

Searching new crystalline substrates for OMBE: topological and energetic aspects of cleavable organic crystals

Pavel N. Zolotarev,^a Massimo Moret,^{b} Silvia Rizzato^c and Davide M. Proserpio^{a,c*}*

^aSamara Center for Theoretical Materials Science (SCTMS), Samara State Aerospace University
(National Research University) named after academician S.P.Korolyev, SSAU, Moskovskoe Shosse
34, Samara 443086, Russia

^bDipartimento di Scienza dei Materiali, Università degli Studi di Milano Bicocca, Via R. Cozzi 53,
20125 Milano, Italy

^dDipartimento di Chimica, Università degli Studi di Milano, Via C. Golgi 19, 20133 Milano, Italy

SUPPORTING INFORMATION

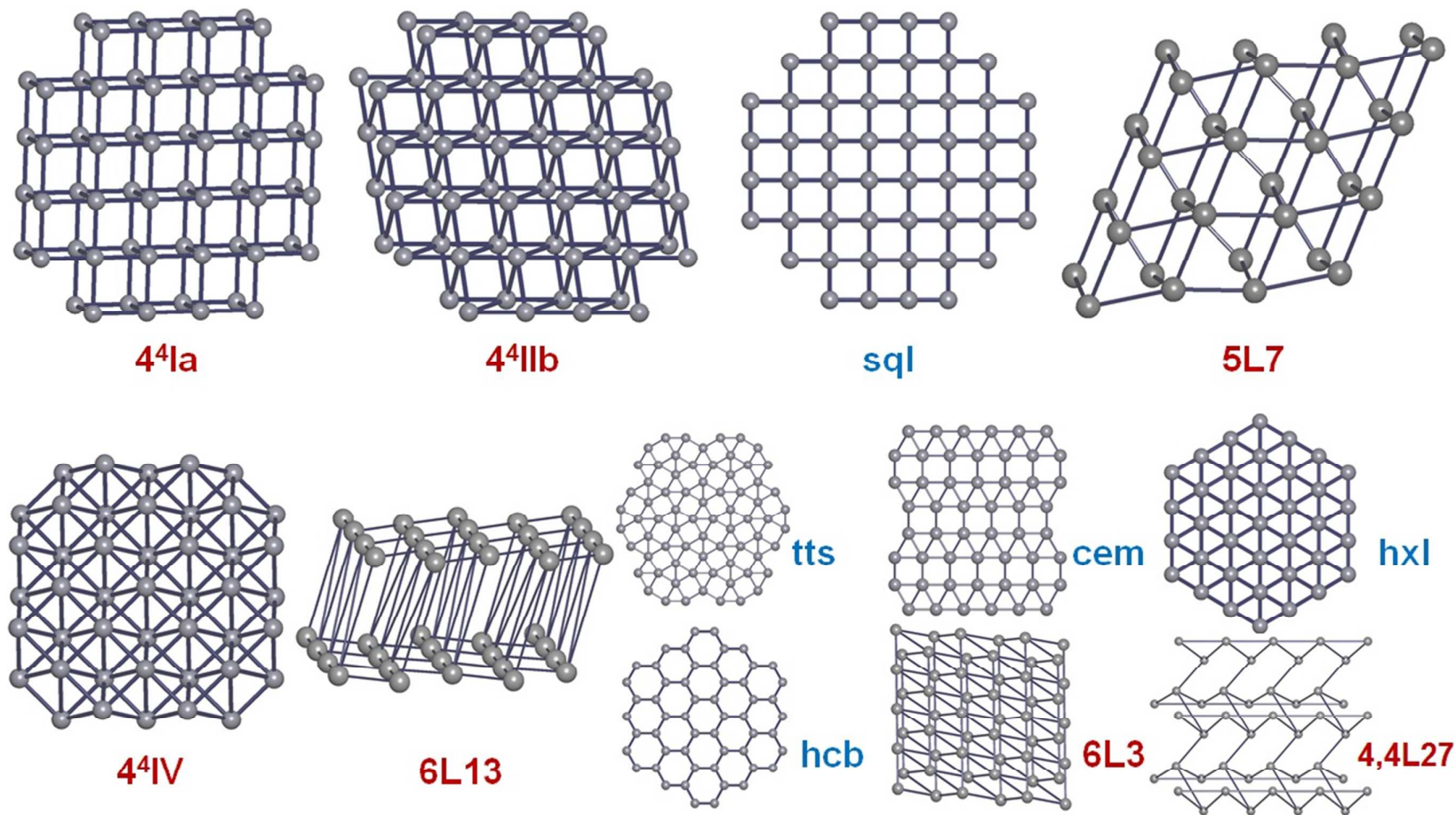


Figure S1. The 12 underlying nets of hydrogen-bonded system found in 199 structures of amino acid derivatives. Topologies corresponding to thick layers are designated in red, those corresponding to simple layers in blue.

Table S1. Distribution of topological types of underlying nets in 199 structures of amino acid derivatives (see Figure S1 above). The 2-periodic 3D thick layers (4^4Ia , 4^4Ib , 5L7, 4^4IV , 6L13, 6L3, 4,4L27); less abundant 2-periodic 2D simple layers (**sql**, **hcb**, **hxl**, **cem**, **tts**).

Topology	Occurrence	Share, %
4^4Ia	71	35.7
4^4Ib	54	27.1
sql	21	10.5
5L7	18	9.0
4^4IV	16	8.0
6L13	7	3.5
cem	4	2.0
hcb	3	1.5
tts	2	1.0
6L3	1	0.5
hxl	1	0.5
4,4L27	1	0.5
Total	199	

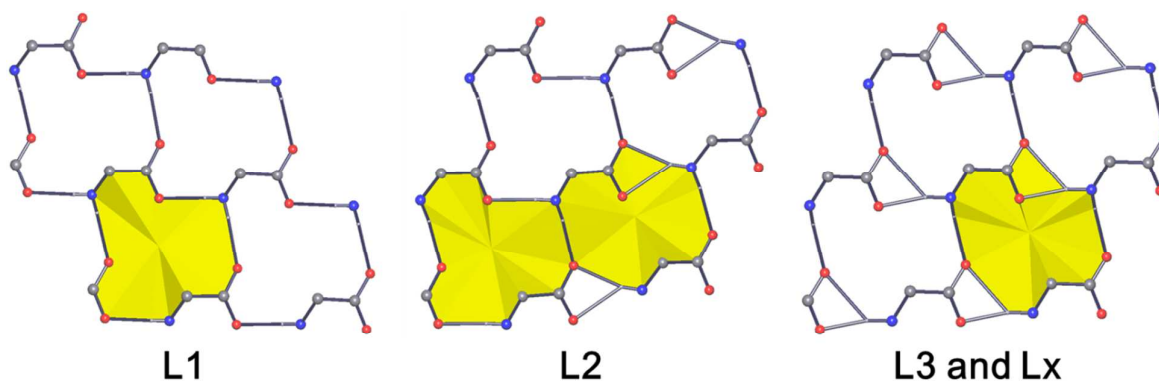


Figure S2. Examples of hydrogen-bonded sheets defined with the nomenclature proposed by Görbitz et al. [1]. Characteristic for each sheet rings are highlighted in yellow.

Table S2. Correspondence between nomenclature proposed by Görbitz et al.¹, and the topological types of underlying net and MCTS of molecules in the structure. See more examples in the Excel table X1.

Görbitz nomenclature	Topology	MCTS	Examples of structures (Refcodes)
LD-LD	4 ⁴ I lb	P ⁶	DLNLUA01
L1-D1	4 ⁴ I a	P ⁴¹	VALIDL03
L1-L1	4 ⁴ I a	P ⁴¹	LEUCIN03
	6L13	P ⁵¹	AZASER10
	5L7	P ⁴¹	QQQAUJ07
L2-L2	5L7	P ³²	LEUCIN02
	6L13	P ⁴²	LVALIN01
L3-L3/Lx-Lx	4 ⁴ I lb	P ⁴²	GAVRAX (L3-L3)
	5L7	P ²³	LNLEUC10 (Lx-Lx)
	6L3	P ⁴²	GLYCIN35
	4 ⁴ I v	P ⁶²	GLYCIN60
	4 ⁴ I a	P ²³	GLYCIN64

(1) Görbitz, C. H.; Vestli, K.; Orlando, R. *Acta Crystallogr.* **2009**, *B65*, 393-400.