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Layer-type Supramolecular Networks from Rosette Ribbons and Bridging Connectors

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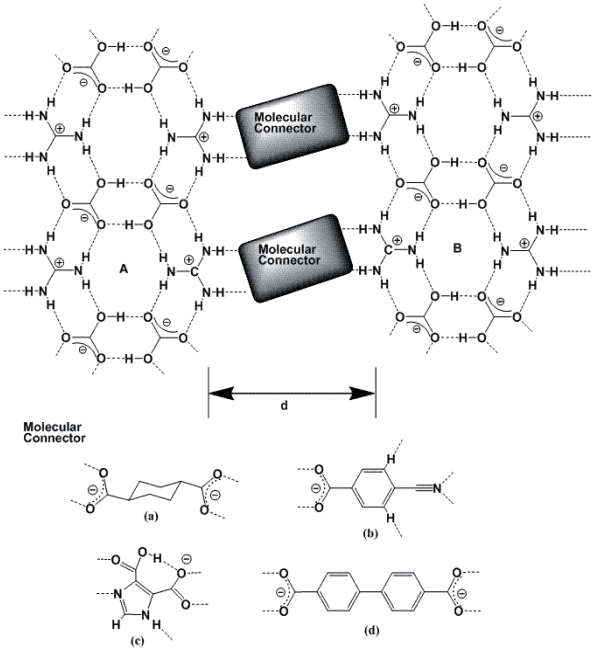
Over the years, chemical systems bearing a rosette motif (often described as hexagonal honeycomb unit or grid) have attracted considerable interest in connection with supramolecular self-assembly.[1] A rosette ribbon consists of a linear arrangement of hexagonal structural units that share fused opposite sides, and a sheet-like network can be generated by bridging an array of parallel ribbons with molecular connectors.[2]

We report the synthesis and X-ray analysis of a family of robust layer-type supramolecular networks featuring an uncharged, linear $GM^+HCO_3^-$ (GM^+ = guanidinium cation) fused-rosette ribbon hemmed with multiple N-H hydrogen-bond donor sites. Bridging of such parallel rosette ribbons by hydrogen-bond acceptors (1,4-cyclohexanedicarboxylate, 1,4-benzenedicarboxylate, 4-cyanobenzate and 1H-imidazole-4,5-dicarboxylate) as anionic molecular connectors is tolerant to a wide inter-ribbon separation ranging from 10.00 to 19.42 Å. Various tetraalkylammonium cations serve as guest templates to construct this series of four inclusion compounds.



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Crystal structures of hydrazinecarbothioamide derivatives

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Thiosemicarbazide compounds exhibit various biological activities such as anti-bacterial, anti-fungal and especially antituberculosis. Besides, thiosemicarbazide derivatives offer special affinity to inhibit corrosion of metals in acidic solutions [1, 2]. In order to search for new thiosemicarbazides, the compounds **I**-**III** have been synthesized and their crystal structures are reported here:

I: *N*-(4-chlorophenyl)-2-[(4-methyl-1,3-thiazol-5-yl)carbonyl]hydrazinecarbothioamide,

II: 2-(2-methyl-3-furoyl)-*N*-(4-methylphenyl)hydrazinecarbothioamide,

III: *N*-{[2-(1*H*-pyrrol-2-ylcarbonyl)hydrazino]carbonothioyl}benzamide hemihydrate.

	I	**II**	**III**
crystal system	monoclinic	triclinic	monoclinic
space group	$P2_1/n$	P-1	$P2/c$
a [Å]	9.899(2)	9.441(3)	14.494(5)
b [Å]	8.059(1)	11.883(4)	4.835(2)
c [Å]	17.702(2)	14.463(6)	19.915(6)
α [º]		74.46(4)	
β [º]	97.51(1)	69.56(3)	96.51(3)
γ [º]		73.93(3)	

In the crystal lattice of **I**, inversion related molcules are joined by chelated N–H···O hydrogen bonds forming the cyclic dimer. The interactions are thioamide···carbonyl and hydrazine···carbonyl, and within this dimer they could be described by the cyclic first-level $R^2_2(10)$ and $R^2_2(14)$ motifs. Moreover, in this crystal, second type of cyclic dimer is observed; molecules are linked by C–H···S (chlorophenyl··· thioamide) interactions – $R^2_2(12)$ graph set. Additionaly, the molecular structure is stabilized by intramolecular N–H···O (hydrazine···carbonyl) hydrogen bond.

Crystals of **II** are triclinic (*P*-1) with Z = 4. Two symmetrically independent V-shaped molecules are linked by N–H···O (thioamide···carbonyl), C–H···O (methyl-furoyl···carbonyl and methylphenyl···carbonyl) and N–H···S (hydrazine···thioamide) hydrogen bonds to form a ribbon.

As in **I**, dimeric arrangement is also observed in the crystal structure of hemihydrate **III**. Nearly planar molecules are associated by inversion-related N–H···O (pyrrol···carbonyl) hydrogen bonds, the dimer is denoted by the cyclic $R^2_2(10)$ graph set. Further, the dimers connected by N–H···O (hydrazine···carbonyl) and π···π interactions built the three-dimensional crystal net. There is second kind of N–H···O hydrogen bond – an intramolecular (hydrazine···carbonyl) which stabilized the molecular structure. In addition to these interactions water···**III** hydrogen bonds are observed, they are N–H···O (thioamide···water) and O–H···S (water···thioamide).