Supporting Information

Ammonium Carboxylate Salts: The Additivity of Intermolecular Interaction Energies in Charged Organic Compounds

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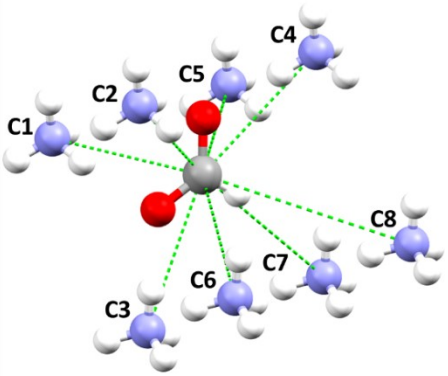
1. Symmetry Codes, Contact Area, Relative Stabilization Energies, and Distances

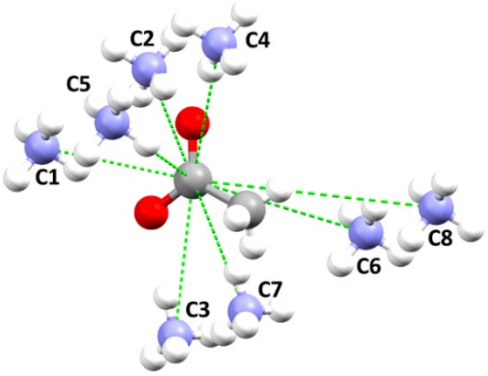
Table S1. Symmetry codes, contact areas, relative stabilization energies, and distances for the possible initial anion-cation pairs of compounds **1**-**12**.

Compound **1**



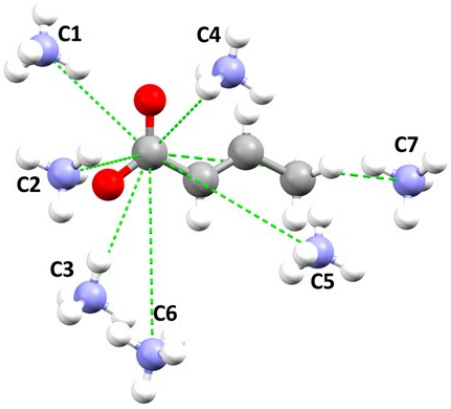
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]
A1···C1	1+x,-y,-1/2+z	8.59	8.59	-154424.563	0.00	3.376
A1···C2	x,-y,-1/2+z	8.80	8.80	-154423.345	1.22	3.332
A1···C3	1+x,y,z	8.41	6.28	-154412.625	11.94	3.634
A1···C4	x,1-y,-1/2+z	8.45	5.98	-154411.630	12.93	3.611
A1···C5	1+x,1-y,-1/2+z	6.49	4.03	-154392.426	32.14	3.652
A1···C6	x,y,z	6.25	3.87	-154391.365	33.20	3.690
A1···C7	1+x,1+y,z	2.49	0.00	-154366.005	58.56	4.708
A1···C8	x,1+y,z	2.80	0.00	-154365.748	58.81	4.751

Compound **2**



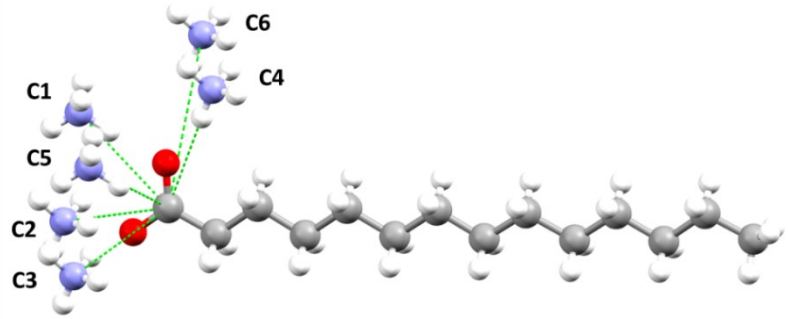
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]
A1···C1	x,y,z	9.34	9.34	-179027.846	0.00	3.427
A1···C2	-x,-y,1-z	8.62	8.62	-179022.255	5.59	3.577
A1···C3	-x,1/2+y,1/2-z	13.39	5.83	-179014.826	13.02	3.556
A1···C4	1-x,-y,1-z	12.24	7.68	-179012.065	15.78	3.695
A1···C5	1+x,y,z	0.46	0.19	-178972.384	55.46	4.771
A1···C6	x,1+y,z	4.47	0.03	-178968.763	59.08	4.718
A1···C7	1-x,1/2+y,1/2-z	6.65	0.00	-178967.939	59.91	4.923
A1···C8	1+x,1+y,z	4.38	0.00	-178958.895	68.95	5.768

Compound **3**



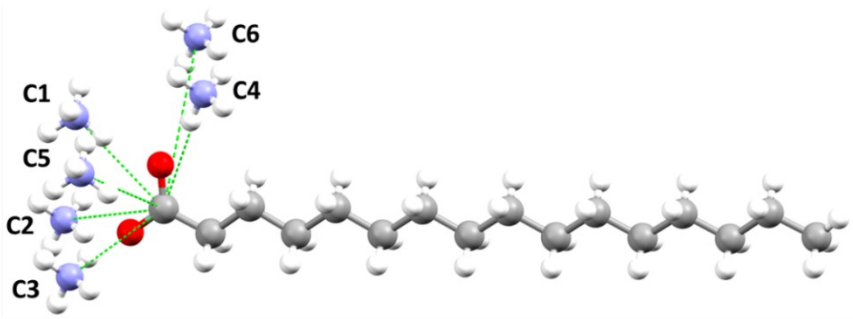
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]
A1···C1	x,1/2-y,-1/2+z	7.84	7.84	-227624.492	0.00	3.540
A1···C2	-x,-1/2+y,1.5-z	11.71	11.71	-227620.049	4.44	3.519
A1···C3	x,-1+y,z	12.24	7.67	-227610.935	13.56	3.737
A1···C4	x,y,z	13.36	8.57	-227610.713	13.78	3.528
A1···C5	x,1/2-y,1/2+z	8.88	0.22	-227568.415	56.08	4.980
A1···C6	-x,-y,2-z	0.92	0.86	-227566.603	57.89	5.335
A1···C7	1-x,-1/2+y,2.5-z	1.07	0.00	-227543.828	80.66	8.384

Compound **4**



A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]
A1···C1	x,y,z	9.41	9.41	-474778.482	0.00	3.581
A1···C2	-1/2+x,1/2-y,-1/2+z	7.04	7.04	-474771.439	7.04	3.776
A1···C3	1/2+x,1/2-y,-1/2+z	10.08	8.05	-474768.809	9.67	3.522
A1···C4	1/2+x,1/2-y,1/2+z	15.67	6.59	-474761.968	16.51	3.855
A1···C5	1+x,y,z	1.88	1.88	-474726.657	51.82	4.794
A1···C6	-1/2+x,1/2-y,1/2+z	0.78	0.78	-474722.061	56.42	5.264

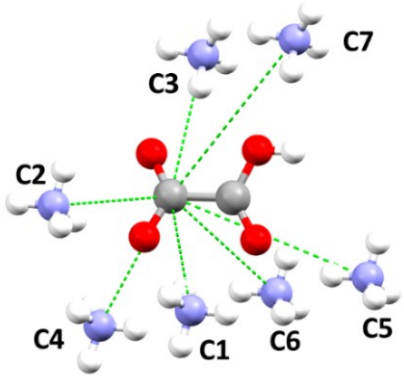
Compound **5**



A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]

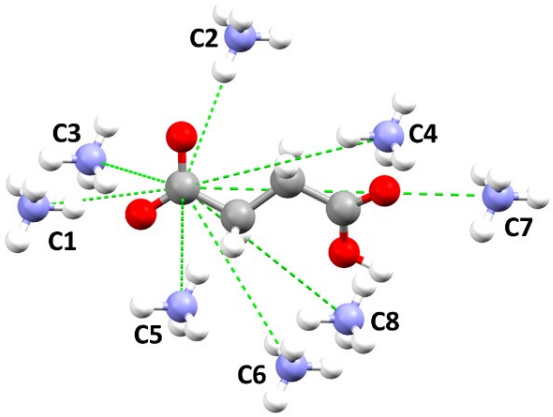
A1···C1	x,y,z	9.58	9.58	-524062.001	0.00	3.601
A1···C2	1/2+x,1/2-y,1/2+z	16.07	6.73	-524053.515	8.49	3.866
A1···C3	-1/2+x,1/2-y,-1/2+z	7.08	7.08	-524052.605	9.40	3.510
A1···C4	1/2+x,1/2-y,-1/2+z	9.58	7.88	-524050.887	11.11	3.800
A1···C5	1+x,y,z	1.76	1.76	-524011.982	50.02	4.762
A1···C6	-1/2+x,1/2-y,1/2+z	0.73	0.73	-524008.524	53.48	5.304

Compound **6**



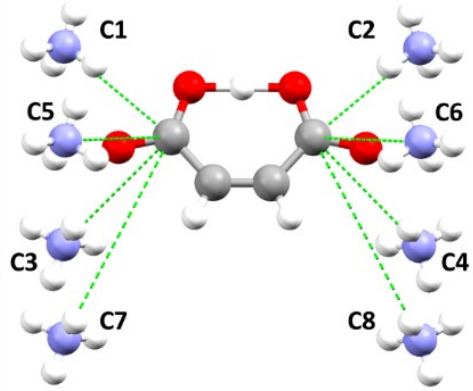
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]
A1···C1	1-x,1/2+y,1/2-z	12.81	6.12	-272753.468	0.00	3.679
A1···C2	x,1.5-y,-1/2+z	6.91	6.91	-272748.694	4.77	3.524
A1···C3	x,y,z	12.48	6.16	-272746.728	6.74	3.781
A1···C4	-x,1/2+y,1/2-z	7.02	6.99	-272736.227	17.24	3.846
A1···C5	1+x,1.5-y,1/2+z	7.49	0.00	-272718.133	35.33	5.268
A1···C6	x,1.5-y,1/2+z	5.32	0.08	-272713.593	39.88	4.467
A1···C7	1+x,y,z	4.70	0.00	-272697.605	55.86	5.382

Compound **7**



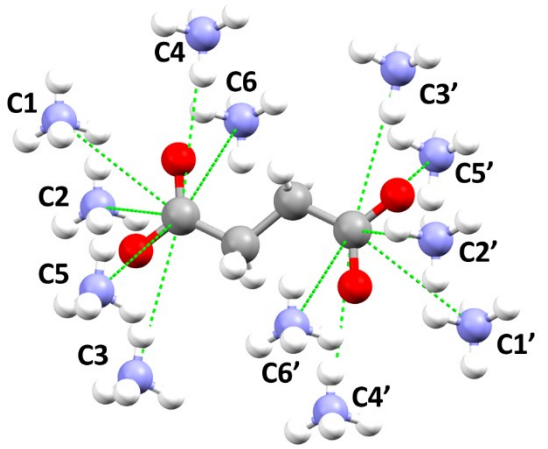
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]
A1···C1	-1+x,1+y,z	5.59	5.59	-322079.517	0.00	3.714
A1···C2	x,1+y,z	12.35	5.12	-322067.598	11.92	3.935
A1···C3	1-x,1-y,-z	6.22	5.87	-322066.390	13.13	3.549
A1···C4	2-x,1-y,1-z	10.58	0.00	-322040.538	38.98	6.027
A1···C5	1-x,1-y,1-z	4.16	0.48	-322028.675	50.84	4.512
A1···C6	-1+x,y,z	10.37	0.00	-322027.077	52.44	5.079
A1···C7	x,y,z	6.88	0.00	-322017.625	61.89	7.676
A1···C8	1-x,-y,-z	3.45	0.00	-322013.330	66.19	6.368

Compound **8**



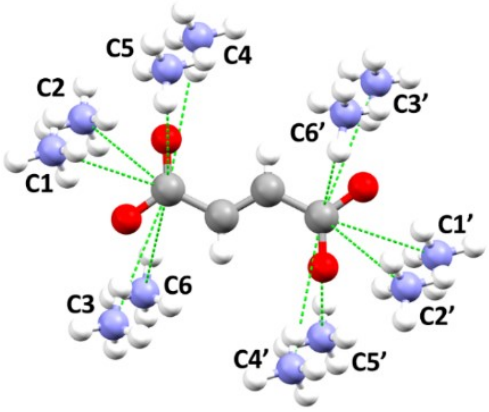
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	$C(O_2^-)\cdots N_f$
A1···C1	x,y,z	12.53	12.53	-321229.885	0.00	3.444
A1···C2	x,y,1/2-z	12.53	12.53	-321229.878	0.01	3.444
A1···C3	1-x,1-y,1-z	10.61	7.65	-321214.673	15.21	3.730
A1···C4	1-x,1-y,-1/2+z	10.61	7.65	-321214.665	15.22	3.740
A1···C5	-1+x,y,z	9.21	7.71	-321210.590	19.29	3.743
A1···C6	-1+x,y,1/2-z	9.21	7.71	-321210.583	19.30	3.743
A1···C7	-x,1-y,1-z	0.74	0.00	-321180.004	49.88	5.923
A1···C8	-x,1-y,-1/2+z	0.74	0.00	-321179.997	49.89	5.923

Compound **9**



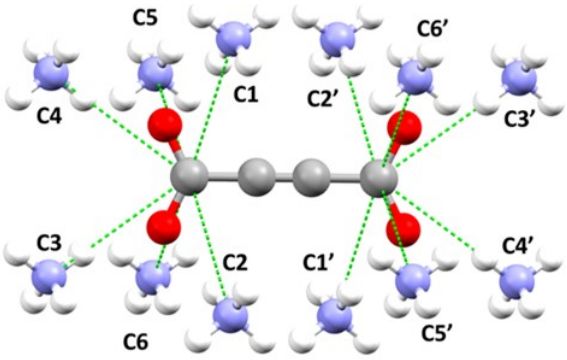
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	$C(O_2^-)\cdots N_f$
A1···C1 / A2···C1′	1-x,-y,1-z / x,1+y,z	15.68	15.68	-357454.989	0.00	3.424
A1···C2 / A2···C2′	-x,-y,1-z / 1+x,1+y,z	15.60	15.60	-357446.674	8.32	3.349
A1···C3 / A2···C3′	x,1/2-y,-1/2+z / 1-x,1/2+y,1.5-z	21.52	12.24	-357443.690	11.30	3.676
A1···C4 / A2···C4′	1+x,y,z / -x,1/2+y,1.5-z	18.00	10.78	-357430.826	24.16	4.011
A1···C5 / A2···C5′	1+x,1/2-y,-1/2+z / -x,1-y,1-z	14.06	8.32	-357390.548	64.44	3.870
A1···C6 / A2···C6′	x,y,z / 1-x,1-y,1-z	11.46	6.54	-357389.456	65.53	4.120

Compound **10**



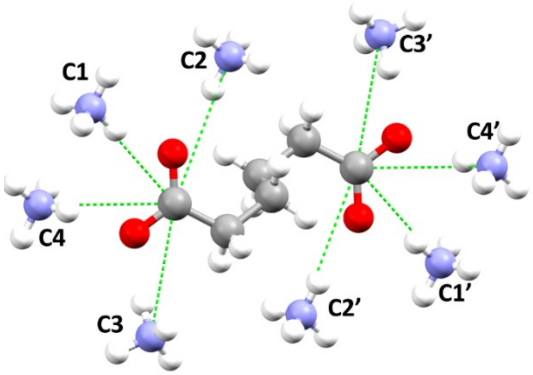
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	$C(O_2^-)\cdots N_f$
A1···C1 / A2-C1′	x,y,z / -x,1-y,1-z	14.50	14.50	-356697.276	0.00	3.369
A1···C2 / A2···C2′	-1+x,y,z / 1-x,1-y,1-z	13.86	13.86	-356696.267	1.01	3.413
A1···C3 / A2···C3′	1-x,1/2+y,1/2-z / -1+x,1/2-y,1/2+z	20.96	12.26	-356692.844	4.43	3.735
A1···C4 / A2···C4′	-x,-y,1-z / x,1+y,z	16.14	9.66	-356676.847	20.43	4.017
A1···C5 / A2···C5′	1-x,-y,1-z / -1+x,1+y,z	13.48	10.56	-356660.601	36.67	3.807
A1···C6 / A2···C6′	-x,1/2+y,1/2-z / x,1/2-y,1/2+z	16.44	9.50	-356651.697	45.58	3.708

Compound **11**



A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	$C(O_2^-)\cdots N_f$
A1···C1 / A2···C1′	1/2-x,1/2-y,2-z / 1/2+x,-1/2+y,-1+z	21.66	13.08	-355966.606	0.00	3.603
A1···C2 / A2···C2′	1/2+x,-1/2+y,z / 1/2-x,1/2-y,1-z	21.66	13.08	-355966.606	0.00	3.603
A1···C3 / A2···C3′	-x,-y,2-z / 1+x,y,-1+z	14.72	14.72	-355955.264	11.34	3.853
A1···C4 / A2···C4′	x,y,z / 1-x,-y,1-z	14.72	14.72	-355955.264	11.34	3.853
A1···C5 / A2···C5′	x,y,-1+z / 1-x,-y,2-z	16.24	15.3	-355935.045	31.56	3.668
A1···C6 / A2···C6′	-x,-y,1-z / 1+x,y,z	16.24	15.3	-355935.045	31.56	3.668

Compound **12**



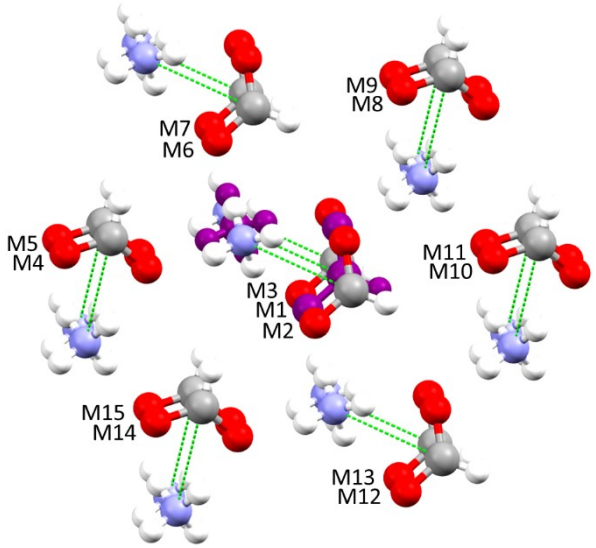
A1···C	Cation symmetry code [a]	$C_{A1\cdots C}$ [b] (total)	$C_{A1\cdots C}$ [c] (COO-)	$G_{A1\cdots C}$ [d]	$\lvert G_{A1\cdots C1} - G_{A1\cdots C}\rvert$ [e]	C(O_2^-)···N [f]
A1···C1 / A2···C1′	x,y,z / -x,2-y,-z	13.78	13.78	-406761.078	0.00	3.593
A1···C2 / A2···C2′	-x,1-y,-z / x,1+y,z	31.38	10.24	-406757.410	3.67	3.925
A1···C3 / A2···C3′	1-x,1/2+y,1/2-z / -1+x,1.5-y,-1/2+z	23.88	11.88	-406751.900	9.18	3.597
A1···C4 / A2···C4′	1-x,1-y,-z / -1+x,1+y,z	14.78	14.78	-406748.561	12.52	3.549

[a] Anion A1 symmetry code: x, y, z. [b] Contact area between A1 and each considered cation, in Å^2. [c] Contact area between the COO^- atoms of A1 and each considered cation, in Å^2. [d] Intermolecular interaction energy (kcal mol$^-$) is determined by the equation $\Sigma G_{M1\cdots MN}$. where $G_{M1\cdots MN} = G_{M1+MN} - (G_{M1} + G_{MN})$, , in kcal mol^{-1}, using ωB97XD/cc-pVDZ level of theory. [e] Difference of absolute energies between the most stable pair and each considered pair ($|G_{A1-C1} - G_{A1-C}|$), in kcal mol^{-1}. [f] Distance between the carbonyl carbon atom of A1 and each ammonium nitrogen cation C, in Å.

2. Supramolecular Clusters Data

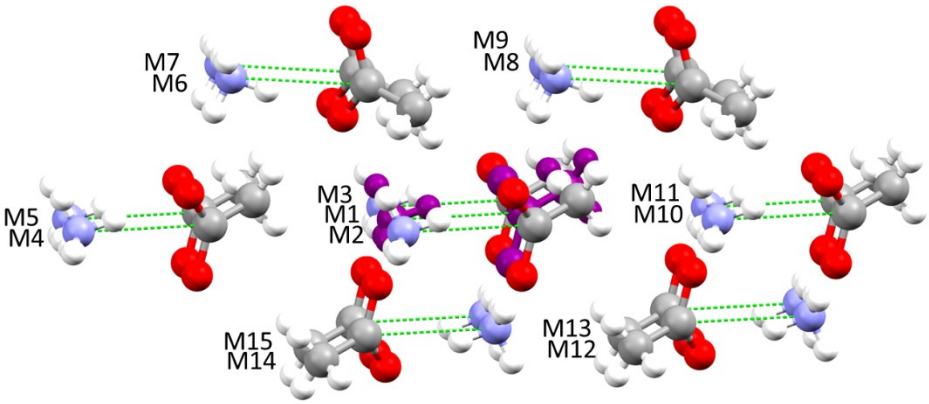
Table S2. Supramolecular cluster and symmetry codes for the monomers of compounds **1**-**12**.

Compound **1**



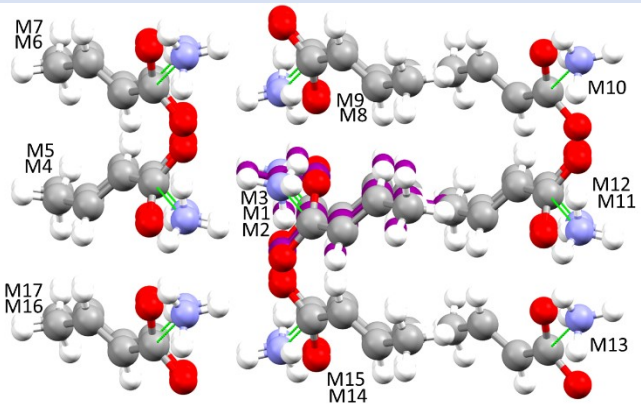
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M9	x,2-y,1/2+z
M2	-1+x,y,z	M10	-1+x,1-y,1/2+z
M3	1+x,y,z	M11	x,1-y,1/2+z
M4	x,2-y,-1/2+z	M12	-1+x,-1+y,z
M5	1+x,2-y,-1/2+z	M13	x,-1+y,z
M6	x,1+y,z	M14	x,1-y,-1/2+z
M7	1+x,1+y,z	M15	1+x,1-y,-1/2+z
M8	-1+x,2-y,1/2+z		

Compound **2**



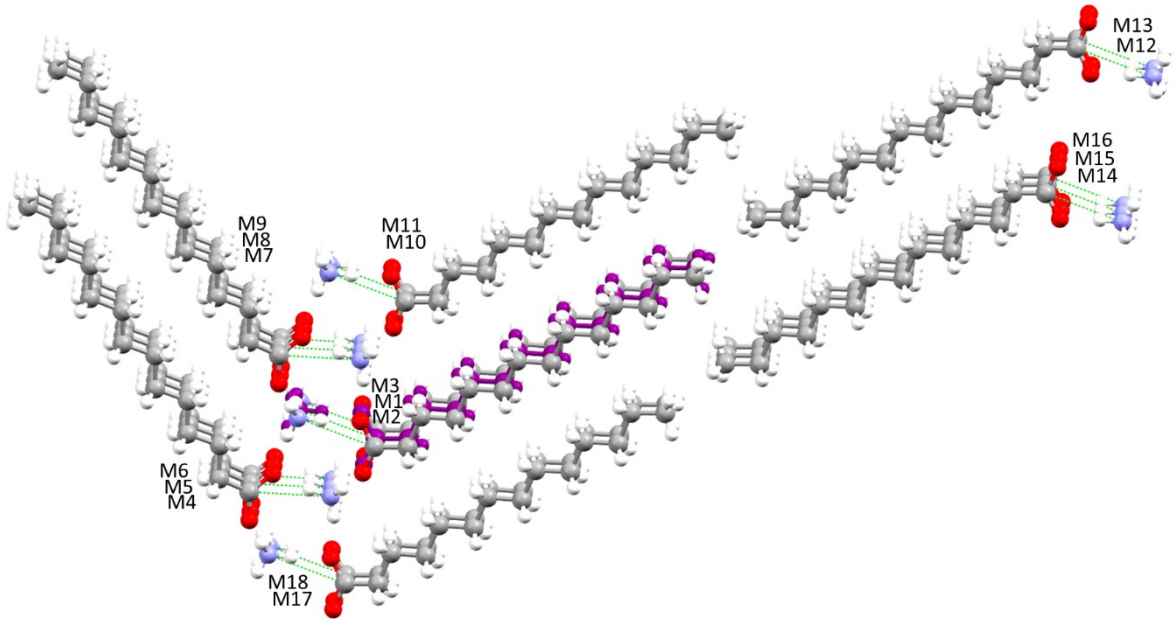
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M9	1-x,1/2+y,1/2-z
M2	-1+x,y,z	M10	x,1+y,z
M3	1+x,y,z	M11	1+x,1+y,z
M4	-1+x,-1+y,z	M12	1-x,1-y,1-z
M5	x,-1+y,z	M13	2-x,1-y,1-z
M6	-x,-1/2+y,1/2-z	M14	-x,-y,1-z
M7	1-x,-1/2+y,1/2-z	M15	1-x,-y,1-z
M8	-x,1/2+y,1/2-z		

Compound **3**



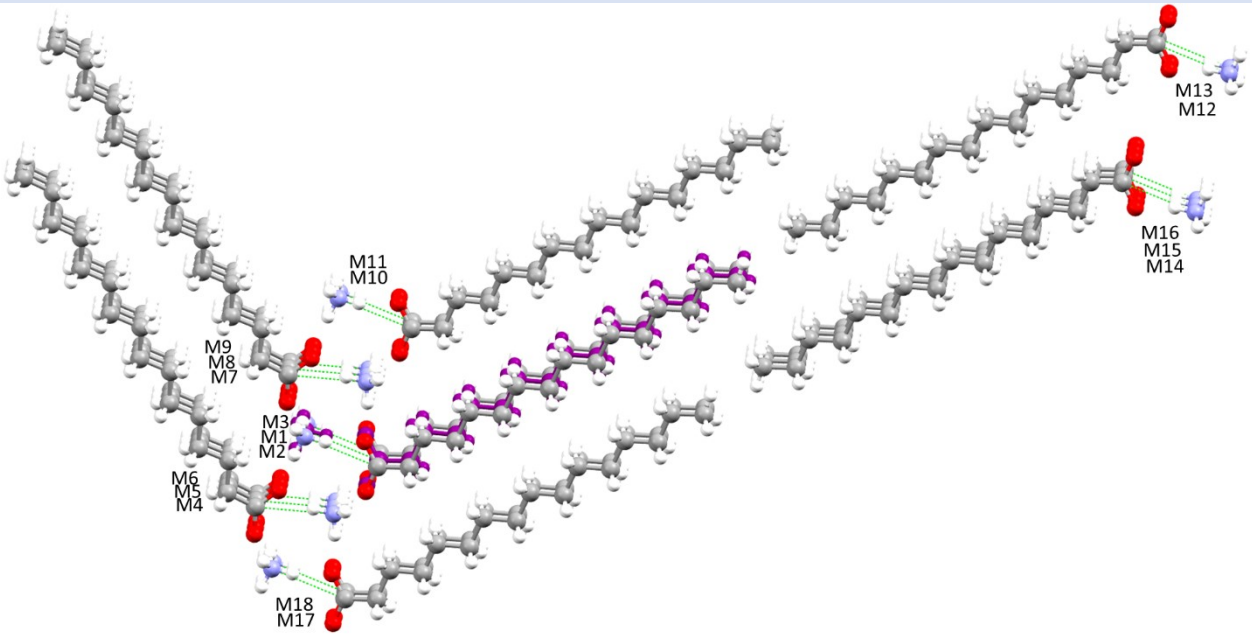
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M10	1-x,1/2+y,2.5-z
M2	x,y,1+z	M11	1-x,-y,3-z
M3	x,y,-1+z	M12	1-x,-y,2-z
M4	-x,-y,1-z	M13	1-x,-1/2+y,2.5-z
M5	-x,-y,-z	M14	x,-1/2-y,1/2+z
M6	-x,1/2+y,1.5-z	M15	x,-1/2-y,-1/2+z
M7	-x,1/2+y,1/2-z	M16	-x,-1/2+y,1.5-z
M8	x,1/2-y,1/2+z	M17	-x,-1/2+y,1/2-z
M9	x,1/2-y,-1/2+z		

Compound **4**



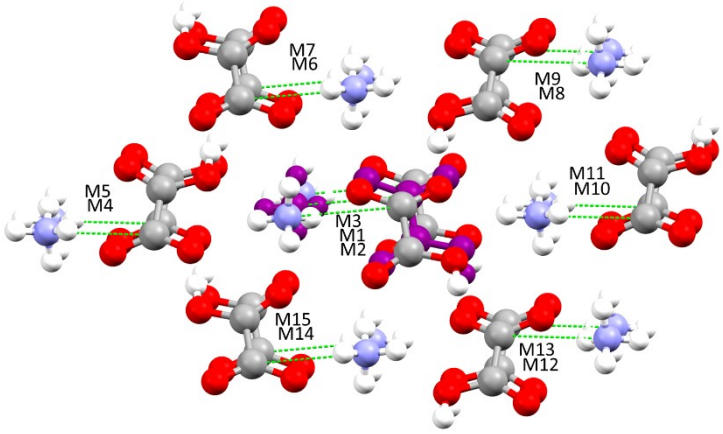
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M10	1+x,y,1+z
M2	1+x,y,z	M11	x,y,1+z
M3	-1+x,y,z	M12	4-x,1-y,3-z
M4	1/2+x,1/2-y,-1/2+z	M13	3-x,1-y,3-z
M5	-1/2+x,1/2-y,-1/2+z	M14	4-x,1-y,2-z
M6	-1.5+x,1/2-y,-1/2+z	M15	3-x,1-y,2-z
M7	1.5+x,1/2-y,1/2+z	M16	2-x,1-y,2-z
M8	1/2+x,1/2-y,1/2+z	M17	x,y,-1+z
M9	-1/2+x,1/2-y,1/2+z	M18	-1+x,y,-1+z

Compound **5**



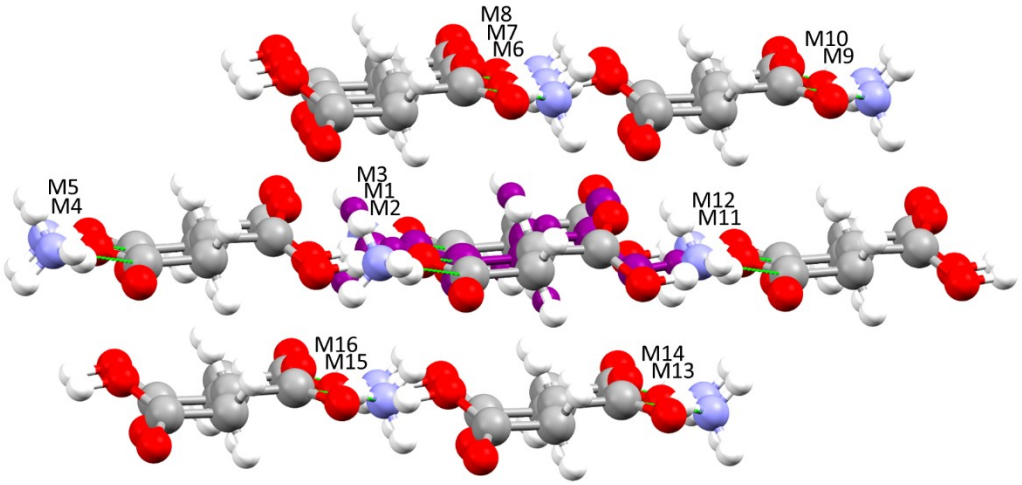
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M10	1+x,y,1+z
M2	1+x,y,z	M11	x,y,1+z
M3	-1+x,y,z	M12	4-x,1-y,3-z
M4	1/2+x,1/2-y,-1/2+z	M13	3-x,1-y,3-z
M5	-1/2+x,1/2-y,-1/2+z	M14	4-x,1-y,2-z
M6	-1.5+x,1/2-y,-1/2+z	M15	3-x,1-y,2-z
M7	1.5+x,1/2-y,1/2+z	M16	2-x,1-y,2-z
M8	1/2+x,1/2-y,1/2+z	M17	x,y,-1+z
M9	-1/2+x,1/2-y,1/2+z	M18	-1+x,y,-1+z

Compound **6**



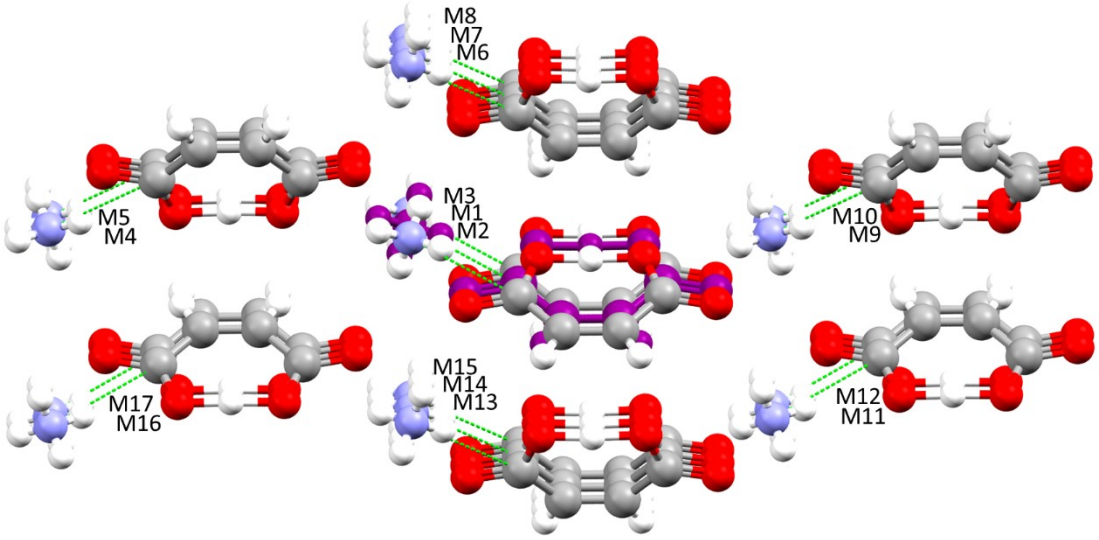
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M9	-1+x,1.5-y,-1/2+z
M2	1+x,y,z	M10	2-x,-1/2+y,1/2-z
M3	-1+x,y,z	M11	1-x,-1/2+y,1/2-z
M4	2-x,1/2+y,1/2-z	M12	1+x,1.5-y,1/2+z
M5	1-x,1/2+y,1/2-z	M13	x,1.5-y,1/2+z
M6	2-x,2-y,-z	M14	2-x,2-y,1-z
M7	1-x,2-y,-z	M15	1-x,2-y,1-z
M8	x,1.5-y,-1/2+z		

Compound **7**



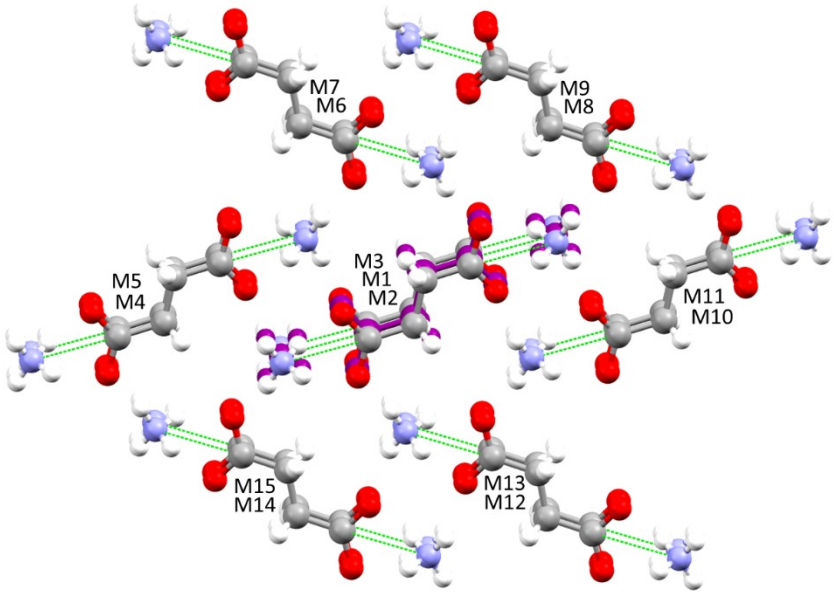
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M10	x,1/2-y,-1/2+z
M2	-1+x,y,z	M11	-x,1-y,-1/2+z
M3	1+x,y,z	M12	1-x,1-y,-1/2+z
M4	x,1/2-y,1/2+z	M13	-x,1/2+y,z
M5	1+x,1/2-y,1/2+z	M14	1-x,1/2+y,z
M6	-x,-1/2+y,z	M15	2-x,1/2+y,z
M7	1-x,-1/2+y,z	M16	-x,1-y,1/2+z
M8	2-x,-1/2+y,z	M17	1-x,1-y,1/2+z
M9	-1+x,1/2-y,-1/2+z		

Compound **8**



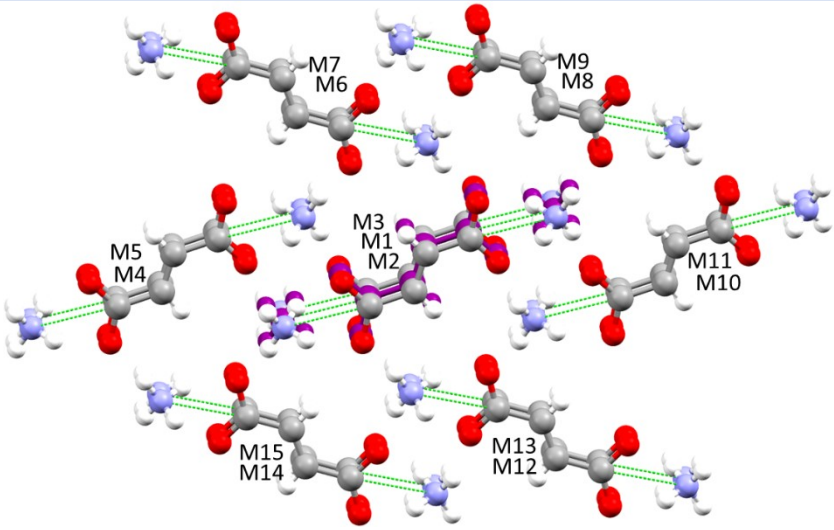
Monomer	Symmetry code [a]	Monomer	Symmetry code [a]
M1	x,y,z	M9	1-x,1-y,1-z
M2	-1+x,y,z	M10	2-x,1-y,1-z
M3	1+x,y,z	M11	x,-1+y,z
M4	-1+x,1+y,z	M12	1+x,-1+y,z
M5	x,1+y,z	M13	-x,1-y,-z
M6	-x,2-y,1-z	M14	1-x,1-y,-z
M7	1-x,2-y,1-z	M15	-x,2-y,-z
M8	2-x,2-y,1-z	M16	1-x,2-y,-z

Compound **9**



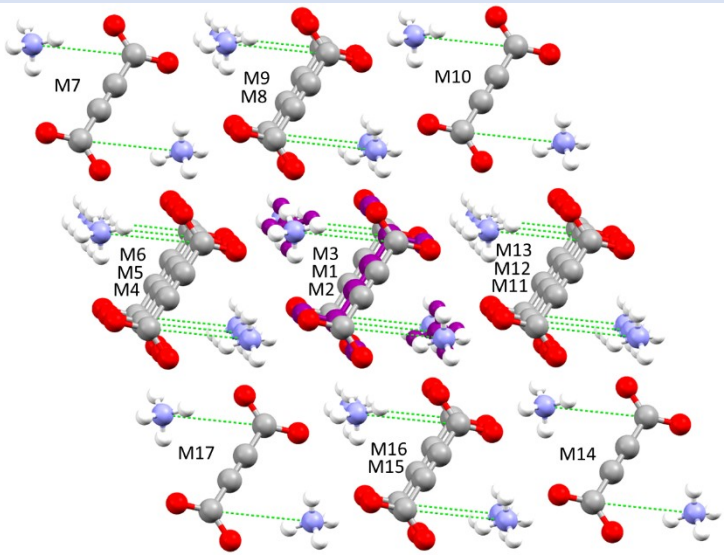
Monomer	Symmetry code [a]		Monomer	Symmetry code [a]	
M1	x,y,z	1-x,1-y,1-z	M9	-x,1/2+y,1.5-z	-1+x,1.5-y,1/2+z
M2	1+x,y,z	2-x,1-y,1-z	M10	x,1+y,z	1-x,2-y,1-z
M3	-1+x,y,z	-x,1-y,1-z	M11	-1+x,1+y,z	-x,2-y,1-z
M4	1+x,-1+y,z	2-x,-y,1-z	M12	2-x,1/2+y,1/2-z	1+x,1.5-y,-1/2+z
M5	x,-1+y,z	1-x,-y,1-z	M13	1-x,1/2+y,1/2-z	x,1.5-y,-1/2+z
M6	1-x,-1/2+y,1.5-z	x,1/2-y,1/2+z	M14	2-x,-1/2+y,1/2-z	1+x,1/2-y,-1/2+z
M7	-x,-1/2+y,1.5-z	-1+x,1/2-y,1/2+z	M15	1-x,-1/2+y,1/2-z	x,1/2-y,-1/2+z
M8	1-x,1/2+y,1.5-z	x,1.5-y,1/2+z			

Compound **10**



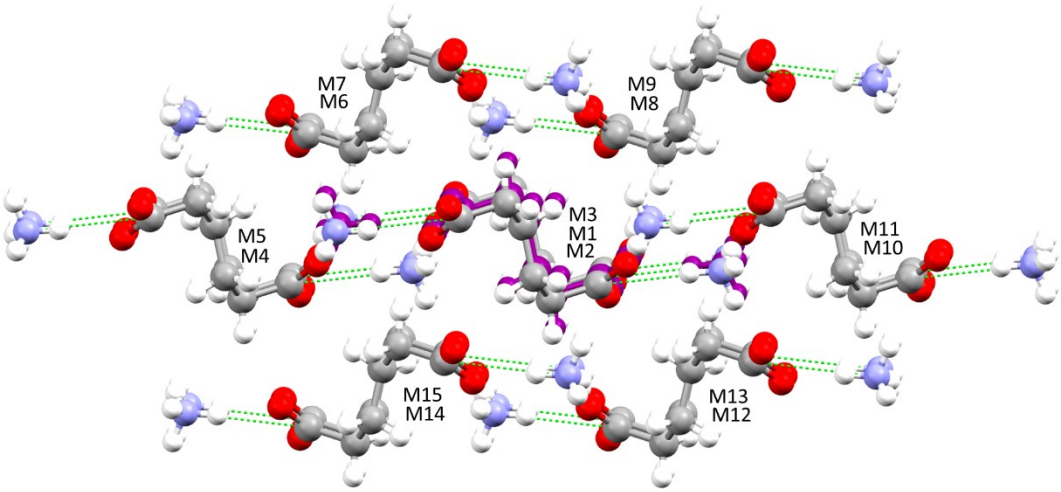
Monomer	Symmetry code [a]		Monomer	Symmetry code [a]	
M1	x,y,z	-x,1-y,1-z	M9	-1-x,1/2+y,1.5-z	-1+x,1.5-y,1/2+z
M2	1+x,y,z	1-x,1-y,1-z	M10	x,1+y,z	-x,2-y,1-z
M3	-1+x,y,z	-1-x,1-y,1-z	M11	-1+x,1+y,z	-1-x,2-y,1-z
M4	1+x,-1+y,z	1-x,-y,1-z	M12	1-x,1/2+y,1/2-z	1+x,1.5-y,-1/2+z
M5	x,-1+y,z	-x,-y,1-z	M13	-x,1/2+y,1/2-z	x,1.5-y,-1/2+z
M6	-x,-1/2+y,1.5-z	x,1/2-y,1/2+z	M14	1-x,-1/2+y,1/2-z	1+x,1/2-y,-1/2+z
M7	-1-x,-1/2+y,1.5-z	-1+x,1/2-y,1/2+z	M15	-x,-1/2+y,1/2-z	x,1/2-y,-1/2+z
M8	-x,1/2+y,1.5-z	x,1.5-y,1/2+z			

Compound **11**



Monomer	Symmetry code [a]		Monomer	Symmetry code [a]	
M1	x,y,z	1-x,y,1-z	M10	1+x,y,z	2-x,y,1-z
M2	x,y,1+z	1-x,y,2-z	M11	1/2+x,-1/2+y,2+z	1.5-x,-1/2+y,3-z
M3	x,y,-1+z	1-x,y,-z	M12	1/2+x,-1/2+y,1+z	1.5-x,-1/2+y,2-z
M4	-1/2+x,1/2+y,z	1/2-x,1/2+y,1-z	M13	1/2+x,-1/2+y,z	1.5-x,-1/2+y,1-z
M5	-1/2+x,1/2+y,-1+z	1/2-x,1/2+y,-z	M14	x,-1+y,1+z	1-x,-1+y,2-z
M6	-1/2+x,1/2+y,-2+z	1/2-x,1/2+y,-1-z	M15	-1/2+x,-1/2+y,1+z	1/2-x,-1/2+y,2-z
M7	x,1+y,-1+z	1-x,1+y,-z	M16	-1/2+x,-1/2+y,z	1/2-x,-1/2+y,1-z
M8	1/2+x,1/2+y,z	1.5-x,1/2+y,1-z	M17	-1+x,y,z	-x,y,1-z
M9	1/2+x,1/2+y,-1+z	1.5-x,1/2+y,-z			

Compound **12**



Monomer	Symmetry code [a]		Monomer	Symmetry code [a]	
M1	x,y,z	-x,2-y,-z	M9	-x,1/2+y,1/2-z	x,2.5-y,1/2+z
M2	1+x,y,z	1-x,2-y,-z	M10	x,1+y,z	-x,3-y,-z
M3	-1+x,y,z	-1-x,2-y,-z	M11	-1+x,1+y,z	-1-x,3-y,-z
M4	1+x,-1+y,z	1-x,1-y,-z	M12	-x,1/2+y,-1/2-z	x,2.5-y,-1/2+z
M5	x,-1+y,z	-x,1-y,-z	M13	-1-x,1/2+y,-1/2-z	-1+x,2.5-y,-1/2+z
M6	1-x,-1/2+y,1/2-z	1+x,1.5-y,1/2+z	M14	-x,-1/2+y,-1/2-z	x,1.5-y,-1/2+z
M7	-x,-1/2+y,1/2-z	x,1.5-y,1/2+z	M15	-1-x,-1/2+y,-1/2-z	-1+x,1.5-y,-1/2+z
M8	1-x,1/2+y,1/2-z	1+x,2.5-y,1/2+z			

[a] The symmetry codes were determined using the carbon atom(s) COO^- of each carboxylate anion(s). Reference molecule M1 is highlighted (purple).

3. Contact Area, Stabilization Energy, and Normalized Data

Table S3. Contact area, stabilization energy, and normalized data of each dimer from the supramolecular cluster for compounds **1**-**12**.

Compound **1**					Compound **2**				
Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]	Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	16.03	-5.78	1.91	0.86	M1···M2	6.81	9.96	0.64	-1.06
M1···M3	16.03	-5.78	1.91	0.86	M1···M3	6.81	9.96	0.64	-1.06
M1···M4	9.39	-12.86	1.12	1.92	M1···M4	4.38	-4.29	0.41	0.46
M1···M5	6.25	-13.32	0.74	1.99	M1···M5	4.47	-6.42	0.42	0.68
M1···M6	10.13	3.82	1.21	-0.57	M1···M6	14.95	-16.78	1.40	1.78
M1···M7	8.45	-20.76	1.01	3.10	M1···M7	13.42	-0.70	1.25	0.07
M1···M8	6.25	-13.32	0.74	1.99	M1···M8	14.95	-16.78	1.40	1.78
M1···M9	9.39	-12.86	1.12	1.92	M1···M9	13.42	-0.70	1.25	0.07
M1···M10	2.80	-2.94	0.33	0.44	M1···M10	4.47	-6.42	0.42	0.68
M1···M11	5.78	4.88	0.69	-0.73	M1···M11	4.38	-4.29	0.41	0.46
M1···M12	8.45	-20.76	1.01	3.10	M1···M12	11.38	5.16	1.06	-0.55
M1···M13	10.13	3.82	1.21	-0.57	M1···M13	1.06	1.16	0.10	-0.12
M1···M14	5.78	4.88	0.69	-0.73	M1···M14	24.03	-55.91	2.25	5.93
M1···M15	2.80	-2.94	0.33	0.44	M1···M15	25.23	-45.98	2.36	4.88
Total	117.66	-93.91	14.00	14.00	Total	149.76	-132.03	14.00	14.00
Compound **3**					Compound **4**				
Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]	Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1···M2	8.88	-7.74	0.72	0.89	M1···M2	88.61	1.16	3.46	-0.12
M1···M3	8.88	-7.74	0.72	0.89	M1···M3	88.61	1.16	3.46	-0.12
M1···M4	30.93	-56.18	2.51	6.46	M1···M4	14.04	-30.73	0.55	3.21
M1···M5	0.04	4.75	0.00	-0.55	M1···M5	27.36	-48.73	1.07	5.09
M1···M6	0.92	-1.00	0.07	0.11	M1···M6	0.52	-5.71	0.02	0.60
M1···M7	1.05	3.56	0.09	-0.41	M1···M7	0.52	-5.71	0.02	0.60
M1···M8	22.80	-16.15	1.85	1.86	M1···M8	27.36	-48.73	1.07	5.09
M1···M9	22.80	-16.16	1.85	1.86	M1···M9	14.04	-30.72	0.55	3.21
M1···M10	13.75	-0.75	1.12	0.09	M1···M10	44.78	0.13	1.75	-0.01
M1···M11	9.12	-0.14	0.74	0.02	M1···M11	23.53	3.29	0.92	-0.34
M1···M12	16.69	-2.40	1.35	0.28	M1···M12	6.83	-0.38	0.27	0.04
M1···M13	13.75	-0.75	1.12	0.09	M1···M13	7.85	-0.31	0.31	0.03
M1···M14	22.82	-20.49	1.85	2.36	M1···M14	1.52	0.10	0.06	-0.01
M1···M15	22.82	-20.49	1.85	2.36	M1···M15	20.91	-1.12	0.82	0.12
M1···M16	0.92	-1.00	0.07	0.11	M1···M16	0.75	0.04	0.03	0.00
M1···M17	1.05	3.56	0.09	-0.41	M1···M17	23.53	3.29	0.92	-0.34
					M1···M18	44.78	0.13	1.75	-0.01
Total	197.22	-139.11	16.00	16.00	Total	435.54	-162.85	17.00	17.00

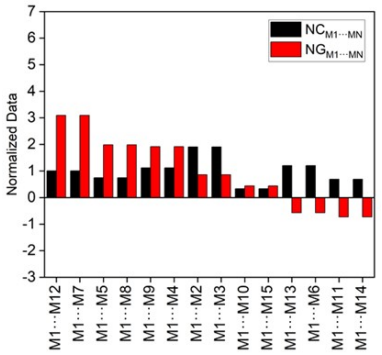
Compound **5**					Compound **6**				
Dimer	$C_{M1\cdots MN}{}^{a}$	$G_{M1\cdots MN}{}^{b}$	$NC_{M1\cdots MN}{}^{c}$	$NG_{M1\cdots MN}{}^{d}$	$C_{M1\cdots MN}{}^{a}$	$G_{M1\cdots MN}{}^{b}$	$NC_{M1\cdots MN}{}^{c}$	$NG_{M1\cdots MN}{}^{d}$	$C_{M1\cdots MN}{}^{a}$
M1⋯M2	99.33	-0.69	3.51	0.07	M1⋯M2	16.05	-0.32	1.53	0.03
M1⋯M3	99.33	-0.69	3.51	0.07	M1⋯M3	16.05	-0.32	1.53	0.03
M1⋯M4	13.36	-30.62	0.47	3.04	M1⋯M4	4.70	-3.05	0.45	0.29
M1⋯M5	27.64	-51.22	0.98	5.08	M1⋯M5	12.48	-28.24	1.19	2.64
M1⋯M6	0.50	-6.18	0.02	0.61	M1⋯M6	1.45	-0.56	0.14	0.05
M1⋯M7	0.50	-6.18	0.02	0.61	M1⋯M7	15.85	-55.37	1.51	5.18
M1⋯M8	27.64	-51.21	0.98	5.08	M1⋯M8	8.65	8.04	0.82	-0.75
M1⋯M9	13.36	-30.62	0.47	3.04	M1⋯M9	8.94	-6.13	0.85	0.57
M1⋯M10	53.37	-1.02	1.89	0.10	M1⋯M10	4.70	-3.05	0.45	0.29
M1⋯M11	26.79	3.27	0.95	-0.32	M1⋯M11	12.48	-28.24	1.19	2.64
M1⋯M12	7.83	-0.46	0.28	0.05	M1⋯M12	8.94	-6.13	0.85	0.57
M1⋯M13	8.83	-0.36	0.31	0.04	M1⋯M13	8.65	8.04	0.82	-0.75
M1⋯M14	1.32	0.10	0.05	-0.01	M1⋯M14	15.91	-21.81	1.51	2.04
M1⋯M15	19.78	-1.14	0.70	-0.11	M1⋯M15	12.43	-12.51	1.18	1.17
M1⋯M16	0.77	0.10	0.03	-0.01					
M1⋯M17	26.79	3.27	0.95	-0.32					
M1⋯M18	53.37	-1.02	1.89	0.10					
Total	480.51	-171.29	17.00	17.00	Total	147.28	-149.64	14.00	14.00

Compound **7**					Compound **8**				
Dimer	$C_{M1\cdots MN}{}^{a}$	$G_{M1\cdots MN}{}^{b}$	$NC_{M1\cdots MN}{}^{c}$	$NG_{M1\cdots MN}{}^{d}$	Dimer	$C_{M1\cdots MN}{}^{a}$	$G_{M1\cdots MN}{}^{b}$	$NC_{M1\cdots MN}{}^{c}$	$NG_{M1\cdots MN}{}^{d}$
M1⋯M2	22.83	2.35	1.91	-0.46	M1⋯M2	17.97	-22.00	1.36	1.77
M1⋯M3	22.83	2.35	1.91	-0.46	M1⋯M3	17.97	-22.00	1.36	1.77
M1⋯M4	12.65	-23.95	1.06	4.69	M1⋯M4	6.88	-8.43	0.52	0.68
M1⋯M5	9.21	-19.61	0.77	3.84	M1⋯M5	17.04	-22.15	1.29	1.78
M1⋯M6	16.76	2.67	1.40	-0.52	M1⋯M6	8.34	-11.92	0.63	0.96
M1⋯M7	21.46	-2.35	1.80	0.46	M1⋯M7	33.94	-36.83	2.56	2.96
M1⋯M8	0.59	13.46	0.05	-2.63	M1⋯M8	0.12	4.54	0.01	-0.37
M1⋯M9	9.21	-19.61	0.77	3.84	M1⋯M9	14.99	-0.91	1.13	0.07
M1⋯M10	12.65	-23.95	1.06	4.69	M1⋯M10	0.26	4.38	0.02	-0.35
M1⋯M11	0.89	2.59	0.07	-0.51	M1⋯M11	17.04	-22.16	1.29	1.78
M1⋯M12	11.09	-16.02	0.93	3.14	M1⋯M12	6.88	-8.43	0.52	0.68
M1⋯M13	16.76	2.67	1.40	-0.52	M1⋯M13	16.66	0.81	1.26	-0.07
M1⋯M14	21.46	-2.35	1.80	0.46	M1⋯M14	24.75	-1.50	1.87	0.12
M1⋯M15	0.59	13.45	0.05	-2.63	M1⋯M15	15.80	-41.59	1.19	3.35
M1⋯M16	0.89	2.59	0.07	-0.51	M1⋯M16	0.27	1.80	0.02	-0.15
M1⋯M17	11.09	-16.02	0.93	3.14					
Total	190.96	-81.73	16.00	16.00	Total	198.91	-186.38	15.00	15.00

Compound **9**					Compound **10**				
Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]	Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1⋯M2	40.22	-19.50	2.39	0.99	M1⋯M2	34.28	-12.54	2.12	0.62
M1⋯M3	40.22	-19.50	2.39	0.99	M1⋯M3	34.28	-12.54	2.12	0.62
M1⋯M4	21.92	-48.57	1.30	2.47	M1⋯M4	17.48	-42.02	1.08	2.07
M1⋯M5	12.02	-14.78	0.71	0.75	M1⋯M5	16.41	-36.28	1.01	1.79
M1⋯M6	13.79	-19.33	0.82	0.98	M1⋯M6	10.83	-20.29	0.67	1.00
M1⋯M7	8.09	-8.19	0.48	0.42	M1⋯M7	11.68	-5.43	0.72	0.27
M1⋯M8	13.79	-19.33	0.82	0.98	M1⋯M8	12.03	-20.28	0.74	1.00
M1⋯M9	8.09	-8.19	0.48	0.42	M1⋯M9	10.48	-5.42	0.65	0.27
M1⋯M10	12.02	-14.78	0.71	0.75	M1⋯M10	16.41	-36.28	1.01	1.79
M1⋯M11	21.92	-48.57	1.30	2.47	M1⋯M11	17.48	-42.02	1.08	2.07
M1⋯M12	8.09	-8.19	0.48	0.42	M1⋯M12	11.68	-5.41	0.72	0.27
M1⋯M13	13.79	-19.33	0.82	0.98	M1⋯M13	10.83	-20.27	0.67	1.00
M1⋯M14	8.09	-8.19	0.48	0.42	M1⋯M14	11.68	-5.42	0.72	0.27
M1⋯M15	13.79	-19.33	0.82	0.98	M1⋯M15	10.83	-20.28	0.67	1.00
Total	235.84	-275.80	14.00	14.00	Total	226.38	-284.49	14.00	14.00
Compound **11**					Compound **12**				
Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]	Dimer	$C_{M1\cdots MN}$[a]	$G_{M1\cdots MN}$[b]	$NC_{M1\cdots MN}$[c]	$NG_{M1\cdots MN}$[d]
M1⋯M2	38.71	-17.45	2.79	0.93	M1⋯M2	12.48	20.23	0.61	-0.96
M1⋯M3	38.71	-17.51	2.79	0.93	M1⋯M3	12.48	20.23	0.61	-0.96
M1⋯M4	14.72	-47.32	1.06	2.52	M1⋯M4	18.18	-61.92	0.89	2.94
M1⋯M5	18.31	-35.54	1.32	1.89	M1⋯M5	32.97	-55.49	1.62	2.63
M1⋯M6	0.38	2.10	0.03	-0.11	M1⋯M6	15.69	-21.36	0.77	1.01
M1⋯M7	5.00	8.05	0.36	-0.43	M1⋯M7	23.79	-3.85	1.17	0.18
M1⋯M8	16.63	-22.88	1.20	1.22	M1⋯M8	15.69	-21.36	0.77	1.01
M1⋯M9	16.79	-52.96	1.21	2.82	M1⋯M9	23.79	-3.85	1.17	0.18
M1⋯M10	0.36	15.89	0.03	-0.85	M1⋯M10	32.97	-61.92	1.62	2.94
M1⋯M11	0.38	2.10	0.03	-0.11	M1⋯M11	18.18	-55.49	0.89	2.63
M1⋯M12	18.31	-35.49	1.32	1.89	M1⋯M12	23.79	-3.85	1.17	0.18
M1⋯M13	14.72	-47.32	1.06	2.52	M1⋯M13	15.69	-21.36	0.77	1.01
M1⋯M14	5.00	8.10	0.36	-0.43	M1⋯M14	23.79	-3.85	1.17	0.18
M1⋯M15	16.79	-52.89	1.21	2.82	M1⋯M15	15.69	-21.36	0.77	1.01
M1⋯M16	16.63	-22.88	1.20	1.22					
M1⋯M17	0.36	15.89	0.03	-0.85					
Total	221.80	-300.10	16.00	16.00	Total	285.18	-295.20	14.00	14.00

[a] Contact area (Å^2). determined by the equation $\Sigma C_{M1\cdots MN}$ using ToposPro. [b] Intermolecular interaction energy (kcal mol^{-1}) is determined by the equation $\Sigma G_{M1\cdots MN}$. where $G_{M1\cdots MN} = G_{M1+MN} - (G_{M1} + G_{MN})$, using ωB97XD/cc-pVDZ level of theory. [c] Normalized contact area (Å^2) determined by the equation $NC_{M1\cdots MN} = (N \times C_{M1\cdots MN})/C_{Cluster}$. [d] Normalized intermolecular interaction energy (kcal mol^{-1}) is determined by the equation $NG_{M1\cdots MN} = (N \times G_{M1\cdots MN})/G_{Cluster}$.

Table S4. Bar graphs for normalized contact area and stabilization energy data of each dimer M1···MN from the supramolecular clusters of compounds **1**-**12**.



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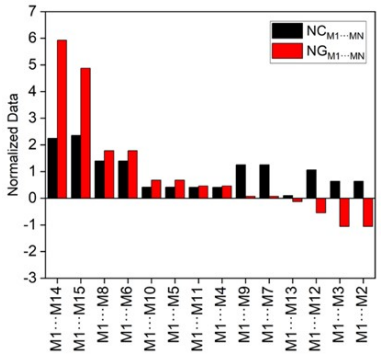

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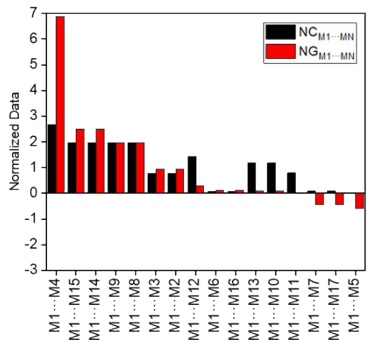

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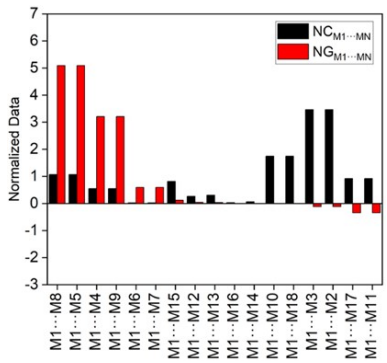

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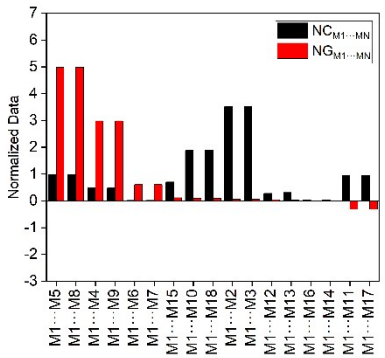

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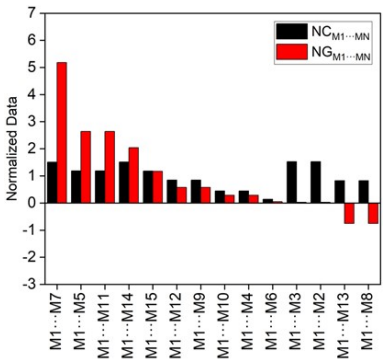

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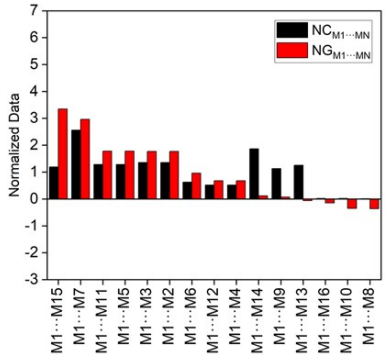

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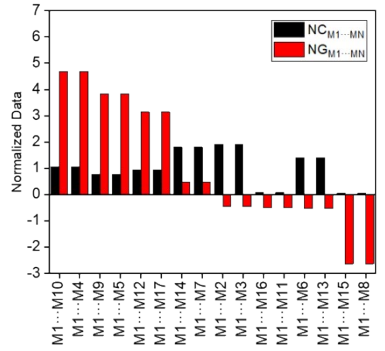

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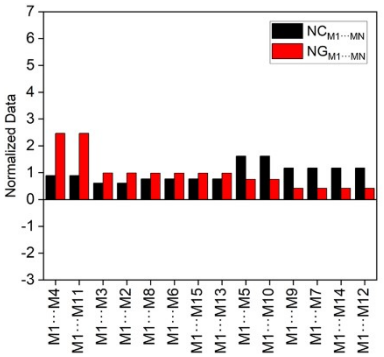

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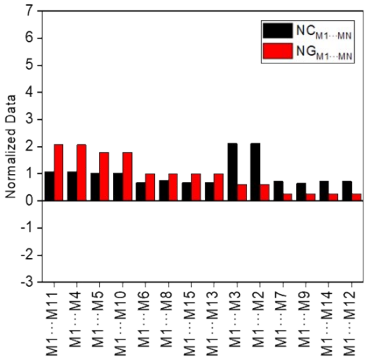

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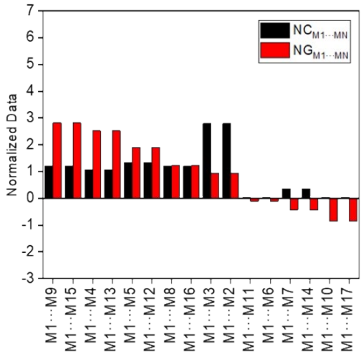

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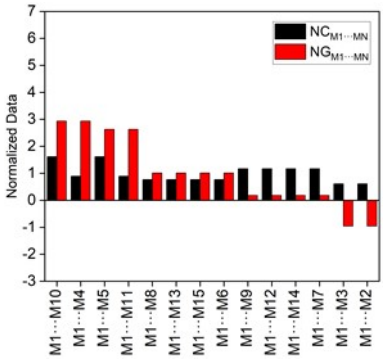
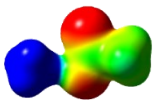
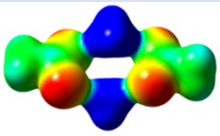
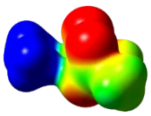
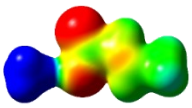
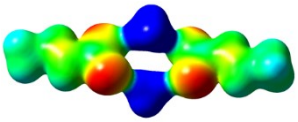
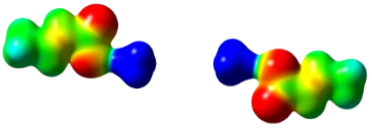
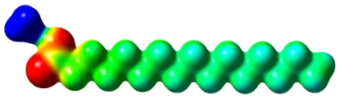
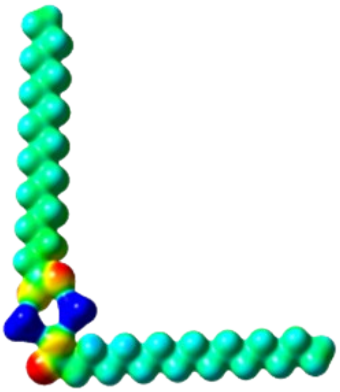
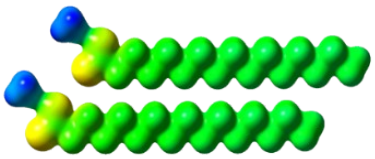
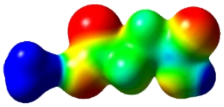
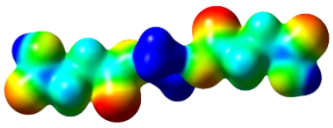
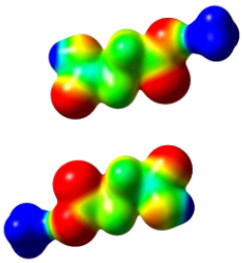
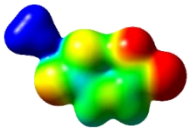
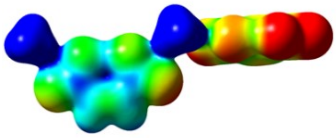
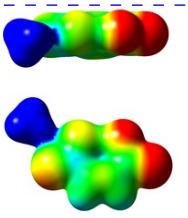
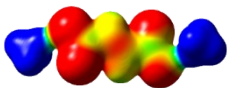
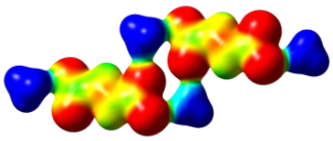
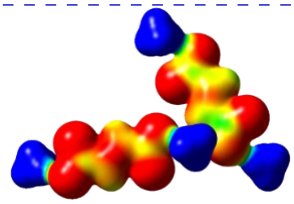
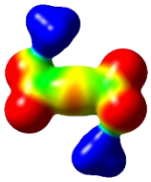
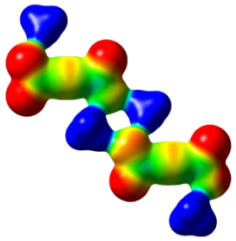
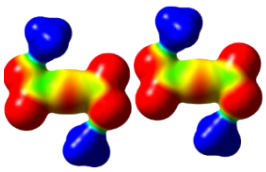
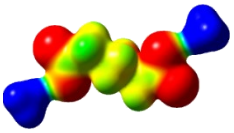
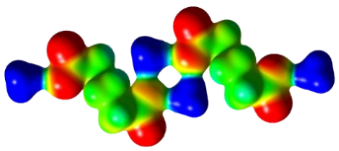
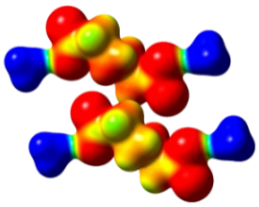


12

4. Molecular Electrostatic Potential – MEP

Table S5. Molecular Electrostatic Potential of compounds **2-3, 5, 7-8,** and **10-12** (red and blue with -0.1 and 0.1 a.u., respectively). *M1···M7/M9/M12/M14 of **10** presents low stabilizing energy, but not a destabilizing one.

Compound	Monomer A–C	Most Stabilizing Dimers	Most Destabilizing Dimers
2	 M1	 M1···M14	 M1···M2
3	 M1	 M1···M4	 M1···M5
5	 M1	 M1···M5	 M1···M11
7	 M1	 M1···M15	 M1···M8
8	 M1	 M1···M4	 M1···M8

10	 M1	 M1···M4	 M1···M7
11	 M1	 M1···M9	 M1···M10
12	 M1	 M1···M4	 M1···M2

5. Cluster Energy Efficiency – CEE

Table S6. Supramolecular cluster stabilization energies ($\sum G_{M1\cdots MN} < 0$), destabilizing energies ($\sum G_{M1\cdots MN} > 0$), $G_{cluster}$[a], and CEE[b] data for the compounds **1**-**12**.

Compound	$\sum G_{M1\cdots MN} < 0$	$\sum G_{M1\cdots MN} > 0$	$G_{cluster}$	CEE
1	-111.33	17.41	-93.91	0.844
2	-158.28	26.24	-132.03	0.834
3	-150.98	11.86	-139.11	0.921
4	-172.15	9.30	-162.85	0.946
5	-180.28	8.99	-171.29	0.950
6	-165.73	16.08	-149.64	0.903
7	-123.85	42.12	-81.73	0.660
8	-197.92	11.54	-186.38	0.942
9	-275.80	0.00	-275.80	1.000
10	-284.49	0.00	-284.49	1.000
11	-352.24	52.14	-300.10	0.852
12	-335.65	40.45	-295.20	0.879

[a] $G_{cluster} = \sum G_{M1\cdots MN}$, in kcal mol^{-1}. [b] Calculated with eqn 6.

6. Crystallization Mechanisms

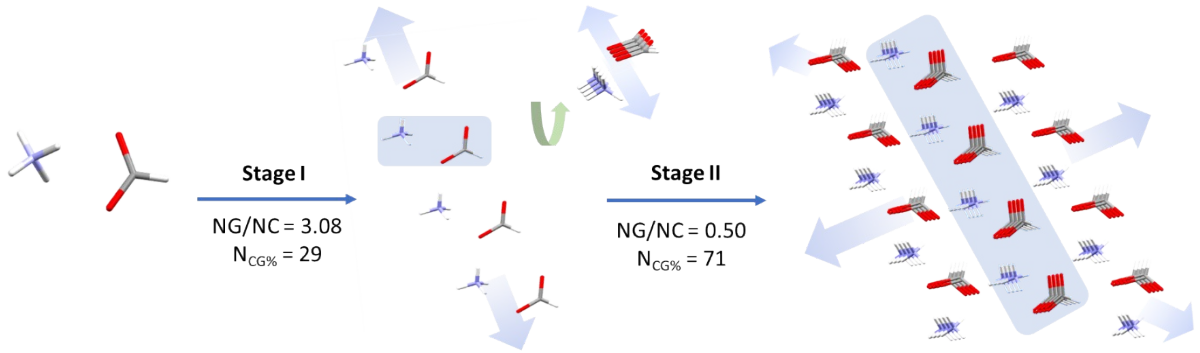


Figure S1. Proposal of crystallization mechanism of compound **1**. The color-shaded area represents the portion in the previous step.

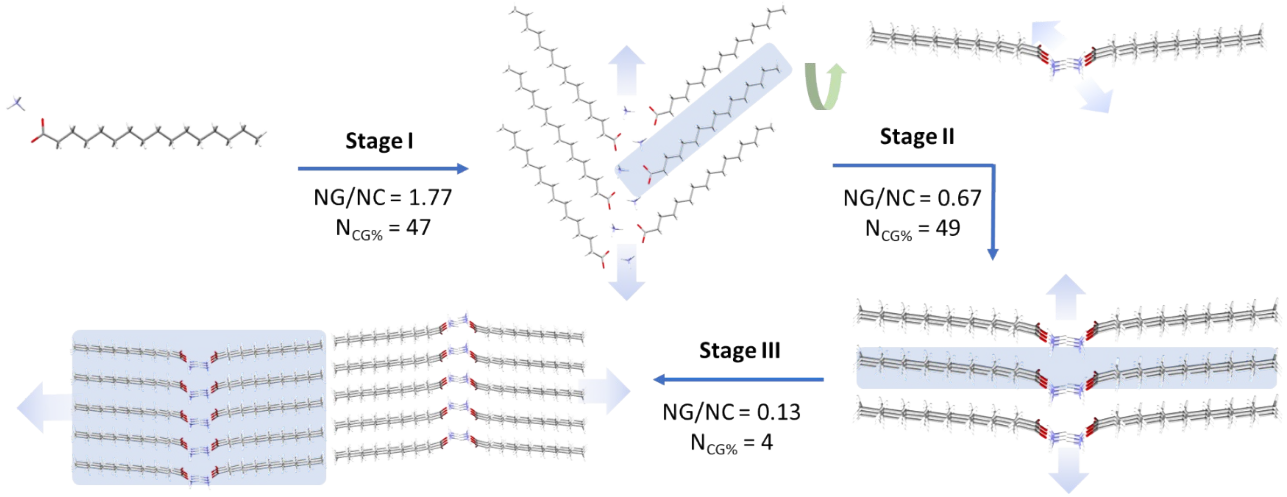


Figure S2. Proposal of crystallization mechanism of compound **5**. The color-shaded area represents the portion in the previous step.

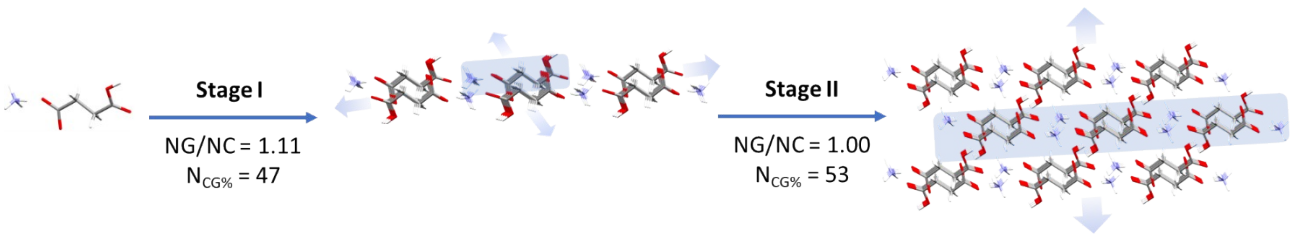


Figure S3. Proposal of crystallization mechanism of compound **7**. The color-shaded area represents the portion in the previous step.

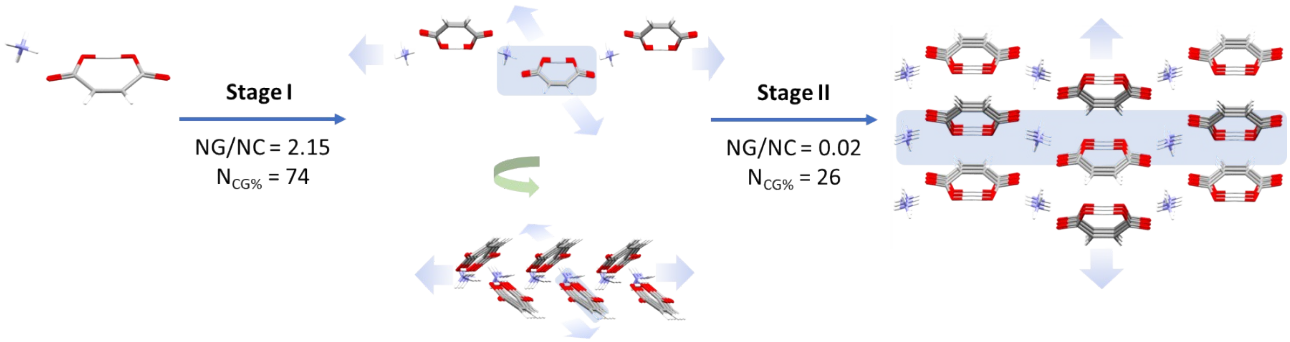


Figure S4. Proposal of crystallization mechanism of compound **8**. The color-shaded area represents the portion in the previous step.

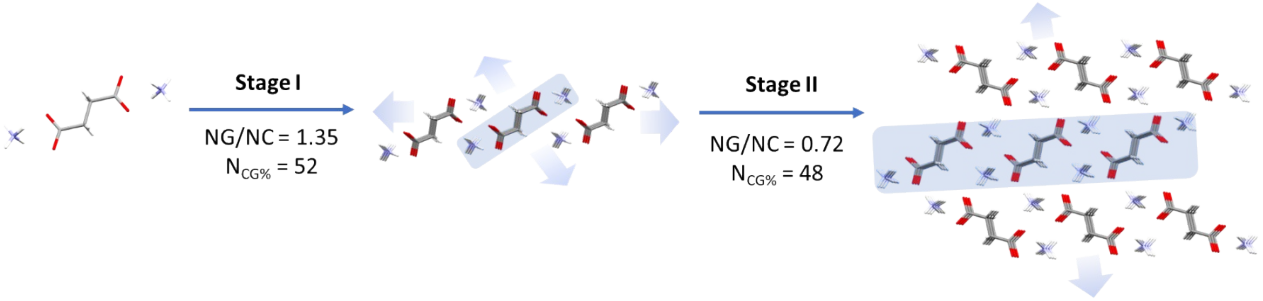


Figure S5. Proposal of crystallization mechanism of compound **9**. The color-shaded area represents the portion in the previous step.

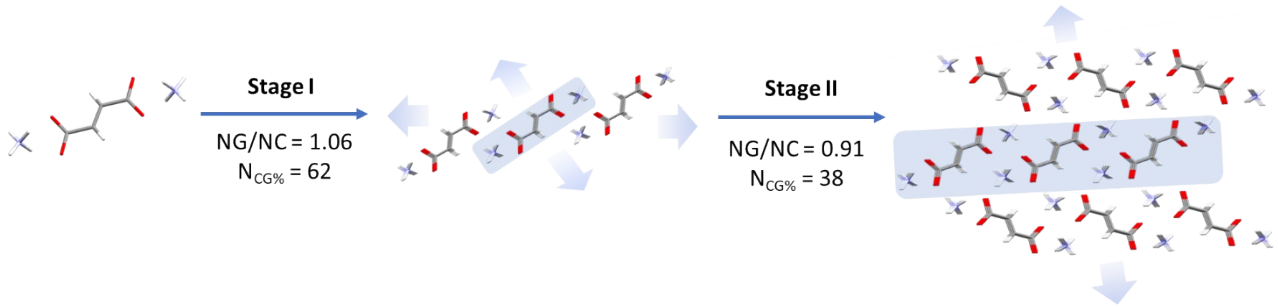


Figure S6. Proposal of crystallization mechanism of compound **10**. The color-shaded area represents the portion in the previous step.

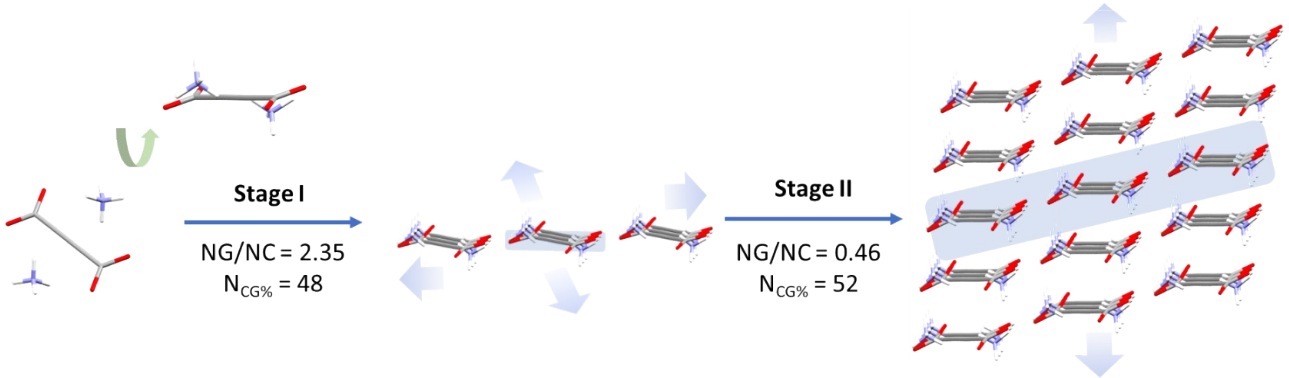


Figure S7. Proposal of crystallization mechanism of compound **11**. The color-shaded area represents the portion in the previous step.