CD chemistry and modeling

THE ROLE OF STRUCTURE IN INCLUSION CAPACITY AND PHYSICAL PROPERTIES OF SOLID CYCLODEXTRINS

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The selection of appropriate cyclodextrin (CD) is one of the main problems in their applications. The problem of such choice is that the applied CD complexes are often prepared in a solid phase. But systematic comparison of different CDs has been made only for complexation in aqueous solutions. For such characterization, structure-property relationships are to be obtained for solid CDs. Also, in most industrial cases water is added to solid CDs to make technological pastes. Here, water acts both as activating agent and competing guest. For various CDs, the ratio of these roles has significant differences as show our studies of hydration Gibbs energies. The highest affinity of α-CD to water can be the main reason why it is not used so often as of β-CD.[1] Such problem can be solved using hydration level/history control. Also, for all native CDs, organic analogues can show better results being applied instead of water.[2] Analysis of the role of water and inclusion thermodynamics allowed to find the recommendation for better preparation method for each native CD.

The roles of water during CD complexation can be explained by the density of crystal packing of CD hydrates. For this study, we performed the powder XRD indexation of unit cell parameters for all natural CDs and their intermediate hydrates. These structural data are also in good agreement with melting parameters and high-temperature behavior of natural CDs using fast scanning calorimetry (FSC). FSC is state-of-the-art method which allowed to find the melting points of natural CDs, also as melting enthalpy of γ-cyclodextrin. Such data are essential for understanding structure-property relationships; for calculations on the energy of the crystal lattice, which has a crucial effect on inclusion properties; for evaluation of the limiting temperatures during the modification of drug complexes by fast heating and cooling.

1. Gatiatulin, A. K.; Osel'skaya, V. Y.; Ziganshin, M. A.; Gorbatchuk, V. V*. RSC Adv*., **2019**, 9, 37778-37787.
2. Gatiatulin, A. K.; Osel'skaya, V. Y.; Ziganshin, M. A.; Gorbatchuk, V. V*. J. Therm. Anal. Calorim*., **2021**, 146, 2417-2422.

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