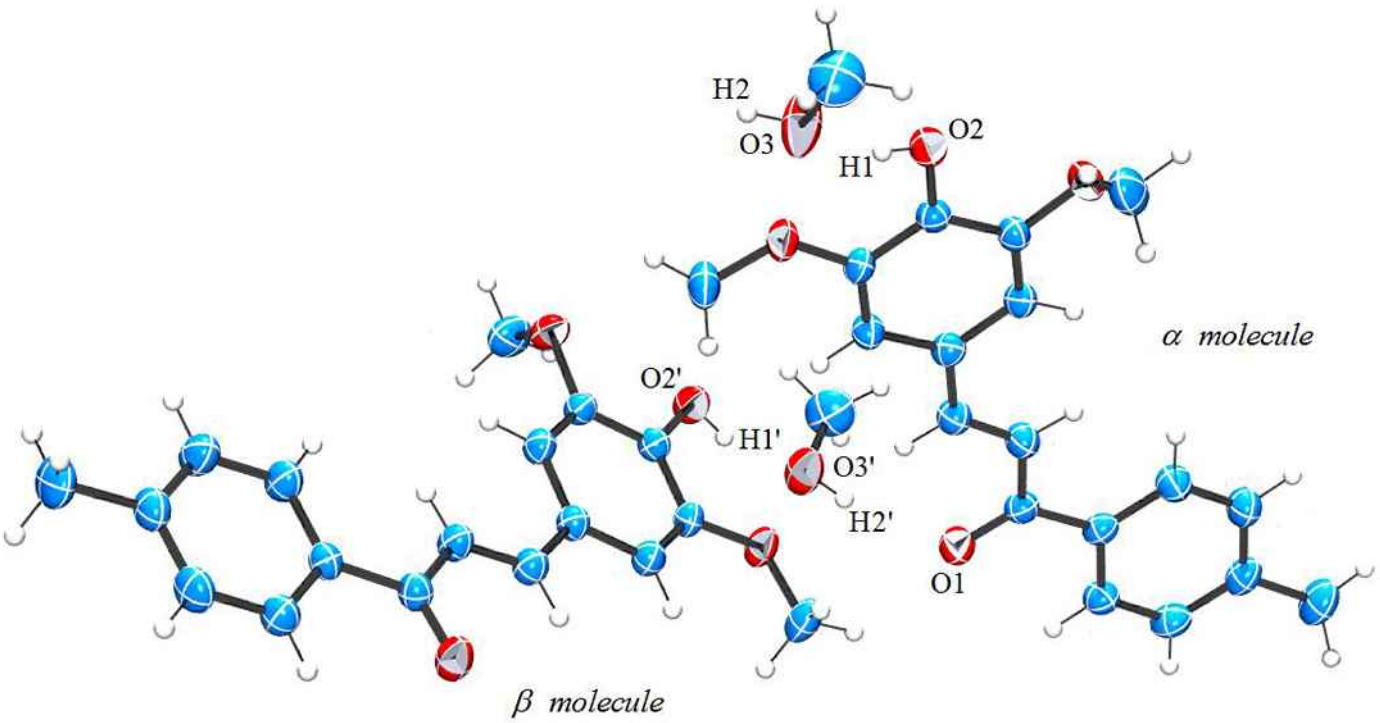
The (E)-3-(4-hydroxy-3,5-dimethoxyphenyl)-1-p-tolylprop-2-en-1-one crystallizes in the triclinic centrossymetric P1̄ space group as a solvate structure (Figure 1). The asymmetric unit is described by a 2[(C18H18O4).(CH3OH)] molecular complex, in which each independent C18H18O4 molecules is bonded to a specific methanol molecule (R1 = 0.1237, wR2 = 0.1869 to all data). The presence of methanol in this crystal lattice results in a unit cell with Z' > 1 which two molecules of methanol and chalcone (alpha molecule and beta molecule) forming a stable molecular complex. With the aim of understanding the process of crystal lattice stabilization, a combination of technique has been used including X-ray diffraction (XRPD), computational molecular modeling and a molecular dynamic. The results show: alpha molecule and beta molecule are sterically barred to form direct hydrogen bond each other. On the another hand, the presence of methanol molecule stabilizes the crystal structure by bifurcated O-H…O interaction acting as a bridge between them. The theoretical thermodynamic parameter and the rigid potential energy surface scan comprise the role of methanol in the energetic stabilization of the crystal. The absence the methanol compound in the asymmetric unit destabilizes the crystalline structure, turning the formation process of the asymmetric unit not spontaneous. The energy difference between alpha and beta molecules is around 0.80 kcal/mol, indicating that both are stable and are equally possible in the crystal lattice. The analyze of the energetic profile of the C14 – O2…H1 – O3 and O2 – H1…O3 – C17 torsion angles in the packing crystal show that the alpha and beta molecules are confined in the stable potential region, in agreement with the two conformer in the asymmetric unit. The MEP show that the methanol have no steric effect that avoid small motion around the torsions angles. The authors would like to acknowledge the Brazilian agencies for financial support: Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and Fundação de Amparo Pesquisa do Estado de Goias (FAPEG).



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