

# Poster Presentations

## [MS25-P08] Melting Point Alternation in the Primary Amines

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The phenomenon of melting point alternation between odd and even alkanes and alkane derivatives has been known since the late 19<sup>th</sup> century [1] but was, for many years, simply ascribed to “packing effects”. Determination of the crystal structures of alkanes, from ethane to nonane, allowed for a geometric rationalisation [2, 3] of this alternation, which can be ascribed to differences in the packing of carbon chains between odd and even membered alkanes. Further work into difunctional alkane derivatives [4-6] has shown that weak hydrogen-bonding and van der Waals interactions are competing driving forces driving the packing of these structures, and it is the ability to strike a balance between these two interactions that leads to the observed differences in melting points. Here, we report, for the first time, the structures of the primary monoamines from ethylamine to decylamine from single crystal data. All of these compounds are liquids at room temperature, so crystals were grown *in situ* by laser-assisted zone refinement. The alternation in melting points arises through differences in hydrogen-bonding and chain packing between odd and even molecules that are known to occur in similar compounds, as described above, and these differences are explored using CrystalExplorer [7] and the various structural tools available in Mercury [8]. A purely geometric analysis of crystal packing can sometimes miss important interactions, and so validation of our results is provided by energy calculations performed using the PIXEL [9] method. By way of this energetic analysis we are able to rationalise the point where hydrogen-bonding ceases to control the crystal packing

and the van der Waals interactions become the driving force. Additionally, we report a structural solution of the low temperature single crystal to powder phase transition observed in the case of ethylamine.

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**Keywords:** low-melting compounds; intermolecular interactions and packing in small-molecule crystals; PIXEL