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Supporting information for article:

Non-covalent interactions in the multicomponent crystal of 1-aminocyclopentane carboxylic acid, oxalic acid and water: a crystallographic and theoretical approach

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Supplementary material

DFT-PBE-PBC optimized atoms coordinates

N	6.89935199	-2.61928091	-6.30556058
H	6.83676978	-2.16405156	-5.36400355
H	7.30928272	2.18195581	-6.16130013
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O	5.09939921	1.73504784	-5.07405865
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C	4.66814076	2.23970646	-6.13018048
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N	-6.59088537	2.28978558	-6.25660356
H	10.02516445	1.67396922	-6.39927912
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H	-5.76105449	1.87928562	-6.74941821
O	9.34917867	-1.61641894	-5.22084504
O	9.52599593	-2.43943889	-3.10417128
C	9.84955833	-2.36913626	-4.34372902
C	-6.41258444	2.48786996	-4.77484209
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H	-4.02674429	0.17159277	8.81405510
H	-7.45476708	-2.69123153	0.15870668
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C	6.21883596	0.91735628	0.39180286
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H	6.68525480	0.56327194	1.32281156
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H	0.26993880	0.99055358	2.20748736
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H	-1.29043400	1.88658885	5.48865811

H	0.26639524	-2.54701838	-4.21903914
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C	-2.05647958	-1.93919900	-0.26366203
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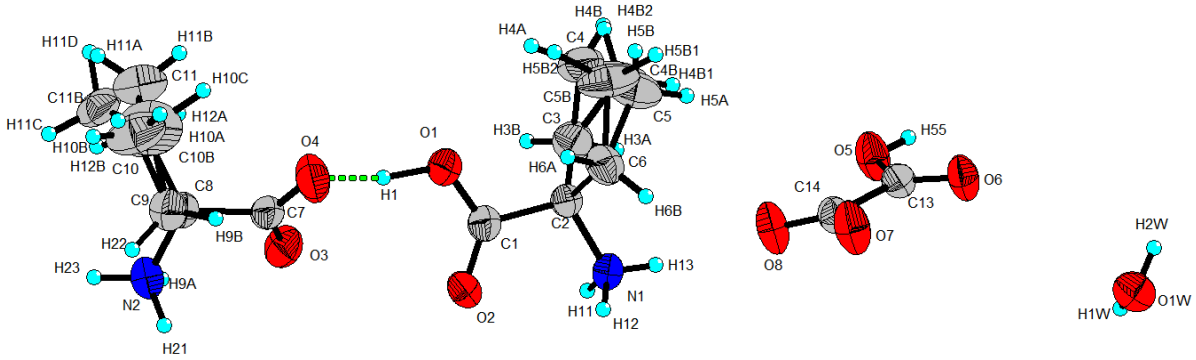
C	2.05825999	1.93003631	0.25921010
O	-2.20517145	1.43241662	-0.17643431

O	3.84505427	1.47949760	8.80045413
O	2.20850348	-1.44172354	0.17578319
H	-1.92128239	0.48059451	-0.51339964
H	4.13684861	2.42747983	8.46128601
H	1.92204808	-0.48959875	0.50946763



O	-0.62950497	2.29921167	-1.58163109
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O	-2.84408413	-1.88634925	0.71826835
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O	2.84679741	1.87812446	-0.72186066
O	2.91687104	-2.06391036	-2.70604574
O	-8.51266915	-0.81213930	6.24752544
O	-2.91169205	2.05977517	2.70611787
H	2.77782202	-2.79612920	-3.36121812
H	-8.64046107	-0.08163100	5.58986777
H	-2.77303423	2.79319678	3.36005027
H	2.92586672	-2.56379772	-1.83756993
H	-8.49830025	-0.30997784	7.11413134
H	-2.92123553	2.55891172	1.83682498
Tv	17.46914598	0.00000000	0.00000000
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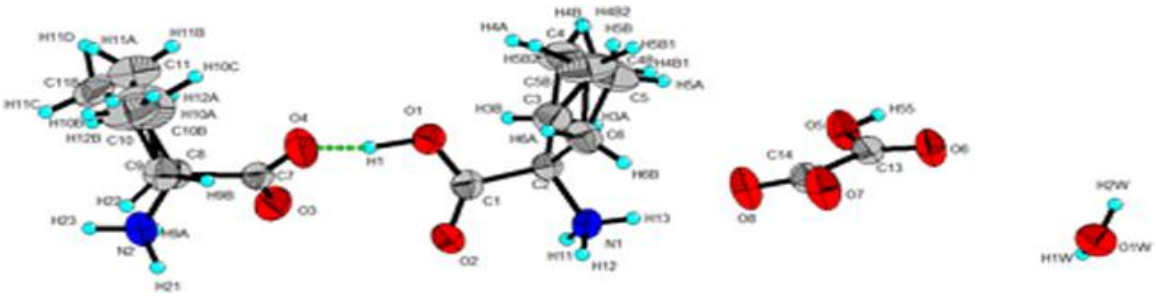

Figure 1A. Asymmetric unit of the 2:1:1 multicomponent crystal of 1-aminocyclopentane carboxylic acid:oxalic acid: water, showing the atom-labeling and the disorder among the cyclopentane ring. Displacement ellipsoids are drawn at 50% probability level. The dimeric cation [Acc5(Z)…Acc5(C)]$^{+}$ linked by a hydrogen bond is displayed.

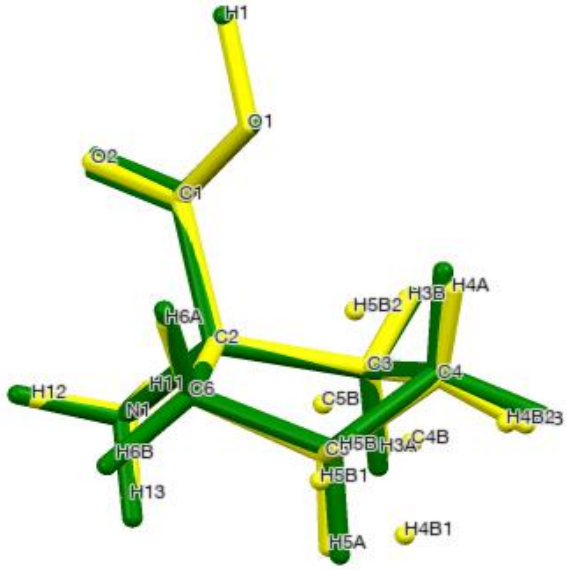

Figure 2A. Optimized geometry at level PBE-PBC (green) of Acc5(C) compared with the crystallographic result (yellow).

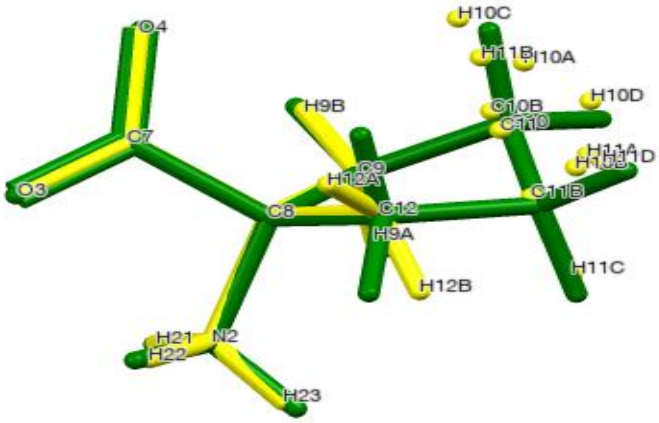

Figure 3A. Optimized geometry at level PBE-PBC (green) of Acc5(Z) compared with the crystallographic result (yellow).