Hydrogen-Deuterium Exchange as a Means of Probing Water-Solid Interactions

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It is well known that water can interact with pharmaceutical materials in a number of different ways. In certain types of hydrated materials e.g. crystal hydrates and hydrophilic amorphous materials, water is not only adsorbed at the surface, but also present in the bulk structure. Using an innovative approach, Saenger and co-workers (1) have used deuterium oxide (D_2O) vapour to probe water diffusion in cyclodextrins. In this presentation, we will discuss the use of this technique to study different types of hydrated materials of pharmaceutical interest. Various model hydrates were exposed to an atmosphere of D_2O and the exchange of hydrate water (and any other exchangeable hydrogens) with D_2O was monitored using Raman spectroscopy. Model compounds included channel hydrates such as caffeine and theophylline, and hydrate forming sugars (as both the crystalline and amorphous phases). It was observed that both the rate and extent of exchange differed between compounds. Amorphous sugars underwent complete exchange, suggesting that D_2O has access to all hydroxyl functions. The crystalline hydrate counterparts only underwent partial exchange, indicating that water access is more limited in the crystal. For the channel hydrates, the kinetics of exchange varied considerably between the different compounds. In all cases, it was possible to rationalize the observed variations in exchange behaviour with the crystal structures. In conclusion, using exchange experiments to investigate hydrates appears to be a useful probe of structure.

Reference

1 T. Steiner, A.M. Dasilva, J.J.C. Teixeiradias, J. Muller and W. Saenger. Angew. Chem.. Int. Ed. Engel. 34:1452-1453