Synthesis and solid state structure for a series of poly(1-pyrrolylmethyl)benzene derivatives. Control of the interplaying π-π and C−H···π interactions?

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Supplementary Material (ESI)

A CSD search for intermolecular C−H···π(heterocycles) interactions.

A Cambridge Structural Database search for non-bonded contacts (Chart 1) was carried out using the program ConQuest (version 1.7).[i] The search criteria (CSD dated February 2005) were error and disorder free only structures (organic and organometallic) with *R* factors less than 0.1 (H normalized). Normalised structures were retrieved from the Cambridge Structural Database and analysed using VISTA (version 2.1).[ii] Of the 104 hits, 89 corresponded to C−H···π(N containing heterocycles).

Chart 1. Parameters used for the search

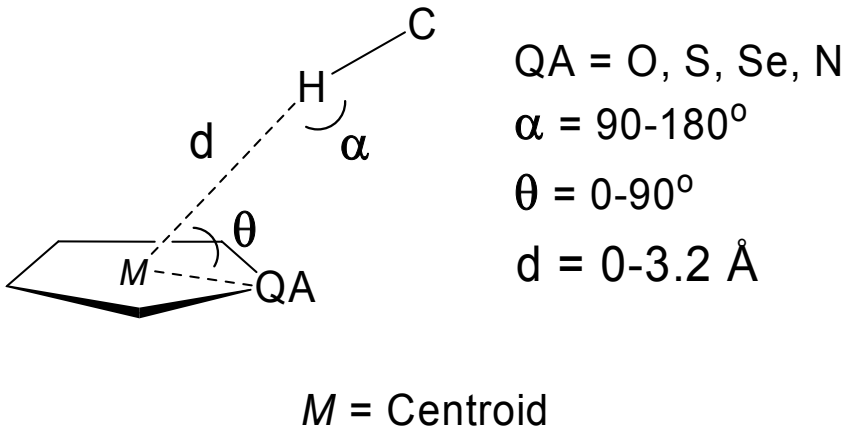


Figure I. Scattergrams for the geometry of the retrieved intermolecular C−H···π(heterocycle) interactions (see Chart 1 for nomenclature).

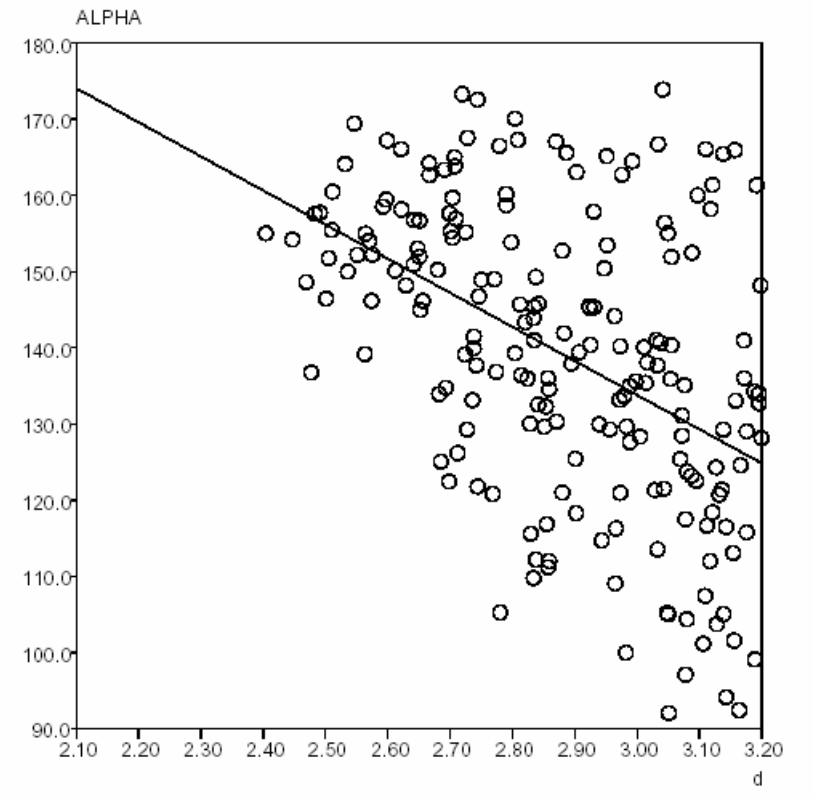
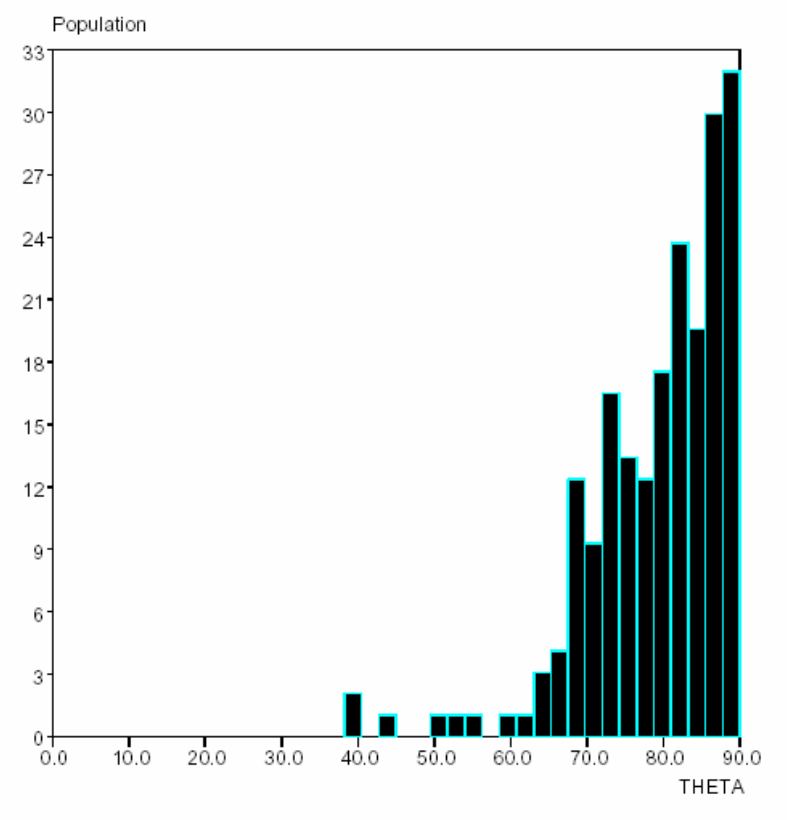


Figure II. Histogram of θ (THETA) angles (º).



(i) Bruno, I. J.; Cole, J. C.; Edgington, P. R.; Kessler, M.; Macrae, C. F.; McCabe, P.; Pearson, J.; Taylor, R. *Acta Cryst.* **2002**, *B58*, 389.

(ii) CCDC (1994). Vista - A Program for the Analysis and Display of Data Retrieved from the CSD. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England.