

Wettability Behaviour of Form I Paracetamol Crystals

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Contact angle measurements have often been used to study the wettability of solids. Current methods of characterising solid particulate materials have relied on powder bed techniques which can be inaccurate and complicated, from both an experimental and a theoretical perspective. This project aims to *directly* measure contact angles and determine surface energy components at different facets on a single macroscopic paracetamol crystal.

Large crystals provides ideally smooth and highly ordered surface for contact angle measurements by sessile drop method. Crystal seeds (1-2 mm) were prepared by cooling of saturated solutions. A single seed was dangled in saturated methanol solution to grow large single crystal (3-5 cm) by solvent evaporation at 20°C over a period of over 20 days. Several contact angle liquids were used. Advancing and receding contact angles recorded by oscillating the droplet volume deposited on facets 011, $10\bar{1}$ and $11\bar{1}$. The dispersive and polar, including acid-base surface energy components were then determined from the contact angle data.

Contact angles of the probe liquids varied on facets examined indicating presence of different functional groups on differing facets. Calculated values of dispersive surface energy, $\tilde{\alpha}_s^d$ varied marginally from 32-35 mJ/m² whilst the polar surface energy, $\tilde{\alpha}_s^p$ ranged from 17-38 mJ/m². It was observed that facets $10\bar{1}$ and $11\bar{1}$ had high polar energies due to probable presence of both hydroxyl and carbonyl functional groups near surface whilst hydroxyl groups were postulated not to be present on the facet 011. An acid-base analysis indicated that surface was relatively more basic, but absolute values were dependant on liquid combination and liquid properties used.

This study shows that the wettability of form I paracetamol crystals is anisotropic and these differences may be attributed to variations in local surface chemistry and molecular orientation. Measurements on powders give surface energy values which may not reflect the detailed surface chemistry of crystalline solids.