Hydrogen Bonds in “Carboxyoximes”: the Case of Bornane Derivatives

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The tendency of forming mixed carboxyl-to-oxime hydrogen bonds was tested on the series of bornane derivatives: one with the acid function only (bornane-2-\textit{endo}-carboxylic acid), one with the oxime function (2,2'-diethylthiobornane-3-oxime), and one with both oxime and carboxylic functions (bornane-2-oxime-3-\textit{endo}-carboxylic acid). The crystal structures of these compounds were determined by means of X-ray diffraction. In bornane-2-\textit{endo}-carboxylic acid and 2,2'-diethylthiobornane-3-oxime ‘homogenic’ hydrogen bonds were found, and these hydrogen bonds close eight- and six-membered rings, respectively. By contrast, in bornane-2-oxime-3-\textit{endo}-carboxylic acid ‘heterogenic’ hydrogen bonds between carboxylic and oxime bonds were found. This carboxylic-oxime, or ‘carboxyoxime’ system is almost always present in compounds which have both oxime and carboxylic groups; therefore it can be regarded as an element of supramolecular structures (synthon). The presence of such synthons can break the tendency of carboxylic acids and oximes towards crystallizing in centrosymmetric structures.