

## Poster Presentation

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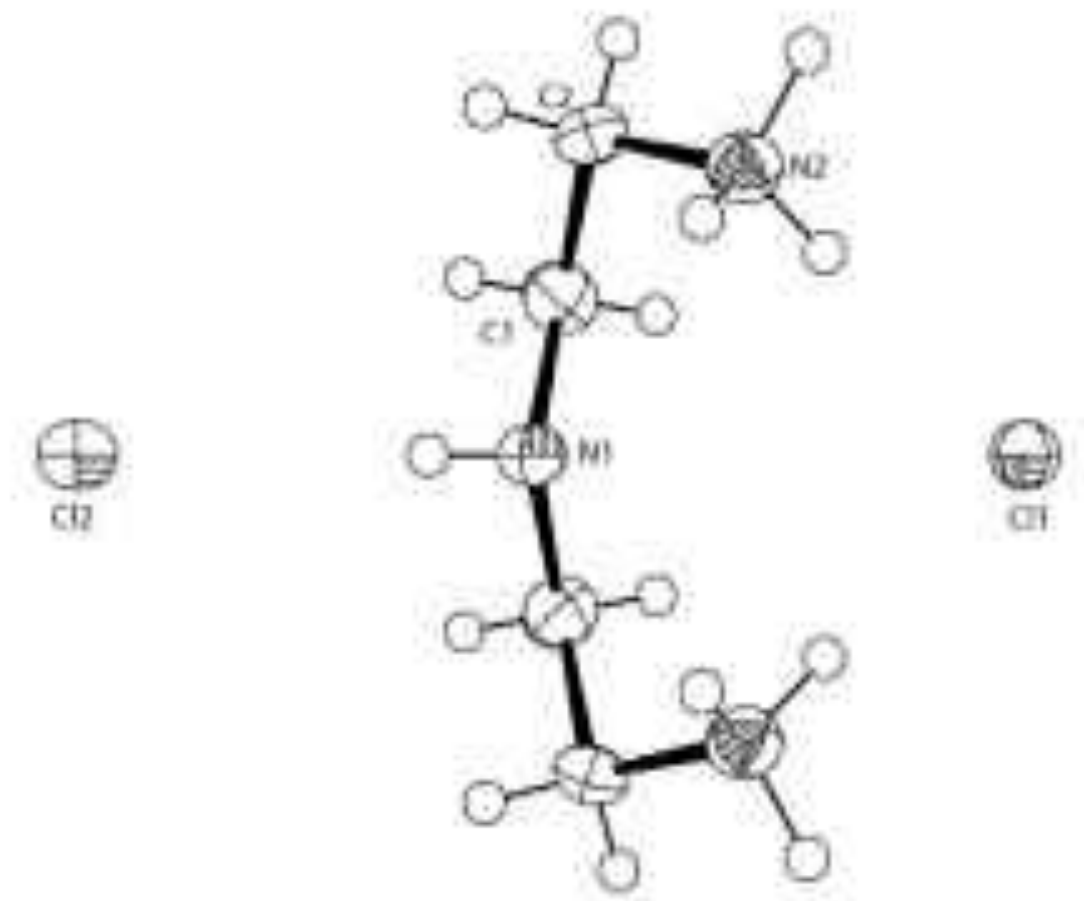
### Crystal structures of di- and tri-hydrochlorides of 1,4,7-triazaheptane

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Four protonated 1,4,8,11-tetraazacyclotetradecane has been characterized as nitrates to show expanded ring structure due to charge repulsion[1]. However, linear polyamine, 1,4,7-triazaheptane (diethylenetriamine=dien) gave di-hydrochloride(1) and tri-hydrochloride(2) and their single crystal structures were examined. In the compound 1, the terminal N atoms are protonated as expected but the dien takes U-shaped conformation with forming double H-bond to a Cl<sup>-</sup> ion at the terminals and the central nitrogen forms another H-bond to the other Cl<sup>-</sup> ion, as shown in the figure. The dien takes linear conformation in the compound 2 as expected.

[1] J. M. Harrowfield, H. Miyamae, T. M. Shand, et al., *Aust. J. Chem.*, 1996, 49, 1051-1066.



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