

# CRYSTALLIZATION MECHANISM OF ORGANIC COMPOUNDS: THE SUPRAMOLECULAR CLUSTER – A DEMARCATION TOOL

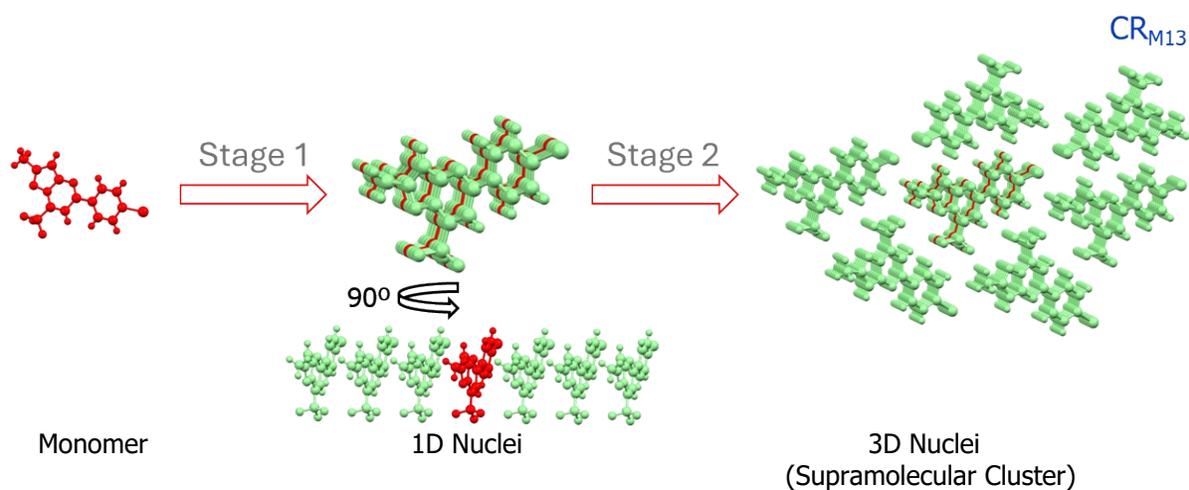
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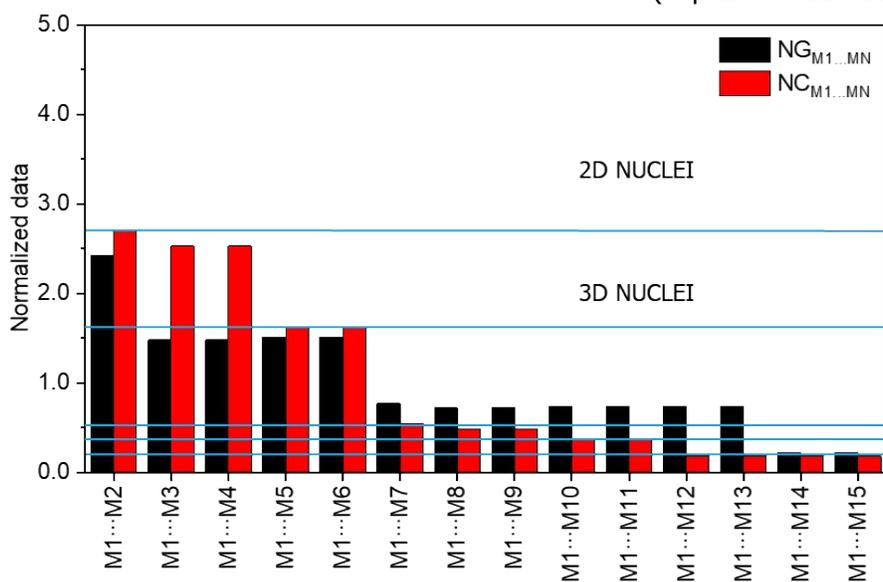
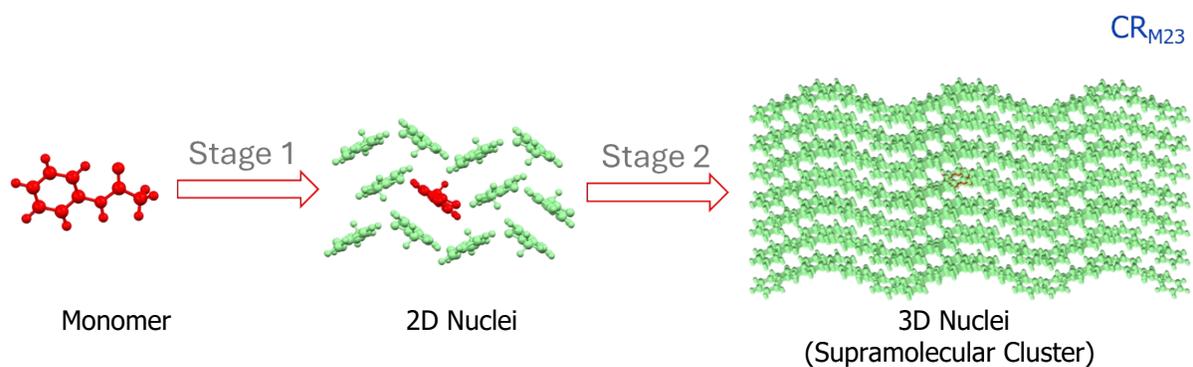
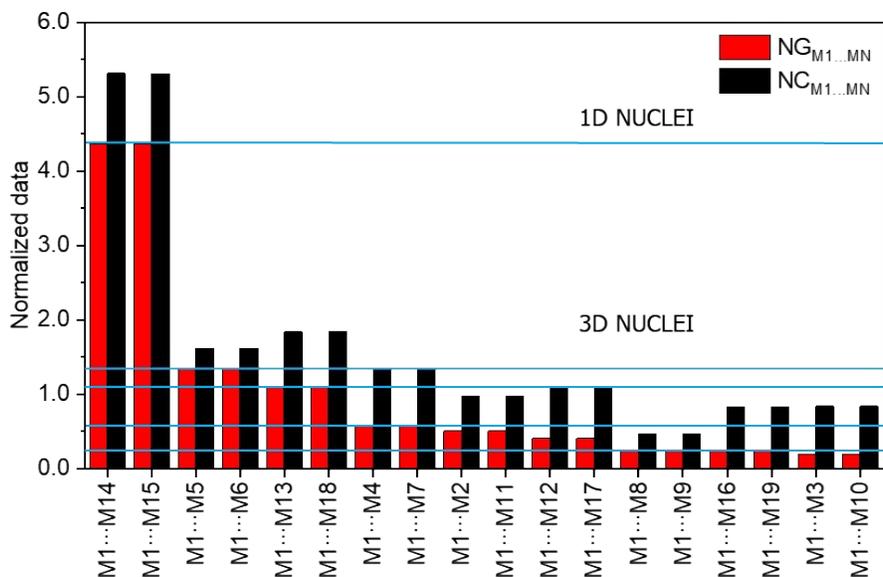
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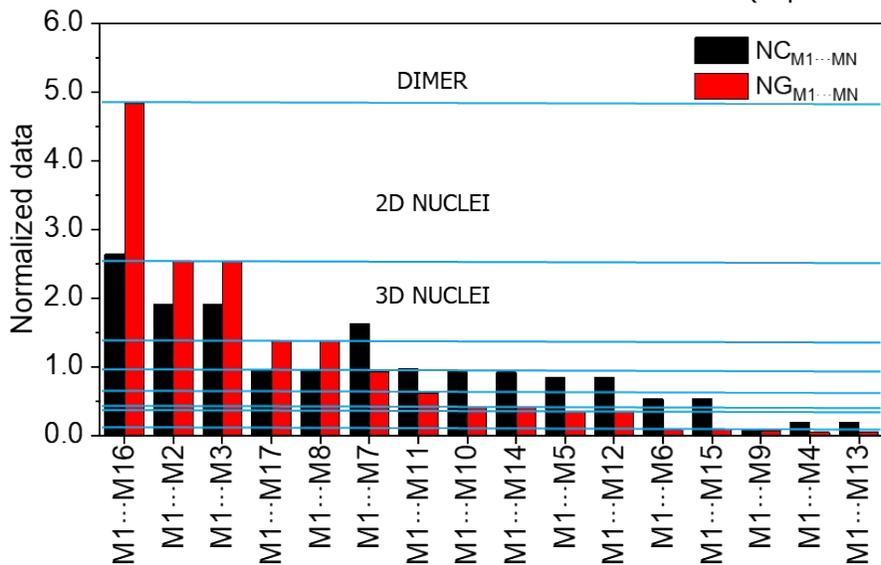
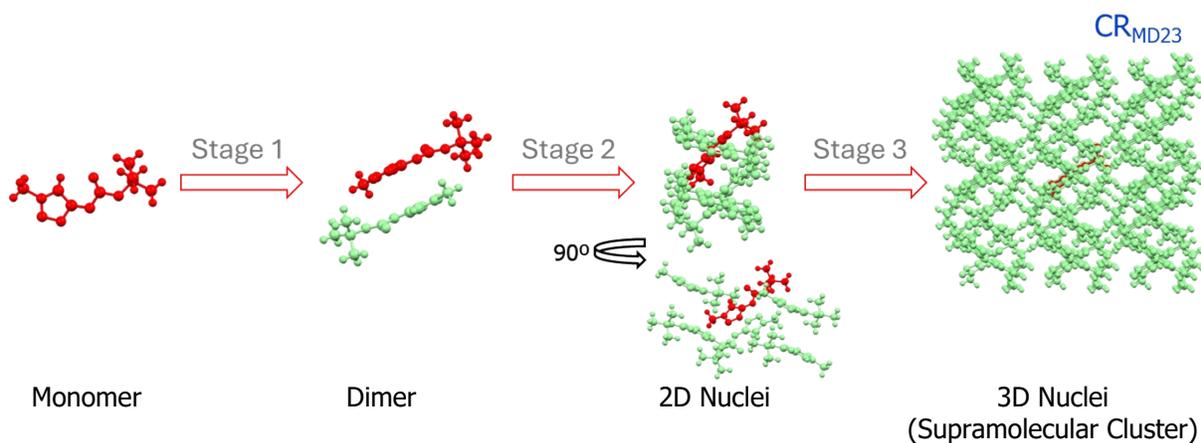
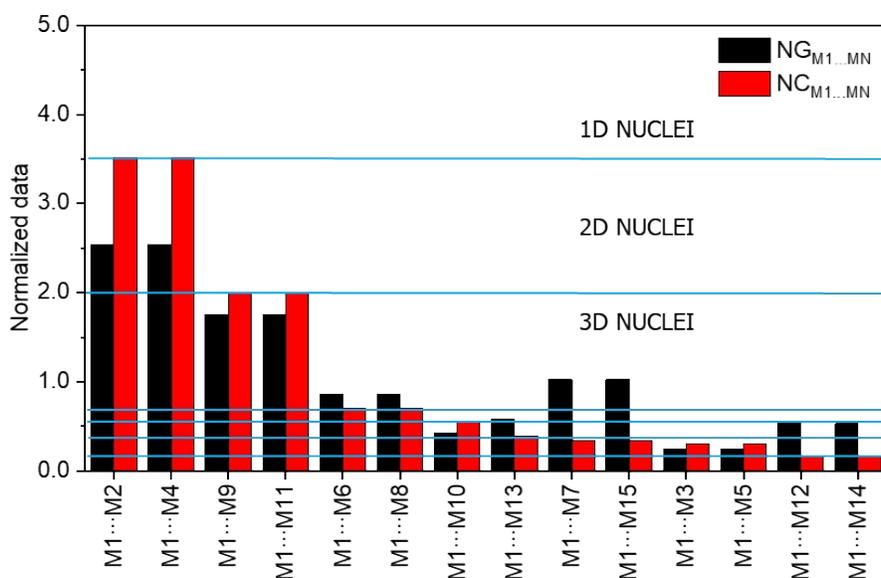
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Monomer      1D Nuclei      2D Nuclei      3D Nuclei (Supramolecular Cluster)



**Figure S1.** Retrocrystallization scheme showing the crystallization process for compound **7**  $CR_{M13}$ ,<sup>63</sup> **1**  $CR_{M23}$ ,<sup>30</sup> **9**  $CR_{M123}$ ,<sup>32</sup> and **12**  $CR_{MD23}$ .<sup>35</sup> This figure presents data on crystallization mechanisms and is based on previously published by the research group itself (see references), therefore maintaining the original numbering of the papers for standardization and comparison purposes.

**Table S1.** Crystallization mechanisms of organic compounds published by our research group.

Crystallization mechanism	Compound <sup>a</sup>	Ref.	Crystallization mechanism	Compound <sup>a</sup>	Ref.
CR <sub>M123</sub>	<b>3, 4, 5, 6</b>	[30]	CR <sub>MD123</sub>	<b>6,11,12</b>	[32]
	<b>1, 2, 3, 4, 5, 6, 11, 12<sup>b</sup></b>	[63]			
	<b>7,9</b>	[32]			
	<b>1b</b>	[33]			
	<b>1b, 2aI, 2aII, 2b, 2c, 2dI, 2dII</b>	[71]			
	<b>2,3,4,12H, 12F</b>	[34]			
	<b>1I,1II</b>	[74]			
	<b>1I,2I,3I,5,9,10</b>	[76]			
CR <sub>M13</sub>	<b>4,5</b>	[75]	CR <sub>MD13</sub>	<b>1, 2, 3, 4, 5A, 5B, 6, 7, 8, 9, 10A, 10B, 11, 12, 14A,<sup>c</sup>14B<sup>c</sup></b>	[37]
	<b>7, 8, 9, 10<sup>b</sup></b>	[63]			
	<b>1,2,3<sup>b</sup></b>	[64]			
	<b>1b, 2c, 2d</b>	[65]			
	<b>2</b>	[30]			
	<b>1II, 6, 7, 13, 15, 17, 23, 24</b>	[76]			
	<b>5,6,7,8</b>	[31]			
	<b>1,2,3,4,10,14</b>	[32]			
	<b>2a,2b,3a</b>	[33]			
	<b>1aI, 1aII, 1c, 1d</b>	[71]			
	<b>1, 2, 3, 4, 5</b>	[72]			
	<b>1a, 3a, 5a, 6a, 8a, 11a, 12a, 13a, 15a, 4b, 8b, 10b, 5c, 12c</b>	[73]			
	<b>1I, 1II, 4, 5, 6, 7, 8</b>	[36]			
<b>2, 5, 6, 8, 13, 14, 16, 17, 19, 20</b>	[35]				
<b>1,2</b>	[75]	CR <sub>MD23</sub>	<b>15, 16, 17, 18</b>	[37]	
<b>1</b>	[30]				
<b>1II</b>	[70]				
<b>2</b>	[74]				
<b>2a, 4a, 7a, 9a, 16a, 17a, 7b, 9b, 7c, 13c, 14c</b>	[73]				
<b>1,2,3,4</b>	[31]				
<b>5</b>	[32]				
<b>3b</b>	[33]				
<b>1</b>	[34]				
<b>1, 3, 10, 11, 21, 22, 23</b>	[35]				
<b>2</b>	[36]				
<b>2II, 3II, 4, 8, 11, 12, 14, 16, 19, 20</b>	[76]				
<b>1, 2,<sup>c</sup> 3,<sup>c</sup> 4</b>	[67]				
CR <sub>M23</sub>	<b>1cA, 1dA</b>	[65]			
	<b>13</b>	[32]			
	<b>2aII</b>	[71]			
	<b>1III</b>	[74]			
	<b>3</b>	[36]			
	<b>9, 12</b>	[35]			
	<b>18, 21, 22</b>	[76]			
	<b>3</b>	[75]			
	<b>5</b>	[67]			
	<b>2</b>	[29]			

	<b>7,8,9,10,11,12</b>	[75]			
CR <sub>M3</sub>	<b>4, 7, 15</b>	[35]	CR <sub>MD3</sub>	<b>5b, 4c</b>	[73]
	<b>1I</b>	[70]		<b>1III</b>	[36]
	<b>8</b>	[32]		<b>6</b>	[75]
			CR <sub>MTt123</sub>	<b>7</b>	[30]

<sup>a</sup> The compound number is the same as in the original reference. <sup>b</sup> The mechanism was currently defined by us based on the data published in the reference. <sup>c</sup> The mechanism was revised by us.