

## Six-Membered Heterocyclic Boronate Esters. Synthesis and Structural Analysis

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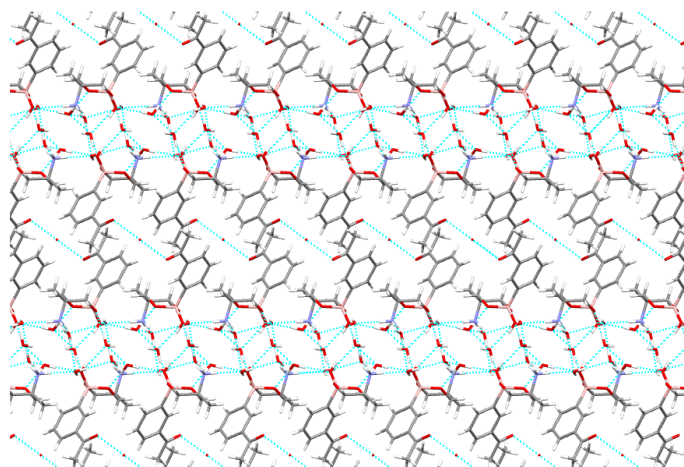
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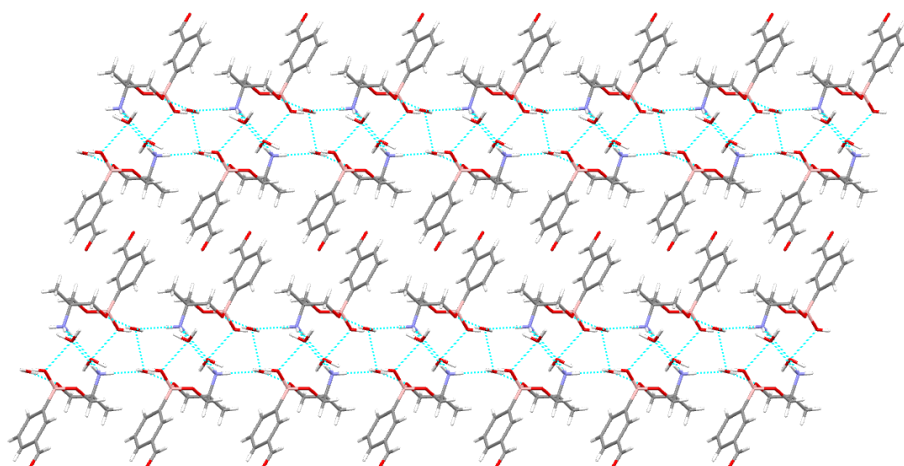
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## Supplementary Information

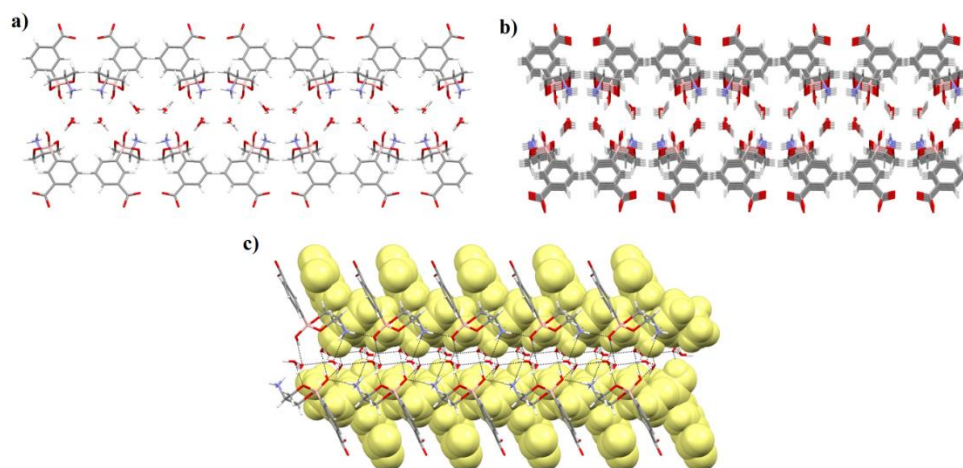
**Table S1.** Selected crystallographic data for compounds **1a**, **1c**, **1e** and **1g**.

	<b>1a</b>	<b>1c</b>	<b>1e</b>	<b>1g</b>
Empirical formula	C <sub>11</sub> H <sub>16</sub> BNO <sub>6</sub>	C <sub>12</sub> H <sub>26</sub> BNO <sub>8</sub>	C <sub>10</sub> H <sub>18</sub> BNO <sub>6</sub>	C <sub>22</sub> H <sub>40</sub> B <sub>2</sub> N <sub>2</sub> O <sub>12</sub>
Fw	269.06	323.15	259.06	546.18
Cryst size [mm <sup>3</sup> ]	.17 x .22 x .35	.26 x .33 x .42	.21 x .28 x .38	.22 x .28 x .37
Cryst syst	Triclinic	Monoclinic	Triclinic	Triclinic
Space group	P1	C2/c	P-1	P-1
Unit cell dimensions				
a [Å]	6.430(2)	31.500(6)	6.829(2)	6.346(4)
b [Å]	7.710(3)	6.1700(12)	12.488(4)	13.518(9)
c [Å]	14.839(5)	17.600(4)	15.153(5)	17.121(12)
α [°]	98.621(7)	90	90.000(6)	68.781(13)
β [°]	90.079(7)	107.00(3)	79.373(6)	81.674(15)
γ [°]	103.978(7)	90	90.000(7)	80.643(14)
V [Å <sup>3</sup> ]	705.2(4)	3271.2(11)	1270.3(8)	1345.0(16)
Z	2	8	4	2
ρ <sub>calcd</sub> [Mg/m <sup>3</sup> ]	1.267	1.312	1.355	1.349
μ [mm <sup>-1</sup> ]	0.101	0.108	0.109	0.107
Collected reflns	5653	12122	9408	8484
Independent reflns (R <sub>int</sub> )	3871 (0.0718)	2402 (0.1551)	3666 (0.2240)	3943 (0.1251)
Number of param	349	235	361	381
R <sub>1</sub> [I > 2σ(I)]	0.1027	0.0831	0.1091	0.0619
wR2 (all data)	0.2382	0.1963	0.2328	0.1759
GOF	0.988	1.183	0.882	0.789

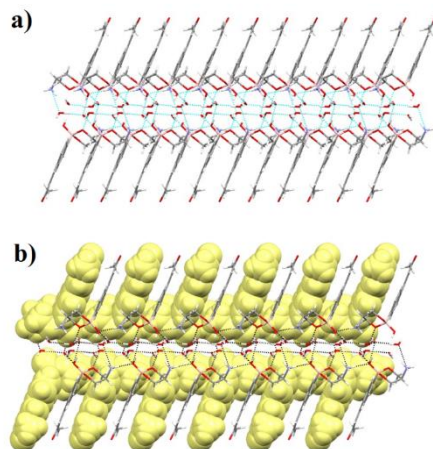
**Fig. S1.** 1D Polymeric chains forming water channels for compound **1d**.



**Fig. S2.** 1D Polymeric chains forming water channels for compound **1b**.



**Fig. S3.** Views of water molecules contained between boronate units in **1f** along the *b* axis.



**Fig. S4.** Two different views of water molecules contained between boronate units in **2e**, viewed along the *c* axis.