

s13.m42.o5 **Stressing a hydrogen-bonded grid: changes in symmetry and topology.** László Fábíán,^a Alajos Kálmán,^a Gyula Argay,^a Gábor Bernáth,^{b,c} and Zsuzsanna Cs. Gyarmati^{b,c}, ^a*Institute of Chemistry, Chemical Research Center of the Hungarian Academy of Sciences, Budapest, Hungary,* ^b*Research Group for Heterocyclic Chemistry, Hungarian Academy of Sciences and University of Szeged, Szeged, Hungary,* and ^c*Institute of Pharmaceutical Chemistry, University of Szeged, Szeged, Hungary.* E-mail: lfabian@chemres.hu

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We have recently combined two ladder-like hydrogen-bond patterns to form a two-dimensional hydrogen-bond grid [1]. The isostructurality of four homologous alicyclic *cis*- β -amino acids [1] suggested that this pattern may be robust enough to be useful in the crystal engineering of bilayer structures. To test the stability of the pattern, the effects of small molecular modifications on the crystal structure were investigated.

The effect of an unsaturated bond was examined via the crystal structure determination of *cis*-2-aminocyclohex-4-enecarboxylic acid. The molecules of this compound form hydrogen bonds in the solid that are analogous to those of its saturated counterpart. The structures differ only in the symmetry relationship between the molecules that form a given hydrogen bond. To stress the original pattern further, *trans* stereoisomers of both the saturated and the unsaturated compound were investigated. The crystals of *trans*-2-aminocyclohexanecarboxylic acid and *trans*-2-amino-cyclohex-4-enecarboxylic acid are isostructural. The hydrogen bonds in the *trans* structures are formed between the same molecules as in the *cis*-2-aminocyclohex-4-enecarboxylic acid crystals, but they involve different atoms. Finally, the grid was destroyed by using norbornane as the alicyclic fragment. The bridging ethylene moiety of *exo*-3-aminobicyclo[2.2.1]heptane-*exo*-2-carboxylic acid sterically inhibits the formation of the original pattern. Nevertheless, this compound still maintains a bilayer arrangement in the solid phase.

Overall, the above crystal structures demonstrate a gradually weakening correspondence to the original pattern. The unsaturated compound loses the symmetry, but maintains the topology of the first grid. The *trans* isomers distort the pattern topology at the atomic level, but preserve it at the molecular level. Finally, the norbornane derivative completely destroys the topology of the hydrogen-bond network, but still affords a similar overall crystal structure, which is based on infinite bilayers.

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- [1] Fábíán, L., Kálmán, A., Argay, Gy., Bernáth, G. & Gyarmati, Zs. (2002). *XIX Congress and General Assembly of the IUCr Abstracts*, C151.