

# SUPRAMOLECULAR CLUSTERS OF IMIDAZOLIUM-BASED IONIC LIQUIDS: THE EFFECT OF THE CATION-ANION STRUCTURE ON CRYSTALLIZATION

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1. Symmetry Codes, Contact Area, Absolute Stabilization Energies and distances of each  $C_1 \cdots A_N$  pairs

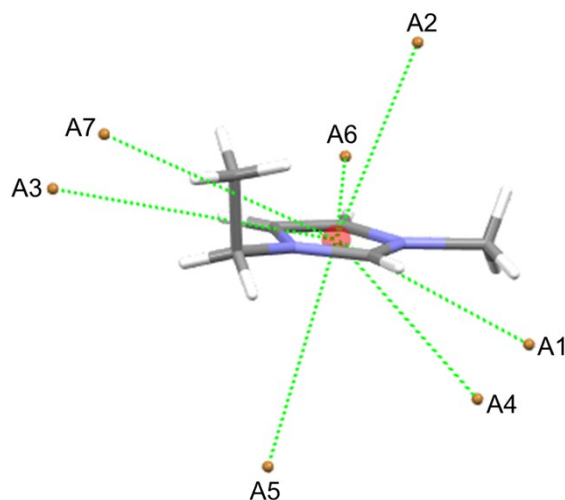


Figure S1- Central cation and all anions with which contact area was established, for compound **1**.

Table S1- Symmetry codes, contact area, absolute stabilization energies and distances  $C \cdots X$  of each  $C_1 \cdots A_N$  pair of **1**.

Pair $C \cdots A_N$	Anion symmetry code <sup>a</sup>	$C_{C \cdots A_N}$ <sup>b</sup>	$G_{C \cdots A_N}$ <sup>c</sup>	$G_{C \cdots A_N} - G_{C \cdots A1}$ <sup>d</sup>	$C \cdots X$ <sup>e</sup>
CA1	2-x,-1/2+y,1/2-z	8.60	-2918.6532	0.00	4.658
CA2	x,1/2-y,1/2+z	8.36	-2918.6488	2.76	3.77
CA3	1+x,y,z	8.18	-2918.6406	7.90	4.867
CA4	x,y,z	6.92	-2918.6312	13.82	4.883
CA5	2-x,1/2+y,1/2-z	3.91	-2918.6306	14.23	5.151
CA6	2-x,1-y,-z	4.87	-2918.6293	15.03	4.947
CA7	1+x,1/2-y,1/2+z	2.10	-2918.6023	31.96	7.570

<sup>a</sup>Cation C symmetry code: x, y, z. <sup>b</sup>Contact area between C1 and each considered anion, in  $\text{\AA}^2$ . <sup>c</sup>Absolute energy of each  $C_1 \cdots A_N$  pair, in a.u. <sup>d</sup>Difference of absolute energies between the most stable pair and each considered pair ( $G_{C \cdots A_N} - G_{C \cdots A1}$ ), in  $\text{kcal mol}^{-1}$ . <sup>e</sup>Distance between the centroid of C1 (cation) and each Br<sup>-</sup> anion, in  $\text{\AA}$ .

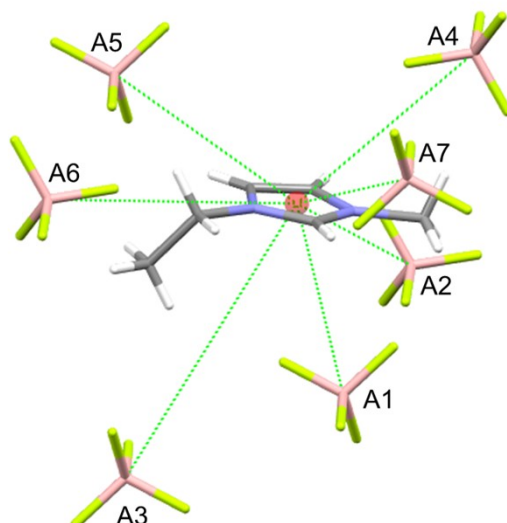


Figure S2- Central cation and all anions with which contact area was established, for compound **2**.

Table S2- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **2**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...A<sub>N</sub></sub> <sup>b</sup>	G <sub>C...A<sub>N</sub></sub> <sup>c</sup>	G <sub>C...A<sub>N</sub></sub> - G <sub>C...A<sub>1</sub></sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	x,y,z	17.39	-768.8084	0.00	4.374
CA2	x,1/2-y,1/2+z	15.77	-768.8078	0.39	4.892
CA3	2-x,1-y,1-z	13.46	-768.7951	8.35	6.584
CA4	2-x,-1/2+y,1.5-z	12.99	-768.7943	8.82	5.104
CA5	-1+x,y,z	12.51	-768.7877	12.95	4.792
CA6	-1+x,1/2-y,-1/2+z	11.12	-768.7768	19.83	6.778
CA7	2-x,-y,1-z	4.55	-768.7635	28.14	4.685

<sup>a</sup>Cation C symmetry code: x, y, z. <sup>b</sup>Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup>Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup>Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-A<sub>N</sub></sub> - G<sub>C-A<sub>1</sub></sub>), in kcal mol<sup>-1</sup>. <sup>e</sup>Distance between the centroid of C1 (cátion) and each B<sub>i</sub><sup>-</sup> anion, in Å.

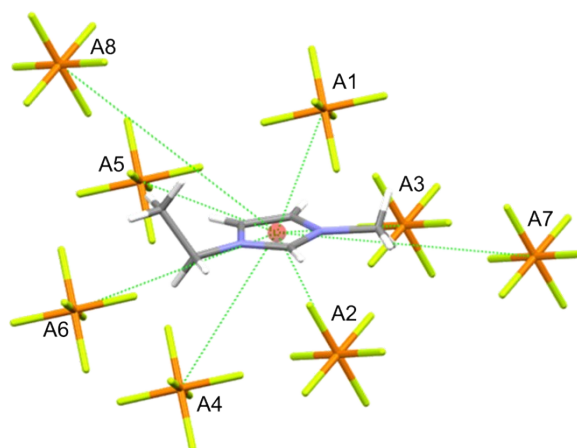


Figure S3- Central cation and all anions with which contact area was established, for compound **3**.

Table S3- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **3**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	1-x,-1/2+y,1.5-z	22.25	-1284.9467	0.00	4.321
CA2	1+x,y,z	17.79	-1284.9448	1.16	5.043
CA3	x,y,z	14.56	-1284.9324	8.96	5.292
CA4	1-x,1/2+y,1.5-z	13.87	-1284.9306	10.08	4.905
CA5	x,1.5-y,-1/2+z	14.21	-1284.9295	10.74	5.246
CA6	1+x,1.5-y,-1/2+z	13.46	-1284.9187	17.53	6.959
CA7	1-x,1-y,2-z	9.40	-1284.9173	18.44	6.723
CA8	1-x,1-y,1-z	6.74	-1284.8992	29.79	7.761

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each P<sup>-</sup> anion, in Å.

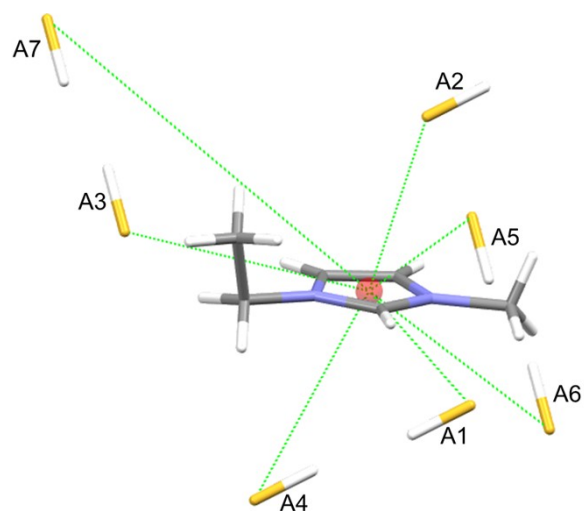


Figure S4- Central cation and all anions with which contact area was established, for compound **4**.

Table S4- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **4**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	1/2+x,1.5-y,-1/2+z	9.00	-743.2415	0.00	4.598
CA2	1/2-x,-1/2+y,1/2-z	8.01	-743.2324	5.67	3.853
CA3	x,y,z	7.32	-743.2278	8.57	4.830
CA4	1/2-x,1/2+y,1/2-z	6.36	-743.2164	15.76	5.056
CA5	1-x,1-y,1-z	5.16	-743.2157	16.17	4.896
CA6	1+x,y,z	8.49	-743.2134	17.6	4.942
CA7	-x,1-y,1-z	1.37	-743.1845	35.79	8.285

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cátion) and each S<sup>-</sup> anion, in Å.

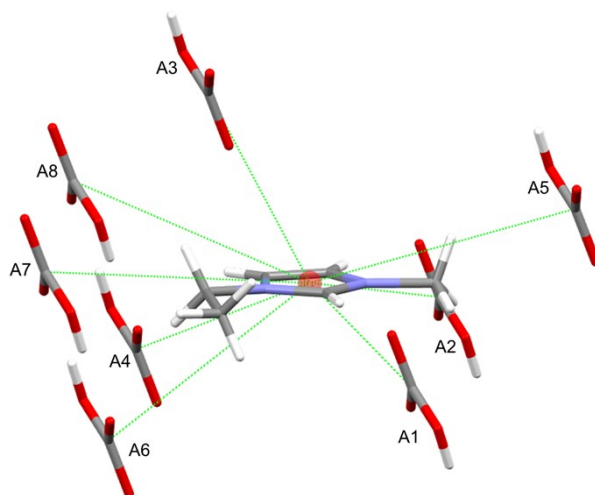


Figure S5- Central cation and all anions with which contact area was established, for compound **5**.

Table S5- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **5**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	-x,1-y,1-z	15.71	-608.8315	0.00	4.445
CA2	1-x,1-y,1-z	12.12	-608.8008	19.28	4.763
CA3	x,y,1+z	6.59	-608.7891	26.62	5.437
CA4	1+x,1+y,1+z	5.18	-608.7844	29.54	5.220
CA5	x,y,z	7.55	-608.7785	33.25	5.89
CA6	x,1+y,1+z	9.28	-608.7682	39.7	6.409
CA7	-x,1-y,2-z	3.86	-608.7632	42.87	7.324
CA8	1-x,1-y,2-z	5.09	-608.7611	44.17	5.806

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each C, anion, in Å.

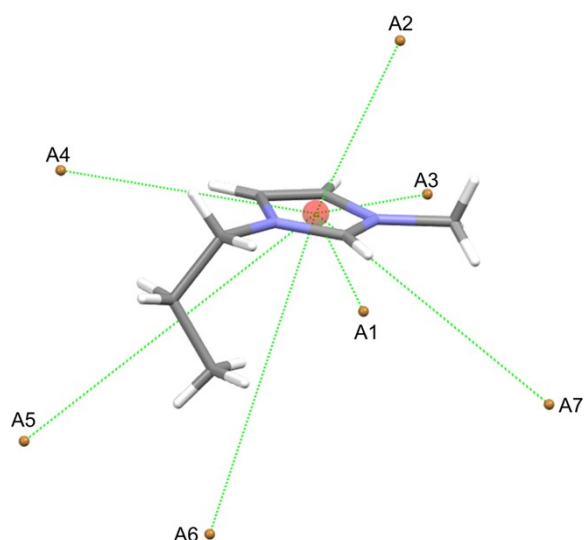


Figure S6- Central cation and all anions with which contact area was established, for compound **6**.

Table S6- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **6**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> – G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	1/2+x,1.5-y,-1/2+z	7.70	-2957.861	0.00	4.667
CA2	1/2-x,-1/2+y,1/2-z	8.03	-2957.8517	5.82	3.633
CA3	1-x,1-y,1-z	7.2	-2957.8486	7.78	4.764
CA4	1+x,y,z	6.46	-2957.846	9.4	4.858
CA5	1/2-x,1/2+y,1/2-z	5.08	-2957.8103	31.8	7.373
CA6	x,y,z	1.74	-2957.8074	33.62	6.45
CA7	-x,1-y,1-z	4.06	-2957.8074	33.62	5.586

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> – G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each Br<sup>-</sup>, anion, in Å.

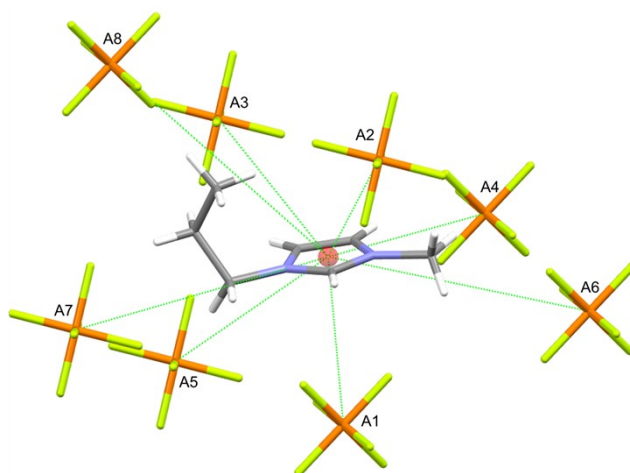


Figure S7- Central cation and all anions with which contact area was established, for compound **7**.

Table S7- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **7**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	1+x,y,z	19.50	-1324.2255	0.00	4.593
CA2	1-x,-1/2+y,1/2-z	24.41	-1324.2221	2.15	4.879
CA3	x,1/2-y,-1/2+z	17.31	-1324.2087	10.54	5.169
CA4	x,y,z	9.96	-1324.2059	12.32	5.494
CA5	1-x,1/2+y,1/2-z	11.55	-1324.2046	13.15	5.502
CA6	1-x,-y,1-z	10.41	-1324.1981	17.18	6.592
CA7	1+x,1/2-y,-1/2+z	14.27	-1324.197	17.92	7.069
CA8	1-x,-y,-z	5.39	-1324.1721	33.53	8.655

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each P<sup>-</sup> anion, in Å.

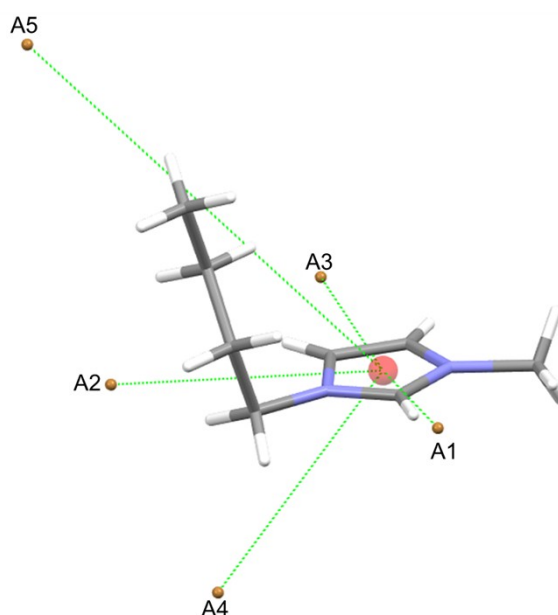


Figure S8- Central cation and all anions with which contact area was established, for compound **8**

Table S8- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **8**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	1/2-x,1/2+y,1/2+z	7.01	-2997.2055	0.00	4.643
CA2	x,y,z	8.30	-2997.1925	8.15	4.847
CA3	1-x,-y,1/2+z	6.40	-2997.1868	11.72	4.544
CA4	-1/2+x,1/2-y,z	3.98	-2997.1782	17.15	5.85
CA5	1/2+x,1/2-y,z	2.54	-2997.1427	39.39	8.178

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each Br<sup>-</sup> anion, in Å.

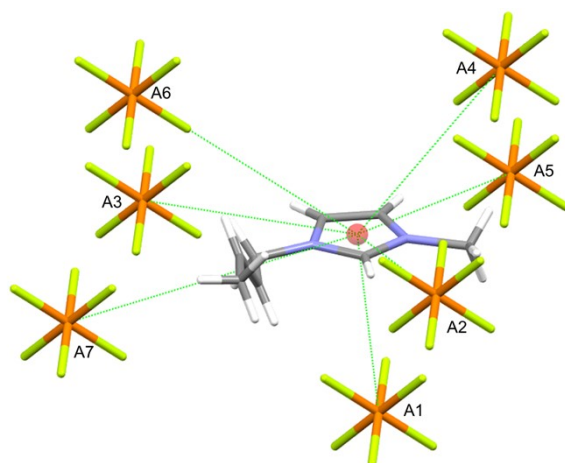


Figure S9- Central cation and all anions with which contact area was established, for compound **9**.

Table S9-Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **9**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	-x,1-y,1-z	24.58	-1362.2175	0.00	4.123
CA2	x,y,-1+z	7.65	-1362.2118	3.57	5.341
CA3	x,-1+y,z	12.59	-1362.1993	11.43	5.390
CA4	1-x,1-y,1-z	9.89	-1362.1978	12.36	5.123
CA5	x,y,z	15.8	-1362.1948	14.28	5.488
CA6	1-x,-y,1-z	13.64	-1362.1859	19.84	6.615
CA7	x,-1+y,-1+z	21.69	-1362.1633	34.01	9.641

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each P<sup>-</sup>, anion, in Å.

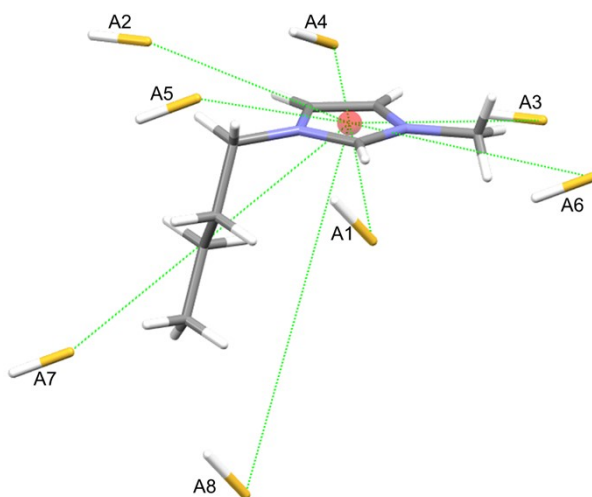


Figure S10- Central cation and all anions with which contact area was established, for compound **10**.

Table S10- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **10**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	1/2-x, -1/2+y, -1/2+z	7.98	-821.8205	0.00	4.615
CA2	x, y, z	7.02	-821.8076	8.10	4.665
CA3	x, y, -1+z	8.7	-821.8018	11.76	4.966
CA4	-x, 2-y, -1/2+z	8.51	-821.7959	15.48	4.62
CA5	1/2+x, 1.5-y, z	4.65	-821.7934	17.06	5.757
CA6	1/2+x, 1.5-y, -1+z	7.53	-821.784	22.91	6.003
CA7	-1/2+x, 1.5-y, z	2.99	-821.7523	42.82	7.960
CA8	-1/2-x, -1/2+y, -1/2+z	0.57	-821.7425	49.10	8.790

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each S<sup>-</sup> anion, in Å.

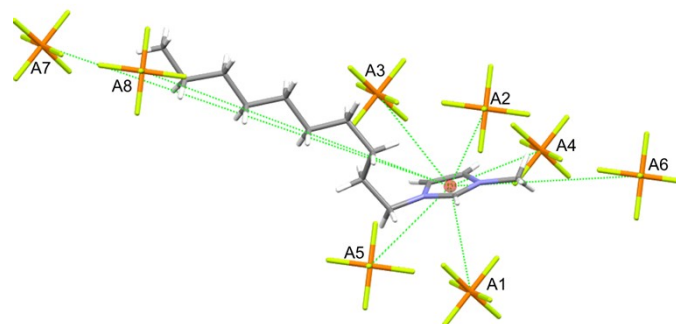


Figure S11- Central cation and all anions with which contact area was established, for compound **11**.

Table S11- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **11**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	$x, 1/2-y, 1/2+z$	20.47	-1598.8719	0.00	4.592
CA2	$x, y, z$	24.05	-1598.869	1.86	4.744
CA3	$x, 1/2-y, -1/2+z$	25.94	-1598.8583	8.55	4.932
CA4	$1-x, -1/2+y, 1/2-z$	14.98	-1598.8575	9.09	5.315
CA5	$x, -1+y, z$	16.02	-1598.8531	11.87	5.206
CA6	$1-x, 1-y, 1-z$	7.09	-1598.8347	23.36	7.319
CA7	$-x, -1/2+y, -1/2-z$	8.73	-1598.7894	51.81	16.942
CA8	$-x, 1-y, -z$	0.10	-1598.7888	52.18	16.018

<sup>a</sup> Cation C symmetry code:  $x, y, z$ . <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each P<sup>-</sup> anion, in Å.

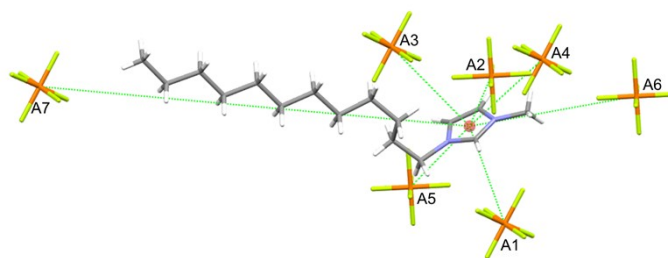


Figure S12- Central cation and all anions with which contact area was established, for compound **12**.

Table S12- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **12**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	1+x,y,z	21.36	-1677.5353	0.00	4.514
CA2	1/2+x,-1/2-y,z	23.51	-1677.5317	2.28	4.779
CA3	x,y,z	26.14	-1677.522	8.35	4.866
CA4	1-x,-y,1-z	14.74	-1677.5194	10.02	5.298
CA5	1/2+x,1/2-y,z	15.75	-1677.5156	12.36	5.203
CA6	1.5-x,-1/2+y,1-z	6.68	-1677.4961	24.61	7.342
CA7	-x,-y,-z	8.50	-1677.4473	55.25	19.359

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each P<sup>-</sup>, anion, in Å.

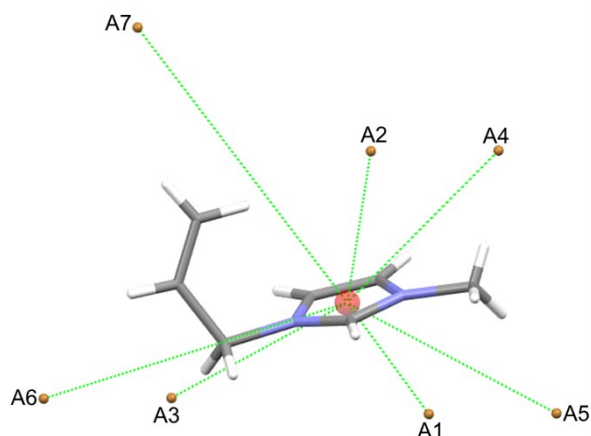


Figure S13- Central cation and all anions with which contact area was established, for compound **13**.

Table S13- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **13**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	x,1+y,z	7.45	-2956.5723	0.00	4.606
CA2	1-x,1/2+y,1-z	9.12	-2956.5706	1.09	3.994
CA3	2-x,1/2+y,2-z	6.89	-2956.5588	8.48	4.759
CA4	2-x,1/2+y,1-z	4.72	-2956.5517	12.95	4.944
CA5	1+x,1+y,z	4.54	-2956.5506	13.61	4.851
CA6	1-x,1/2+y,2-z	4.55	-2956.5356	23.05	6.679
CA7	x,y,z	4.10	-2956.5219	31.61	6.801

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each Br<sup>-</sup> anion, in Å.

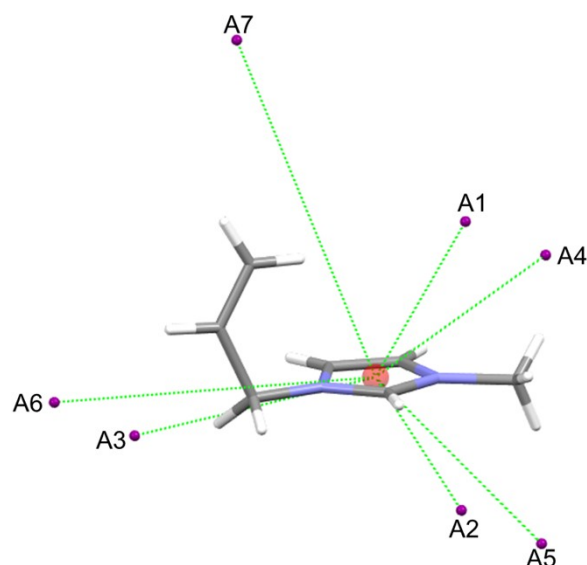


Figure S14- Central cation and all anions with which contact area was established, for compound **14**.

Table S14- Symmetry codes, contact area, absolute stabilization energies and C...X distances of each C<sub>1</sub>...A<sub>N</sub> pair of **14**.

Pair C...A <sub>N</sub>	Anion symmetry code <sup>a</sup>	C <sub>C...AN</sub> <sup>b</sup>	G <sub>C...AN</sub> <sup>c</sup>	G <sub>C...AN</sub> - G <sub>C...A1</sub> <sup>d</sup>	C...X <sup>e</sup>
CA1	-1+x,y,-1+z	10.33	-678.357053	0.00	4.291
CA2	1-x,1/2+y,1-z	8.72	-678.356561	0.31	4.818
CA3	x,y,z	7.28	-678.345918	6.99	4.984
CA4	x,y,-1+z	6.78	-678.342641	9.04	5.082
CA5	2-x,1/2+y,1-z	5.51	-678.341248	9.92	4.858
CA6	-1+x,y,z	5.04	-678.320024	23.24	7.163
CA7	1-x,-1/2+y,1-z	3.62	-678.310583	29.16	6.986

<sup>a</sup> Cation C symmetry code: x, y, z. <sup>b</sup> Contact area between C1 and each considered anion, in Å<sup>2</sup>. <sup>c</sup> Absolute energy of each C<sub>1</sub>...A<sub>N</sub> pair, in a.u. <sup>d</sup> Difference of absolute energies between the most stable pair and each considered pair (G<sub>C-AN</sub> - G<sub>C-A1</sub>), in kcal mol<sup>-1</sup>. <sup>e</sup> Distance between the centroid of C1 (cation) and each I<sup>-</sup> anion, in Å.

## 2. Symmetry Codes, Contact Area, Stabilization and Destabilization Energies and Normalized Data

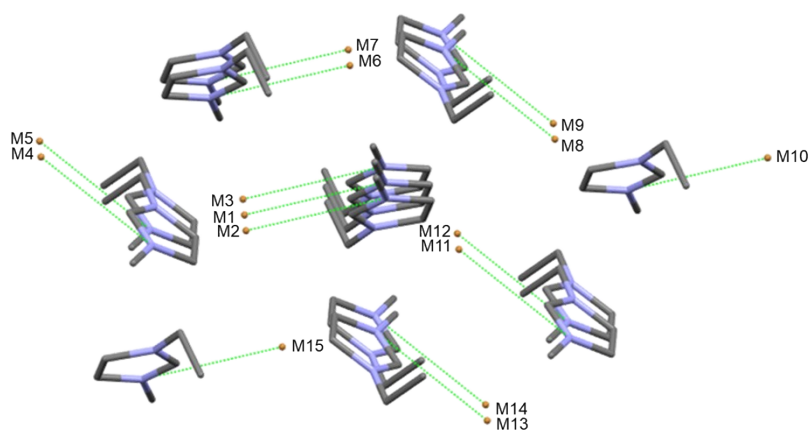


Figure S15- Supramolecular cluster of compound **1<sub>CA1</sub>**, based on the CA1 cation-anion pair.

Table S15- Symmetry codes for the monomers of compound **1<sub>CA1</sub>**.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1+x,1/2-y,1/2+z$
M2	$1+x,y,z$	$2+x,1/2-y,1/2+z$
M3	$-1+x,y,z$	$x,1/2-y,1/2+z$
M3	$1+x,1/2-y,1/2+z$	$2+x,y,1+z$
M4	$x,1/2-y,1/2+z$	$1+x,y,1+z$
M5	$3-x,1-y,1-z$	$2-x,1/2+y,1/2-z$
M6	$2-x,1-y,1-z$	$1-x,1/2+y,1/2-z$
M7	$3-x,1/2+y,1/2-z$	$2-x,1-y,-z$
M8	$2-x,1/2+y,1/2-z$	$1-x,1-y,-z$
M9	$2-x,1-y,-z$	$1-x,1/2+y,-1/2-z$
M10	$x,1/2-y,-1/2+z$	$1+x,y,z$
M11	$-1+x,1/2-y,-1/2+z$	$x,y,z$
M12	$3-x,-1/2+y,1/2-z$	$2-x,-y,-z$
M13	$2-x,-1/2+y,1/2-z$	$1-x,-y,-z$
M14	$3-x,-y,1-z$	$2-x,-1/2+y,1/2-z$
M15	$x,y,z$	$1+x,1/2-y,1/2+z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S16- Contact area ( $C_{M_1 \dots M_N}$ ) and stabilization energy ( $G_{M_1 \dots M_N}$ ) and normalized contact area and stabilization energy data area ( $NC_{M_1 \dots M_N}$  and  $NG_{M_1 \dots M_N}$ ) between the dimers of the supramolecular cluster for **1**<sub>CA1</sub>.

Dimer	$C_{M_1 \dots M_N}$ (Å <sup>2</sup> )	$G_{M_1 \dots M_N}$ (kcal mol <sup>-1</sup> )	$NC_{M_1 \dots M_N}$	$NG_{M_1 \dots M_N}$
M1...M6	39.54	-33.15	2.41	3.9
M1... M15	7.86	-19.82	0.48	2.33
M1...M8	25.41	-15.15	1.55	1.78
M1...M13	25.41	-15.15	1.55	1.78
M1...M4	8.18	-15.1	0.5	1.77
M1...M12	21.68	-15.1	1.32	1.77
M1...M5	20.41	-2.61	1.24	0.31
M1...M11	6.92	-2.61	0.42	0.31
M1...M7	9.44	-2.46	0.58	0.29
M1...M2	10.84	-1.79	0.66	0.21
M1...M3	10.84	-1.79	0.66	0.21
M1...M9	20.42	0.70	1.24	-0.08
M1...M14	20.42	0.70	1.24	-0.08
M1...M10	2.26	4.20	0.14	-0.49
TOTAL	229.63	-119.13	14	14

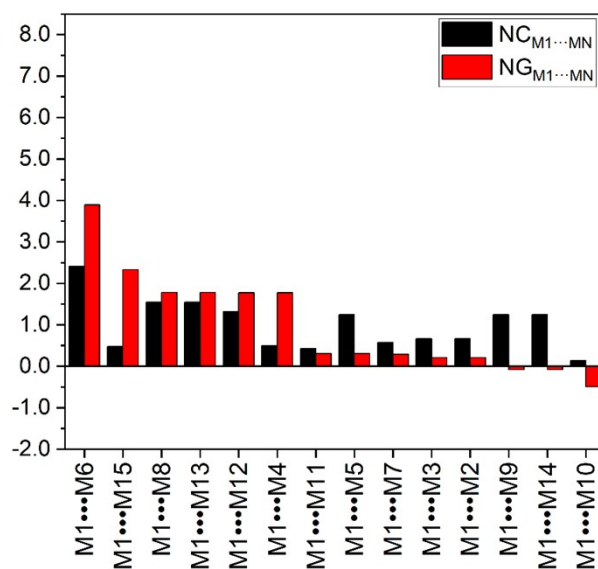


Figure S16- Normalized contact ( $NC_{M_1 \dots M_N}$ ) area and stabilization energy ( $NG_{M_1 \dots M_N}$ ) data of each dimer from the supramolecular cluster of compound **1**<sub>CA1</sub>.

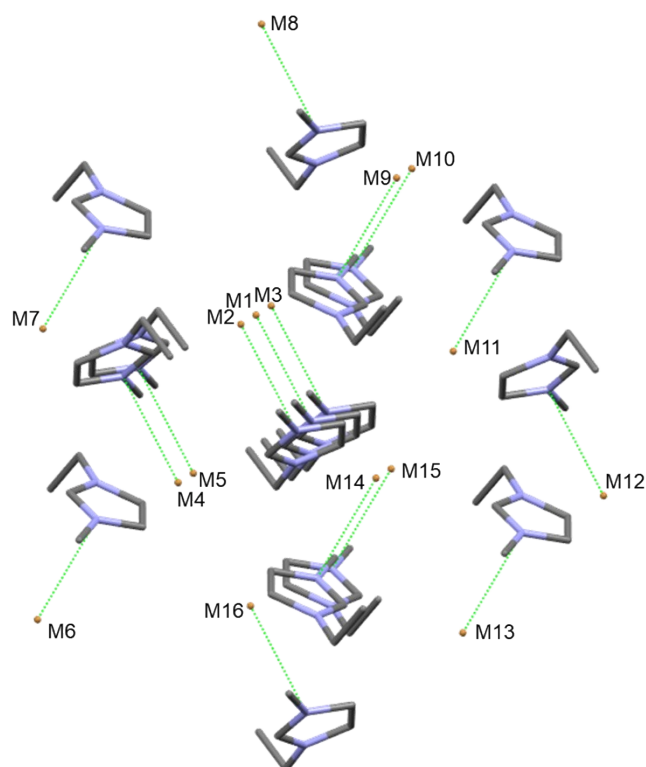


Figure S17- Supramolecular cluster of compound  $\mathbf{1}_{CA2}$ , based on the CA2 cation-anion pair.

Table S17- Symmetry codes for the monomers of compound  $\mathbf{1}_{CA2}$ .

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x, y, z$	$2-x, 1/2+y, 1/2-z$
M2	$1+x, y, z$	$3-x, 1/2+y, 1/2-z$
M3	$-1+x, y, z$	$1-x, 1/2+y, 1/2-z$
M3	$x, 1/2-y, 1/2+z$	$2-x, -y, 1-z$
M4	$3-x, 1-y, 1-z$	$1+x, 1/2-y, 1/2+z$
M5	$2-x, 1-y, 1-z$	$x, 1/2-y, 1/2+z$
M6	$x, 1.5-y, 1/2+z$	$2-x, 1-y, 1-z$
M7	$x, 1+y, z$	$2-x, 1.5+y, 1/2-z$
M8	$3-x, 1/2+y, 1/2-z$	$1+x, 1+y, z$
M9	$2-x, 1/2+y, 1/2-z$	$x, 1+y, z$
M10	$1+x, 1.5-y, -1/2+z$	$3-x, 1-y, -z$
M11	$3-x, 1-y, -z$	$1+x, 1/2-y, -1/2+z$
M12	$x, 1/2-y, -1/2+z$	$2-x, -y, -z$
M13	$4-x, -1/2+y, 1/2-z$	$2+x, y, z$
M14	$3-x, -1/2+y, 1/2-z$	$1+x, y, z$

M15	$x, -1+y, z$	$2-x, -1/2+y, 1/2-z$
M16	$x, y, z$	$2-x, 1/2+y, 1/2-z$

<sup>a</sup>Symmetry codes were taken using the N2 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br atom of the anion as reference.

Table S18- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **1**<sub>CA2</sub>.

Dimer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M4	13.5	-38.67	0.88	5.43
M1...M5	40.01	-13.53	2.61	1.9
M1...M7	4.87	-11.21	0.32	1.57
M1...M8	3.91	-10.5	0.25	1.48
M1... M16	3.91	-10.5	0.25	1.48
M1...M10	28.6	-9.72	1.86	1.37
M1...M9	27.46	-7.93	1.79	1.11
M1... M15	28.6	-7.93	1.86	1.11
M1...M11	4.87	-1.6	0.32	0.23
M1...M6	13.63	-1.05	0.89	0.15
M1...M13	13.5	-1.05	0.88	0.15
M1...M12	2.26	0.25	0.15	-0.04
M1...M14	27.46	0.7	1.79	-0.1
M1...M2	8.74	2.98	0.57	-0.42
M1...M3	8.74	2.98	0.57	-0.42
TOTAL	230.06	-106.81	15	15

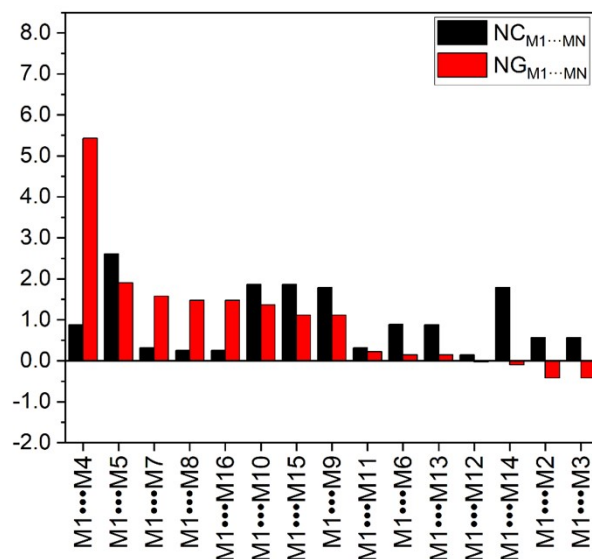


Figure S18- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **1**<sub>CA2</sub>.

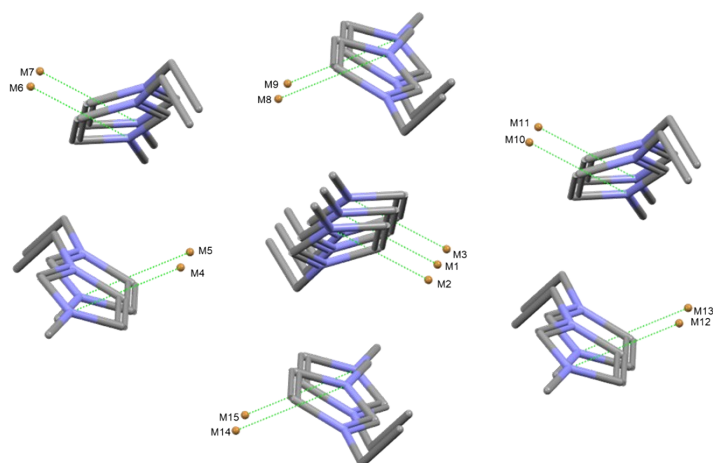


Figure S19- Supramolecular cluster of compound **1**<sub>CA3</sub>, based on the CA3 cation-anion pair.

Table S19- Symmetry codes for the monomers of compound **1**<sub>CA3</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x, y, z$	$x, y, z$
M2	$1+x, y, z$	$1+x, y, z$
M3	$-1+x, y, z$	$-1+x, y, z$
M4	$1+x, 1/2-y, 1/2+z$	$1+x, 1/2-y, 1/2+z$
M5	$x, 1/2-y, 1/2+z$	$x, 1/2-y, 1/2+z$
M6	$3-x, 1-y, 1-z$	$3-x, 1-y, 1-z$

M7	2-x,1-y,1-z	2-x,1-y,1-z
M8	3-x,1/2+y,1/2-z	3-x,1/2+y,1/2-z
M9	2-x,1/2+y,1/2-z	2-x,1/2+y,1/2-z
M10	2-x,1-y,-z	2-x,1-y,-z
M11	1-x,1-y,-z	1-x,1-y,-z
M12	x,1/2-y,-1/2+z	x,1/2-y,-1/2+z
M13	-1+x,1/2-y,-1/2+z	-1+x,1/2-y,-1/2+z
M14	3-x,-1/2+y,1/2-z	3-x,-1/2+y,1/2-z
M15	2-x,-1/2+y,1/2-z	2-x,-1/2+y,1/2-z

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S20- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{C_{M1...MN}}$  and  $N_{G_{M1...MN}}$ ) between the dimers of the supramolecular cluster for **1**<sub>CA3</sub>.

Dimer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{C_{M1...MN}}$	$N_{G_{M1...MN}}$
M1...M9	28.78	-37.75	1.73	3.31
M1... M15	24.33	-37.75	1.46	3.31
M1...M10	9.79	-33.39	0.59	2.93
M1...M4	22.09	-20.88	1.33	1.83
M1...M13	22.09	-20.88	1.33	1.83
M1...M2	16.92	-11.49	1.02	1.01
M1...M3	16.92	-11.49	1.02	1.01
M1...M6	22.82	-7.49	1.37	0.66
M1...M7	9.44	-7.49	0.57	0.66
M1...M8	24.45	0.59	1.47	-0.05
M1...M14	28.9	0.59	1.74	-0.05
M1...M5	2.1	8.01	0.13	-0.7
M1...M12	2.1	8.01	0.13	-0.7
M1...M11	2.26	11.97	0.14	-1.05
TOTAL	232.99	-159.44	14	14

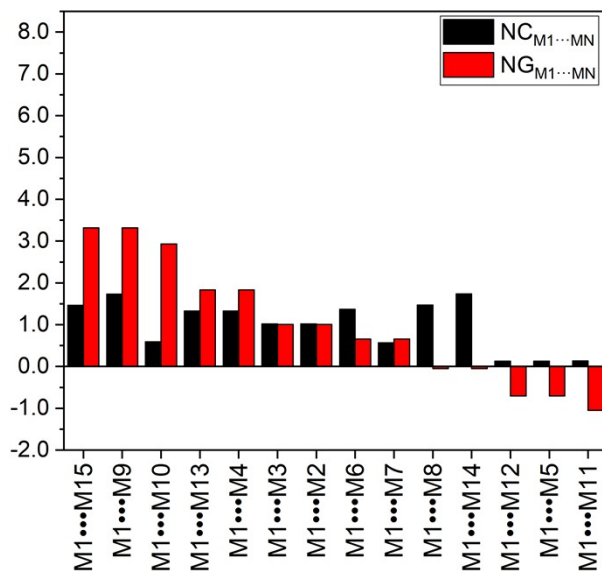


Figure S20- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **1**<sub>CA3</sub>.

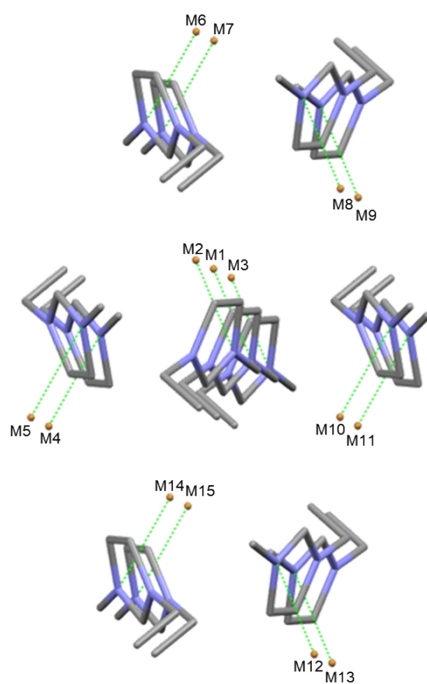


Figure S21- Supramolecular cluster of compound **1**<sub>CA4</sub>, based on the CA4 cation-anion pair.

Table S21- Symmetry codes for the monomers of compound **1**<sub>CA4</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	x,y,z	1+x,y,z
M2	-1+x,y,z	x,y,z
M3	1+x,y,z	2+x,y,z
M3	2-x,-1/2+y,1/2-z	1-x,-1/2+y,1/2-z
M4	3-x,-1/2+y,1/2-z	2-x,-1/2+y,1/2-z
M5	x,1/2-y,-1/2+z	1+x,1/2-y,-1/2+z
M6	1+x,1/2-y,-1/2+z	2+x,1/2-y,-1/2+z
M7	3-x,1-y,-z	2-x,1-y,-z
M8	4-x,1-y,-z	3-x,1-y,-z
M9	2-x,1/2+y,1/2-z	1-x,1/2+y,1/2-z
M10	3-x,1/2+y,1/2-z	2-x,1/2+y,1/2-z
M11	2-x,1-y,1-z	1-x,1-y,1-z
M12	3-x,1-y,1-z	2-x,1-y,1-z
M13	-1+x,1/2-y,1/2+z	x,1/2-y,1/2+z
M14	x,1/2-y,1/2+z	1+x,1/2-y,1/2+z
M15	x,y,z	1+x,y,z

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S22- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{C_{M1...MN}}$  and  $N_{G_{M1...MN}}$ ) between the dimers of the supramolecular cluster for **1**<sub>CA4</sub>.

Dimer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{C_{M1...MN}}$	$N_{G_{M1...MN}}$
M1...M5	28.9	-42.43	1.74	3.49
M1...M11	24.45	-42.43	1.47	3.49
M1...M8	2.26	-25.47	0.14	2.09
M1...M2	16.92	-16.65	1.02	1.37
M1...M3	16.92	-16.65	1.02	1.37
M1...M7	2.1	-11.41	0.13	0.94
M1...M14	2.1	-11.41	0.13	0.94
M1...M6	22.09	-10.4	1.33	0.85
M1...M15	22.09	-10.4	1.33	0.85
M1...M13	22.82	0.79	1.37	-0.07

M1...M4	24.33	2.25	1.46	-0.18
M1...M10	28.78	2.25	1.73	-0.18
M1...M12	9.44	4.55	0.57	-0.37
M1...M9	9.79	6.96	0.59	-0.57
TOTAL	232.99	-170.44	14	14

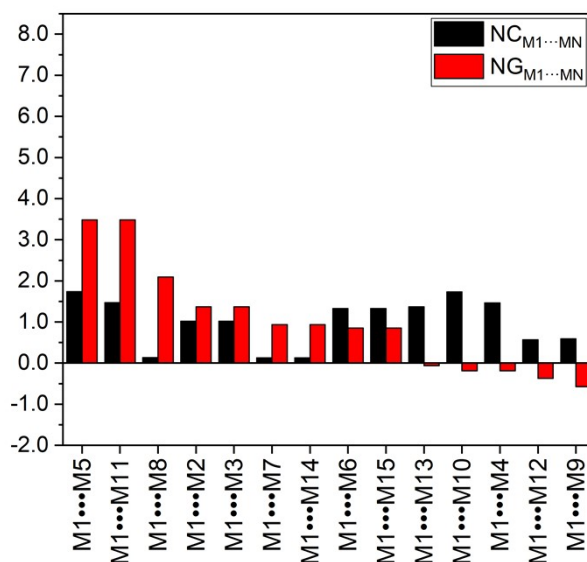


Figure S22- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **1**<sub>CA4</sub>.

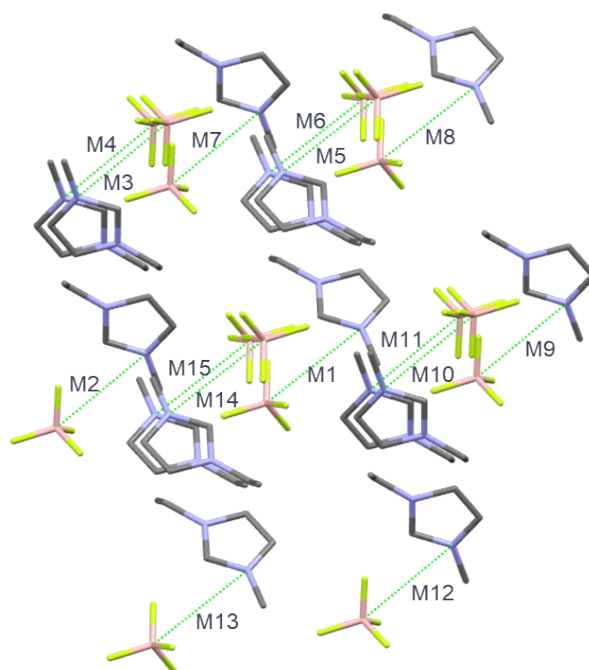


Figure S23- Supramolecular cluster of compound **2**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S23- Symmetry codes for the monomers of compound **2**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$x,y,z$
M2	$x,1/2-y,-1/2+z$	$x,1/2-y,-1/2+z$
M3	$1-x,-1/2+y,1/2-z$	$1-x,-1/2+y,1/2-z$
M3	$1-x,1/2+y,1/2-z$	$1-x,1/2+y,1/2-z$
M4	$1-x,-y,1-z$	$1-x,-y,1-z$
M5	$1-x,1-y,1-z$	$1-x,1-y,1-z$
M6	$-1+x,1/2-y,-1/2+z$	$-1+x,1/2-y,-1/2+z$
M7	$-1+x,y,z$	$-1+x,y,z$
M8	$x,1/2-y,1/2+z$	$x,1/2-y,1/2+z$
M9	$2-x,-1/2+y,1.5-z$	$2-x,-1/2+y,1.5-z$
M10	$2-x,1/2+y,1.5-z$	$2-x,1/2+y,1.5-z$
M11	$1+x,1/2-y,1/2+z$	$1+x,1/2-y,1/2+z$
M12	$1+x,y,z$	$1+x,y,z$
M13	$2-x,-y,1-z$	$2-x,-y,1-z$
M14	$2-x,1-y,1-z$	$2-x,1-y,1-z$
M15	$x,y,z$	$x,y,z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the B1 atom of the anion as reference.

Table S24- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **2**<sub>CA1</sub>.

Dimer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M14	33.71	-34.59	1.85	3.66
M1...M10	27.68	-15.52	1.52	1.64
M1...M11	27.68	-15.52	1.52	1.64
M1...M8	13.46	-14.47	0.74	1.53
M1...M13	13.46	-14.47	0.74	1.53
M1...M2	24.13	-6.08	1.32	0.64
M1...M9	24.13	-6.08	1.32	0.64
M1...M7	18.41	-4.55	1.01	0.48
M1...M12	18.41	-4.55	1.01	0.48
M1... M15	11.19	-4.58	0.61	0.48

M1...M6	13.14	-4.39	0.72	0.46
M1...M3	2.72	-3.83	0.15	0.41
M1...M4	2.72	-3.83	0.15	0.41
M1...M5	24.61	0.03	1.35	0.00
TOTAL	255.45	-132.43	14.00	14.00

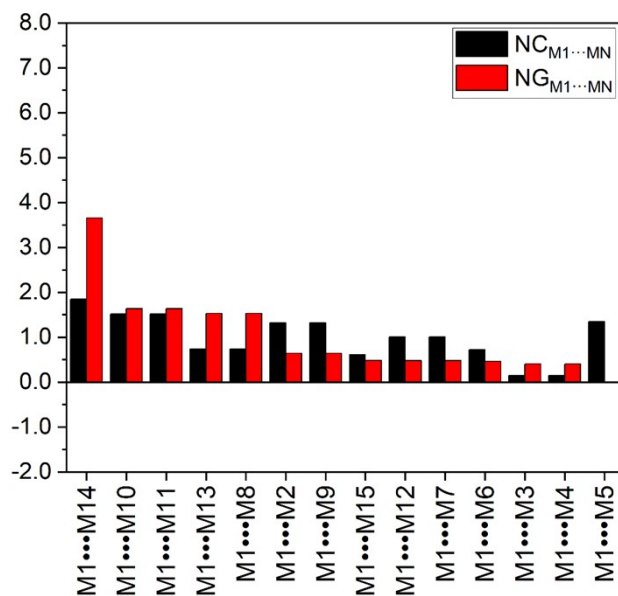


Figure S24- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **2**<sub>CA1</sub>.

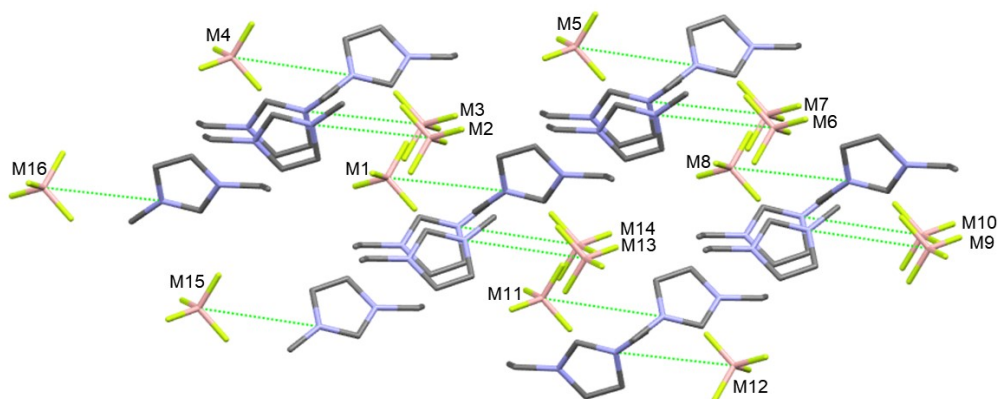


Figure S25- Supramolecular cluster of compound **2**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S25- Symmetry codes for the monomers of compound **2**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$x,1/2-y,1/2+z$
M2	$2-x,1-y,2-z$	$2-x,1/2+y,1.5-z$
M3	$2-x,-y,2-z$	$2-x,-1/2+y,1.5-z$
M3	$x,1/2-y,1/2+z$	$x,y,1+z$
M4	$-1+x,1/2-y,-1/2+z$	$-1+x,y,z$
M5	$1-x,1-y,1-z$	$1-x,1/2+y,1/2-z$
M6	$1-x,-y,1-z$	$1-x,-1/2+y,1/2-z$
M7	$-1+x,y,-1+z$	$-1+x,1/2-y,-1/2+z$
M8	$1-x,1/2+y,1/2-z$	$1-x,1-y,-z$
M9	$1-x,-1/2+y,1/2-z$	$1-x,-y,-z$
M10	$x,1/2-y,-1/2+z$	$x,y,z$
M11	$2-x,-y,1-z$	$2-x,-1/2+y,1/2-z$
M12	$2-x,1/2+y,1.5-z$	$2-x,1-y,1-z$
M13	$2-x,-1/2+y,1.5-z$	$2-x,-y,1-z$
M14	$1+x,1/2-y,1/2+z$	$1+x,y,1+z$
M15	$1+x,y,1+z$	$1+x,1/2-y,1.5+z$
M16	$x,y,z$	$x,1/2-y,1/2+z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the B1 atom of the anion as reference.

Table S26- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **2**<sub>CA2</sub>.

Dimer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1•••M14	35.49	-32.29	2.01	3.21
M1•••M13	35.49	-32.29	2.01	3.21
M1•••M3	27.11	-25.95	1.54	2.58
M1•••M16	11.12	-15.13	0.63	1.50
M1•••M8	11.12	-15.13	0.63	1.50
M1•••M11	28.53	-10.66	1.62	1.06
M1•••M4	28.53	-10.66	1.62	1.06
M1•••M5	20.75	-10.40	1.18	1.03
M1•••M15	20.75	-10.39	1.18	1.03

M1•••M6	13.14	-4.00	0.75	0.40
M1•••M2	0.30	1.85	0.02	-0.18
M1•••M7	24.61	1.95	1.40	-0.19
M1•••M12	1.86	3.31	0.11	-0.33
M1•••M9	2.72	4.36	0.15	-0.43
M1•••M10	2.72	4.36	0.15	-0.43
TOTAL	264.24	-151.07	15.00	15.00

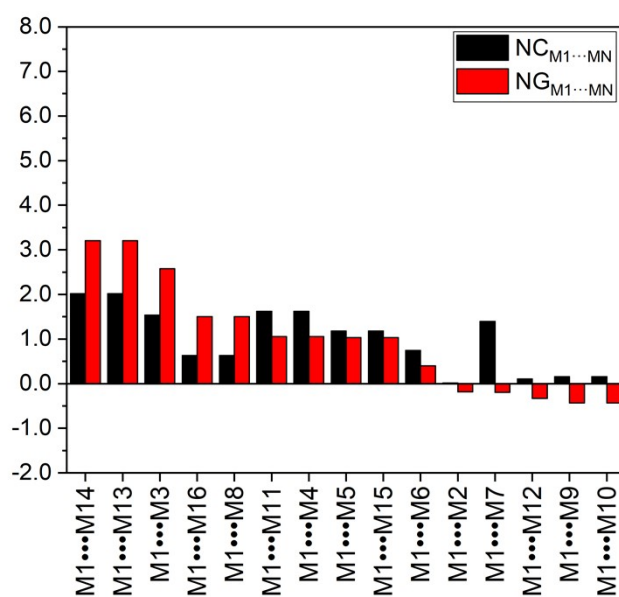


Figure S26- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **2**<sub>CA2</sub>

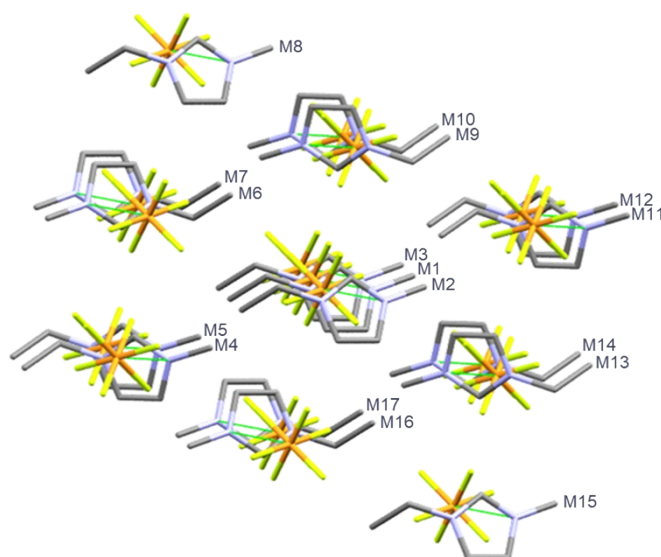


Figure S27- Supramolecular cluster of compound **3**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S27- Symmetry codes for the monomers of compound **3**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1-x,-1/2+y,1.5-z$
M2	$x,1+y,z$	$1-x,1/2+y,1.5-z$
M3	$x,-1+y,z$	$1-x,-1.5+y,1.5-z$
M4	$x,1.5-y,-1/2+z$	$1-x,2-y,1-z$
M5	$x,1/2-y,-1/2+z$	$1-x,1-y,1-z$
M6	$2-x,1-y,1-z$	$1+x,1.5-y,-1/2+z$
M7	$2-x,-y,1-z$	$1+x,1/2-y,-1/2+z$
M8	$1+x,y,z$	$2-x,-1/2+y,1.5-z$
M9	$2-x,1/2+y,1.5-z$	$1+x,y,z$
M10	$2-x,-1/2+y,1.5-z$	$1+x,-1+y,z$
M11	$x,1.5-y,1/2+z$	$1-x,2-y,2-z$
M12	$x,1/2-y,1/2+z$	$1-x,1-y,2-z$
M13	$1-x,1/2+y,1.5-z$	$x,y,z$
M14	$1-x,-1/2+y,1.5-z$	$x,-1+y,z$
M15	$-1+x,y,z$	$-x,-1/2+y,1.5-z$
M16	$1-x,1-y,1-z$	$x,1.5-y,-1/2+z$
M17	$1-x,-y,1-z$	$x,1/2-y,-1/2+z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P atom of the anion as reference.

Table S28- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **3**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1... M16	48.05	-28.48	2.85	4.08
M1...M6	42.11	-22.91	2.5	3.28
M1...M5	16.14	-14.71	0.96	2.11
M1...M12	16.14	-14.71	0.96	2.11
M1...M2	13.87	-13.46	0.82	1.93
M1...M3	13.87	-13.46	0.82	1.93
M1...M9	22.11	-7.37	1.31	1.06
M1...M10	22.11	-7.37	1.31	1.06
M1...M13	22.63	-6.75	1.34	0.97

M1...M14	22.63	-6.75	1.34	0.97
M1...M4	13.56	0.85	0.8	-0.12
M1...M11	13.56	0.85	0.8	-0.12
M1...M7	0.59	5.07	0.03	-0.73
M1...M8	0.18	5.79	0.01	-0.83
M1... M15	0.18	5.79	0.01	-0.83
M1... M17	2.11	5.95	0.13	-0.85
TOTAL	269.84	-111.70	16.00	16.00

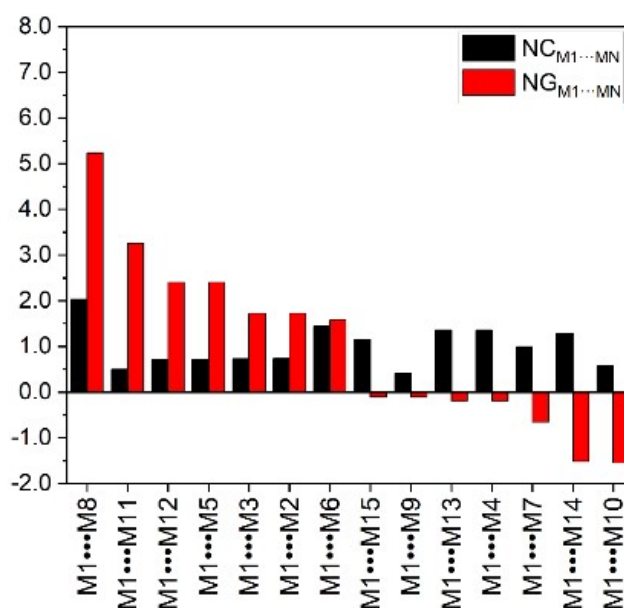


Figure S28- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **3**<sub>CA1</sub>.

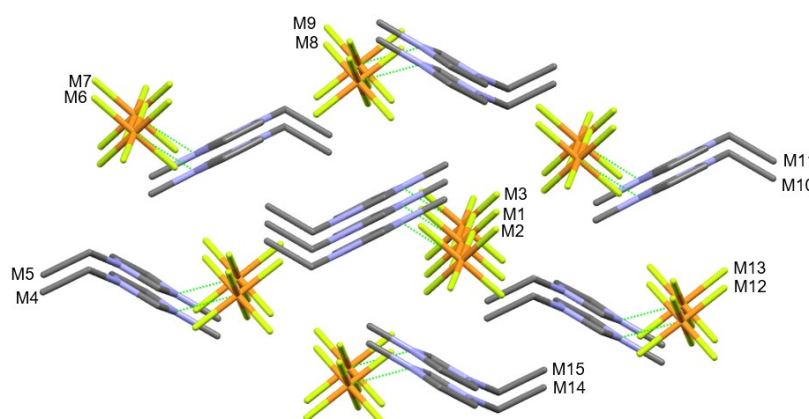


Figure S29- Supramolecular cluster of compound **3**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S29- Symmetry codes for the monomers of compound **3**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1+x,y,z$
M2	$1+x,y,z$	$2+x,y,z$
M3	$-1+x,y,z$	$x,y,z$
M4	$x,1.5-y,-1/2+z$	$1+x,1.5-y,-1/2+z$
M5	$-1+x,1.5-y,-1/2+z$	$x,1.5-y,-1/2+z$
M6	$2-x,1-y,1-z$	$1-x,1-y,1-z$
M7	$1-x,1-y,1-z$	$-x,1-y,1-z$
M8	$2-x,-1/2+y,1.5-z$	$1-x,-1/2+y,1.5-z$
M9	$1-x,-1/2+y,1.5-z$	$-x,-1/2+y,1.5-z$
M10	$3-x,1-y,2-z$	$2-x,1-y,2-z$
M11	$2-x,1-y,2-z$	$1-x,1-y,2-z$
M12	$1+x,1.5-y,1/2+z$	$2+x,1.5-y,1/2+z$
M13	$x,1.5-y,1/2+z$	$1+x,1.5-y,1/2+z$
M14	$2-x,1/2+y,1.5-z$	$1-x,1/2+y,1.5-z$
M15	$1-x,1/2+y,1.5-z$	$-x,1/2+y,1.5-z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P atom of the anion as reference.

Table S30- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **3**<sub>CA2</sub>.

Dimer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M8	40.45	-32.93	2.03	5.23
M1...M11	9.99	-20.53	0.5	3.26
M1...M5	14.21	-15.12	0.71	2.4
M1...M12	14.21	-15.12	0.71	2.4
M1...M2	14.73	-10.83	0.74	1.72
M1...M3	14.56	-10.83	0.73	1.72
M1...M6	28.67	-9.97	1.44	1.58
M1...M9	8.07	0.7	0.41	-0.11
M1... M15	22.9	0.7	1.15	-0.11
M1...M4	27.03	1.19	1.36	-0.19
M1...M13	27.03	1.19	1.36	-0.19

M1...M7	19.64	4.14	0.99	-0.66
M1...M14	25.62	9.57	1.29	-1.52
M1...M10	11.5	9.77	0.58	-1.55
TOTAL	278.61	-88.08	14.00	14.00

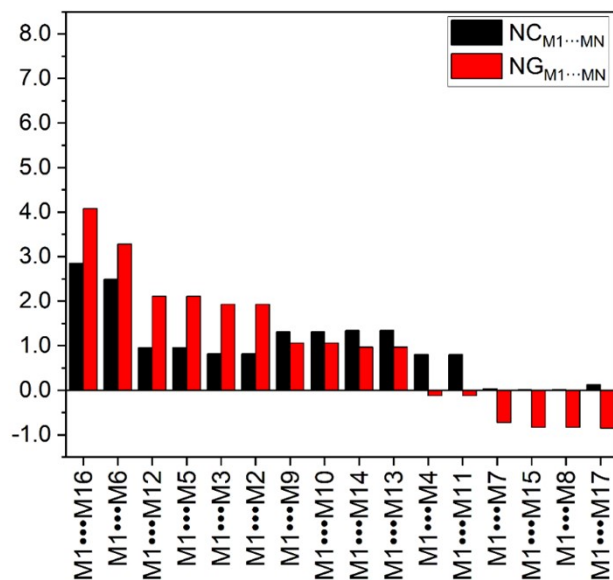


Figure S30- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **3**<sub>CA2</sub>.

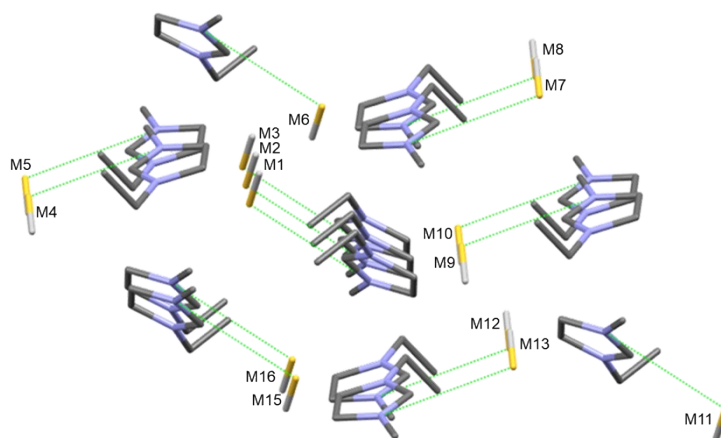


Figure S31- Supramolecular cluster of compound **4**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S31- Symmetry codes for the monomers of compound **4**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	x,y,z	-x,1-y,1-z
M2	1+x,y,z	1-x,1-y,1-z
M3	-1+x,y,z	-1-x,1-y,1-z
M4	1/2+x,1/2-y,1/2+z	1/2-x,-1/2+y,1.5-z
M5	-1/2+x,1/2-y,1/2+z	-1/2-x,-1/2+y,1.5-z
M6	-x,1-y,1-z	x,y,z
M7	1/2-x,1/2+y,1/2-z	1/2+x,1.5-y,-1/2+z
M8	-1/2-x,1/2+y,1/2-z	-1/2+x,1.5-y,-1/2+z
M9	1/2+x,1/2-y,-1/2+z	1/2-x,-1/2+y,1/2-z
M10	-1/2+x,1/2-y,-1/2+z	-1/2-x,-1/2+y,1/2-z
M11	-x,-y,-z	x,-1+y,-1+z
M12	1/2-x,-1/2+y,1/2-z	1/2+x,1/2-y,-1/2+z
M13	-1/2-x,-1/2+y,1/2-z	-1/2+x,1/2-y,-1/2+z
M14	1-x,-y,1-z	1+x,-1+y,z
M15	-x,-y,1-z	x,-1+y,z

<sup>a</sup>Symmetry codes were taken using the N2 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the S1 atom of the anion as reference.

Table S32- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **4**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1... M15	37.54	-29.58	2.27	3.64
M1...M6	17.57	-19.9	1.06	2.45
M1...M5	7.32	-14.98	0.44	1.84
M1...M9	7.32	-14.98	0.44	1.84
M1...M8	23.8	-14.5	1.44	1.78
M1...M13	23.8	-14.5	1.44	1.78
M1...M14	8.98	-2.87	0.54	0.35
M1...M4	18.4	-2.22	1.11	0.27
M1...M10	18.4	-2.22	1.11	0.27
M1...M2	11.05	-1.07	0.67	0.13
M1...M3	11.05	-1.07	0.67	0.13

M1...M7	21.68	0.08	1.31	-0.01
M1...M12	21.68	0.08	1.31	-0.01
M1...M11	3.21	3.84	0.19	-0.47
TOTAL	231.80	-113.90	14	14

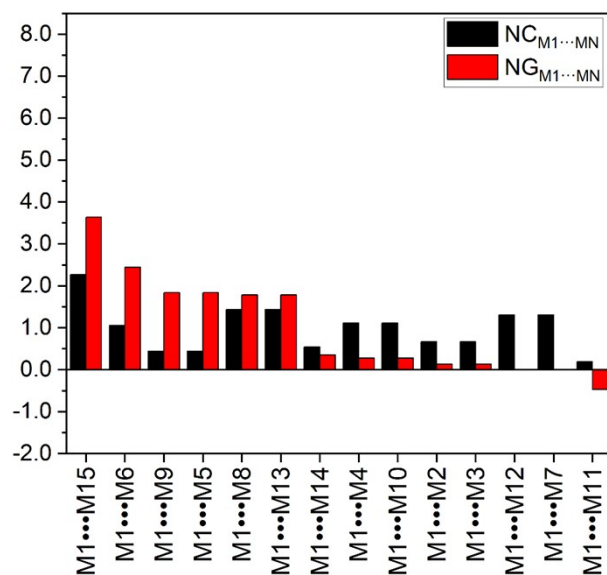


Figure S32- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **4**<sub>CA1</sub>.

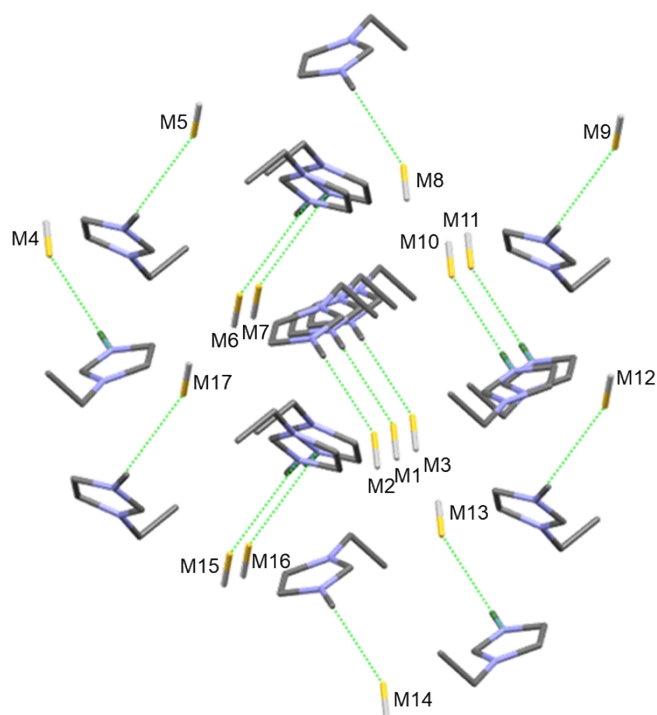


Figure S33- Supramolecular cluster of compound **4**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S33- Symmetry codes for the monomers of compound **4**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1/2-x,-1/2+y,1/2-z$
M2	$1+x,y,z$	$1.5-x,-1/2+y,1/2-z$
M3	$-1+x,y,z$	$-1/2-x,-1/2+y,1/2-z$
M4	$1-x,1-y,1-z$	$1/2+x,1.5-y,1/2+z$
M5	$1/2+x,1.5-y,1/2+z$	$1-x,2-y,1-z$
M6	$1.5-x,1/2+y,1/2-z$	$1+x,y,z$
M7	$1/2-x,1/2+y,1/2-z$	$x,y,z$
M8	$x,1+y,z$	$1/2-x,1/2+y,1/2-z$
M9	$-1/2+x,1.5-y,-1/2+z$	$-x,2-y,-z$
M10	$1-x,1-y,-z$	$1/2+x,1.5-y,-1/2+z$
M11	$-x,1-y,-z$	$-1/2+x,1.5-y,-1/2+z$
M12	$-1/2+x,1/2-y,-1/2+z$	$-x,1-y,-z$
M13	$1-x,-y,-z$	$1/2+x,1/2-y,-1/2+z$
M14	$x,-1+y,z$	$1/2-x,-1.5+y,1/2-z$
M15	$1.5-x,-1/2+y,1/2-z$	$1+x,-1+y,z$
M16	$1/2-x,-1/2+y,1/2-z$	$x,-1+y,z$
M17	$1/2+x,1/2-y,1/2+z$	$1-x,1-y,1-z$

<sup>a</sup>Symmetry codes were taken using the N2 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the S1 atom of the anion as reference.

Table S34- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **4**<sub>CA2</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M10	39.52	-40.93	2.70	5.20
M1...M11	11.71	-13.03	0.8	1.66
M1...M7	29.00	-11.43	1.98	1.45
M1... M16	29.00	-11.43	1.98	1.45
M1...M12	5.16	-11.36	0.35	1.44
M1... M17	5.16	-11.36	0.35	1.44
M1...M8	6.36	-9.77	0.44	1.24
M1...M14	6.36	-9.77	0.44	1.24
M1...M6	27.12	-7.73	1.86	0.98

M1... M15	27.12	-7.73	1.86	0.98
M1...M5	9.91	-1.24	0.68	0.16
M1...M9	9.91	-1.24	0.68	0.16
M1...M4	3.21	-1.1	0.22	0.14
M1...M2	9.69	2.89	0.66	-0.37
M1...M3	9.69	2.89	0.66	-0.37
M1...M13	4.85	6.41	0.33	-0.81
TOTAL	233.77	-125.94	16	16

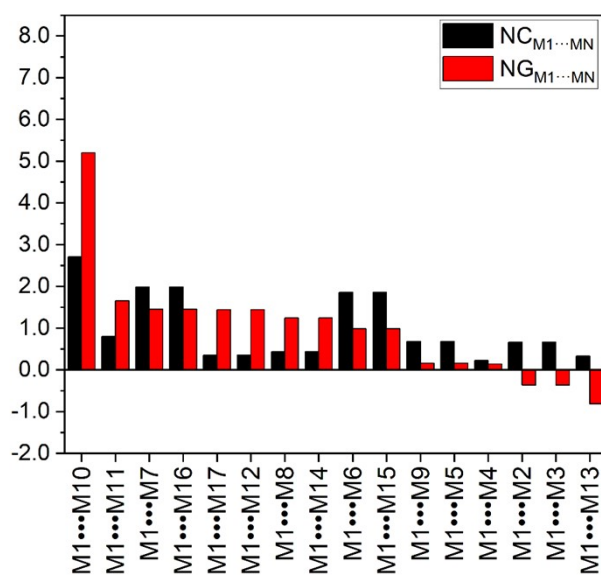


Figure S34- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **4**<sub>CA2</sub>.

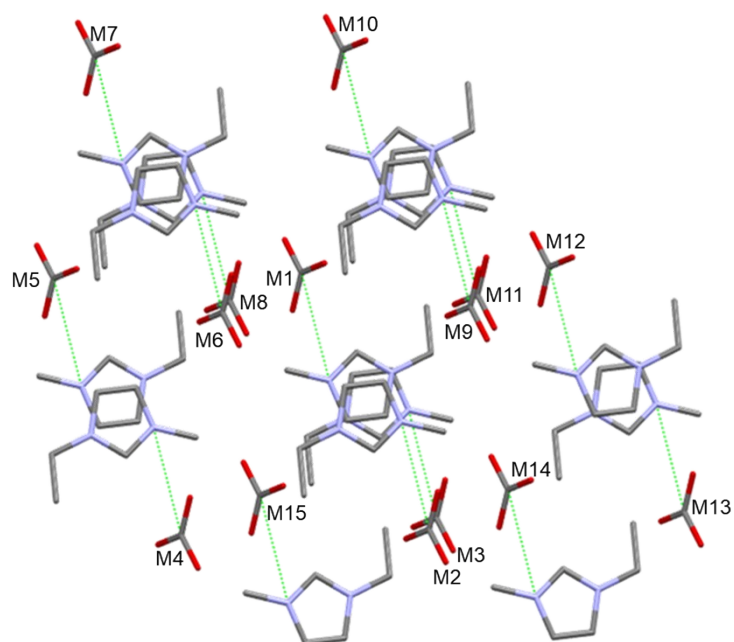


Figure S35- Supramolecular cluster of compound **5**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S35- Symmetry codes for the monomers of compound **5**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$-x,1-y,1-z$
M2	$1-x,1-y,2-z$	$1+x,y,1+z$
M3	$1-x,2-y,2-z$	$1+x,1+y,1+z$
M4	$1-x,1-y,1-z$	$1+x,y,z$
M5	$x,y,-1+z$	$-x,1-y,-z$
M6	$-x,1-y,1-z$	$x,y,z$
M7	$-1+x,y,-1+z$	$-1-x,1-y,-z$
M8	$-x,2-y,1-z$	$x,1+y,z$
M9	$-x,1-y,2-z$	$x,y,1+z$
M10	$-1+x,y,z$	$-1-x,1-y,1-z$
M11	$-x,2-y,2-z$	$x,1+y,1+z$
M12	$x,y,1+z$	$-x,1-y,2-z$
M13	$1-x,2-y,3-z$	$1+x,1+y,2+z$
M14	$1+x,y,1+z$	$1-x,1-y,2-z$
M15	$1+x,y,z$	$1-x,1-y,1-z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the C1 atom of the anion as reference.

Table S36- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **5**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M3	42.6	-22.33	2.52	2.84
M1...M9	32.64	-20.85	1.93	2.65
M1...M6	17.59	-12.51	1.04	1.59
M1...M11	22.51	-11.65	1.33	1.48
M1...M10	21.47	-10.08	1.27	1.28
M1... M15	21.47	-10.08	1.27	1.28
M1...M8	12.17	-6.38	0.72	0.81
M1...M7	5.09	-5.1	0.3	0.65
M1...M14	5.09	-5.1	0.3	0.65
M1...M2	24.2	-2.99	1.43	0.38
M1...M4	4.32	-1.47	0.26	0.19
M1...M5	12.7	-1.31	0.75	0.17
M1...M12	12.7	-1.31	0.75	0.17
M1...M13	2.15	1.11	0.13	-0.14
TOTAL	236.7	-110.06	14.00	14.00

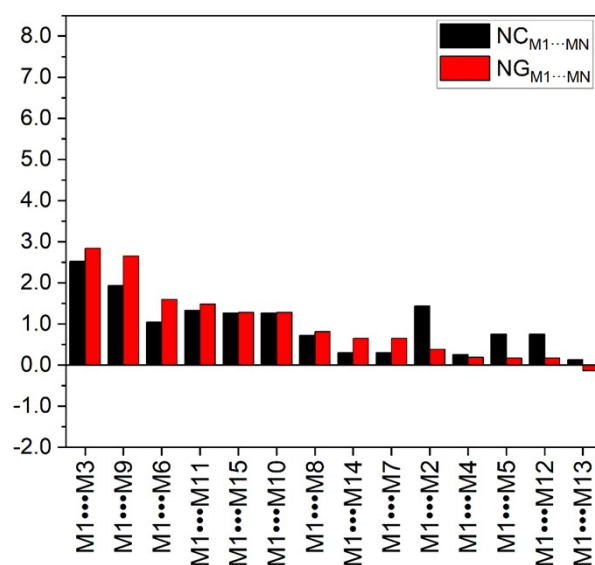


Figure S36- Normalized contact ( $N_{CM1...MN}$ ) area and stabilization energy ( $N_{GM1...MN}$ ) data of each dimer from the supramolecular cluster of compound **5**<sub>CA1</sub>.

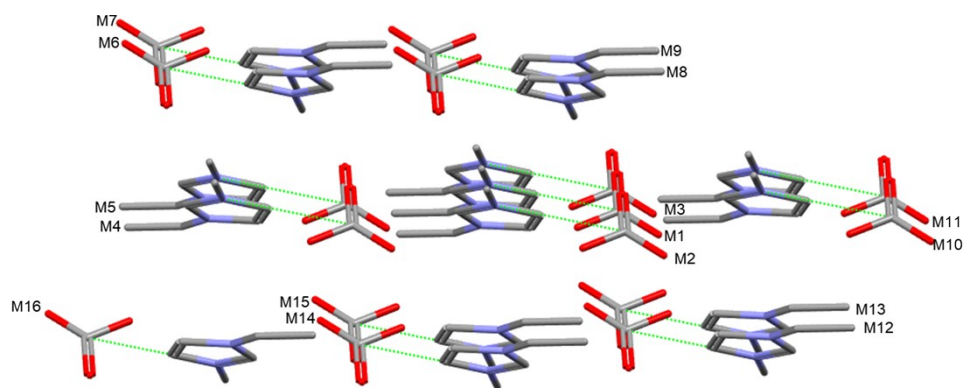


Figure S37- Supramolecular cluster of compound **5**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S37- Symmetry codes for the monomers of compound **5**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x, y, z$	$1-x, 1-y, 1-z$
M2	$x, y, -1+z$	$1-x, 1-y, -z$
M3	$x, y, 1+z$	$1-x, 1-y, 2-z$
M4	$-1+x, y, z$	$-x, 1-y, 1-z$
M5	$-1+x, y, 1+z$	$-x, 1-y, 2-z$
M6	$-x, 1-y, 2-z$	$-1+x, y, 1+z$
M7	$-x, 1-y, 3-z$	$-1+x, y, 2+z$
M8	$1-x, 1-y, 1-z$	$x, y, z$
M9	$1-x, 1-y, 2-z$	$x, y, 1+z$
M10	$1+x, y, -1+z$	$2-x, 1-y, -z$
M11	$1+x, y, z$	$2-x, 1-y, 1-z$
M12	$2-x, 2-y, 1-z$	$1+x, 1+y, z$
M13	$2-x, 2-y, 2-z$	$1+x, 1+y, 1+z$
M14	$1-x, 2-y, 2-z$	$x, 1+y, 1+z$
M15	$1-x, 2-y, 1-z$	$x, 1+y, z$
M16	$-x, 2-y, 2-z$	$-1+x, 1+y, 1+z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the C1 atom of the anion as reference.

Table S38- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{C_{M1...MN}}$  and  $N_{G_{M1...MN}}$ ) between the dimers of the supramolecular cluster for **5**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{C_{M1...MN}}$	$N_{G_{M1...MN}}$
M1...M9	37.38	-35.14	2.30	2.86
M1...M13	5.18	-32.70	0.32	2.66
M1...M8	19.43	-23.78	1.20	1.94
M1...M4	25.06	-23.12	1.54	1.88
M1...M11	25.06	-23.12	1.54	1.88
M1...M14	50.79	-19.85	3.12	1.62
M1...M12	17.34	-11.19	1.07	0.91
M1...M5	3.86	-11.16	0.24	0.91
M1...M10	3.86	-11.16	0.24	0.91
M1...M15	2.15	-9.48	0.13	0.77
M1...M3	13.94	2.52	0.86	-0.21
M1...M2	13.94	2.52	0.86	-0.21
M1...M7	19.46	2.75	1.20	-0.22
M1...M16	3.96	3.89	0.24	-0.32
M1...M6	2.48	4.96	0.15	-0.40
TOTAL	243.89	-184.08	15.00	15.00

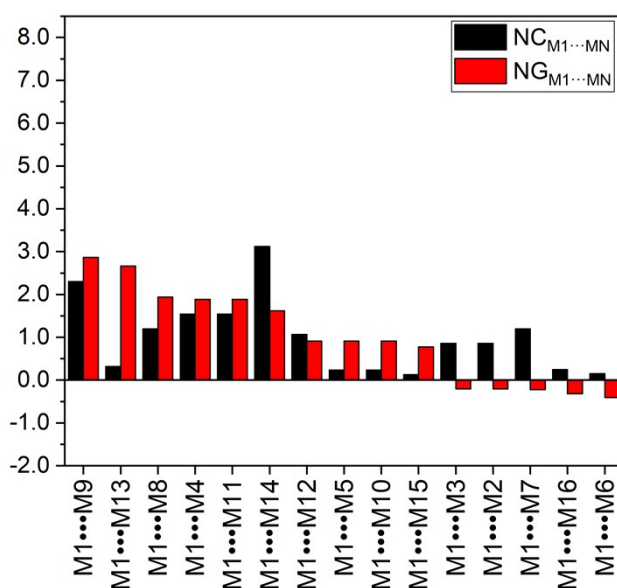


Figure S38- Normalized contact ( $N_{C_{M1...MN}}$ ) area and stabilization energy ( $N_{G_{M1...MN}}$ ) data of each dimer from the supramolecular cluster of compound **5**<sub>CA2</sub>.

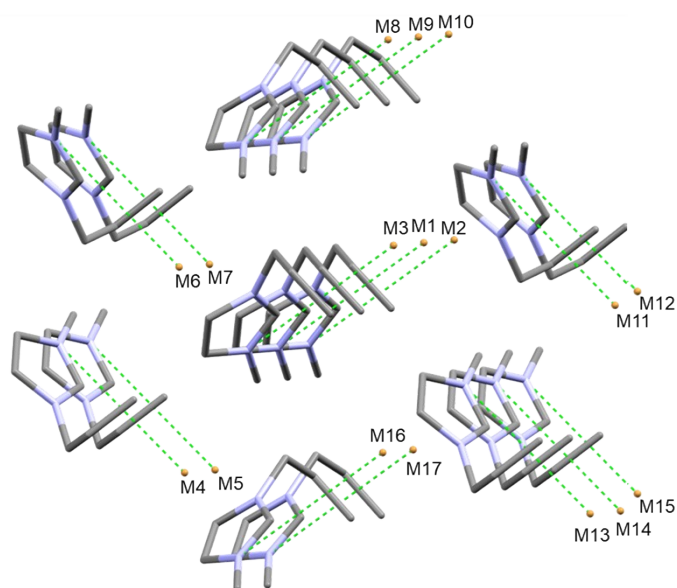


Figure S39- Supramolecular cluster of compound **6**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S39- Symmetry codes for the monomers of compound **6**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x, y, z$	$-x, 1-y, 1/2+z$
M2	$x, -1+y, z$	$-x, -y, 1/2+z$
M3	$x, 1+y, z$	$-x, 2-y, 1/2+z$
M4	$1/2-x, y, -1/2+z$	$1/2+x, 1-y, z$
M5	$1/2-x, 1+y, -1/2+z$	$1/2+x, 2-y, z$
M6	$-x, 1-y, -1/2+z$	$x, y, z$
M7	$-x, 2-y, -1/2+z$	$x, 1+y, z$
M8	$-1/2+x, -y, z$	$-1/2-x, -1+y, 1/2+z$
M9	$-1/2+x, 1-y, z$	$-1/2-x, y, 1/2+z$
M10	$-1/2+x, 2-y, z$	$-1/2-x, 1+y, 1/2+z$
M11	$-x, 1-y, 1/2+z$	$x, y, 1+z$
M12	$-x, 2-y, 1/2+z$	$x, 1+y, 1+z$
M13	$1/2-x, -1+y, 1/2+z$	$1/2+x, -y, 1+z$
M14	$1/2-x, y, 1/2+z$	$1/2+x, 1-y, 1+z$
M15	$1/2+x, 2-y, z$	$1/2-x, 1+y, 1/2+z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S40- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **6**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M4	22.86	-14.96	1.35	3.00
M1...M14	15.65	-14.96	0.93	3.00
M1...M6	20.86	-13.54	1.24	2.71
M1...M11	6.46	-13.54	0.38	2.71
M1...M7	8.03	-12.49	0.48	2.50
M1...M12	22.42	-12.49	1.33	2.50
M1...M13	14.29	-0.93	0.85	0.19
M1...M5	7.09	-0.93	0.42	0.19
M1...M10	12.68	0.59	0.75	-0.12
M1... M16	16.74	0.59	0.99	-0.12
M1...M9	26.19	1.14	1.55	-0.23
M1... M15	23.87	1.14	1.41	-0.23
M1...M8	1.74	1.24	0.10	-0.25
M1...M2	27.1	2.13	1.61	-0.43
M1...M3	27.1	2.13	1.61	-0.43
TOTAL	253.08	-74.90	15.00	15.00

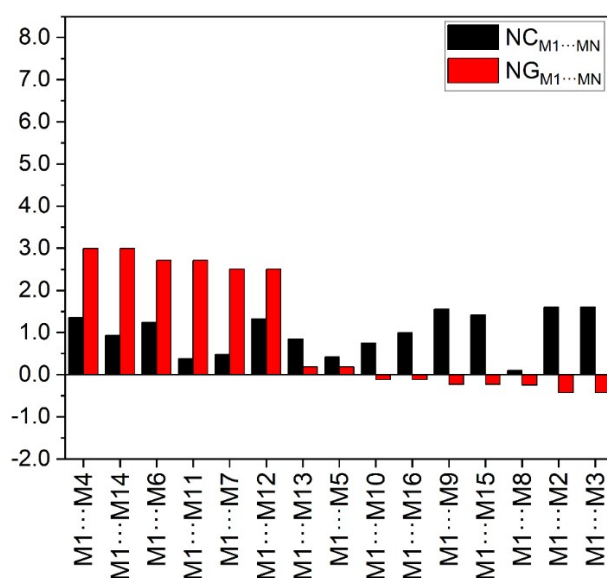


Figure S40- Normalized contact ( $N_{CM1...MN}$ ) area and stabilization energy ( $N_{GM1...MN}$ ) data of each dimer from the supramolecular cluster of compound **6**<sub>CA1</sub>.

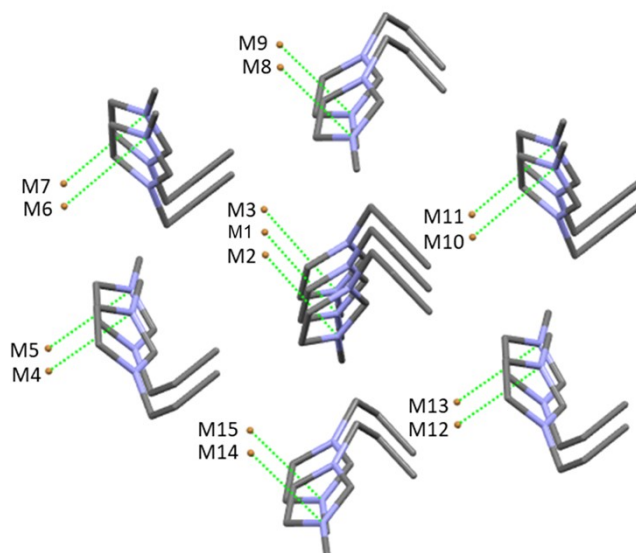


Figure S41- Supramolecular cluster of compound **6**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S41- Symmetry codes for the monomers of compound **6**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$x,1+y,z$
M2	$x,-1+y,z$	$x,y,z$
M3	$x,1+y,z$	$x,2+y,z$
M4	$1/2-x,y,-1/2+z$	$1/2-x,1+y,-1/2+z$
M5	$1/2-x,1+y,-1/2+z$	$1/2-x,2+y,-1/2+z$
M6	$-x,1-y,-1/2+z$	$-x,-y,-1/2+z$
M7	$-x,2-y,-1/2+z$	$-x,1-y,-1/2+z$
M8	$-1/2+x,1-y,z$	$-1/2+x,-y,z$
M9	$-1/2+x,2-y,z$	$-1/2+x,1-y,z$
M10	$-x,1-y,1/2+z$	$-x,-y,1/2+z$
M11	$-x,2-y,1/2+z$	$-x,1-y,1/2+z$
M12	$1/2-x,-1+y,1/2+z$	$1/2-x,y,1/2+z$
M13	$1/2-x,y,1/2+z$	$1/2-x,1+y,1/2+z$
M14	$1/2+x,1-y,z$	$1/2+x,-y,z$
M15	$1/2+x,2-y,z$	$1/2+x,1-y,z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S42- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $NC_{M1...MN}$  and  $NG_{M1...MN}$ ) between the dimers of the supramolecular cluster for **6**<sub>CA2</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$NC_{M1...MN}$	$NG_{M1...MN}$
M1...M7	7.70	-17.24	0.44	2.16
M1...M11	7.70	-17.24	0.44	2.16
M1...M2	25.85	-10.00	1.46	1.25
M1...M3	25.85	-10.00	1.46	1.25
M1...M9	19.88	-9.81	1.13	1.23
M1... M15	19.88	-9.81	1.13	1.23
M1...M6	19.48	-6.55	1.1	0.82
M1...M10	19.48	-6.55	1.1	0.82
M1...M4	19.71	-6.05	1.12	0.76
M1...M13	19.71	-6.05	1.12	0.76
M1...M5	8.83	-5.59	0.50	0.70
M1...M12	8.83	-5.59	0.50	0.70
M1...M8	22.13	-0.72	1.25	0.09
M1...M14	22.13	-0.72	1.25	0.09
TOTAL	247.16	-111.93	14.00	14.00

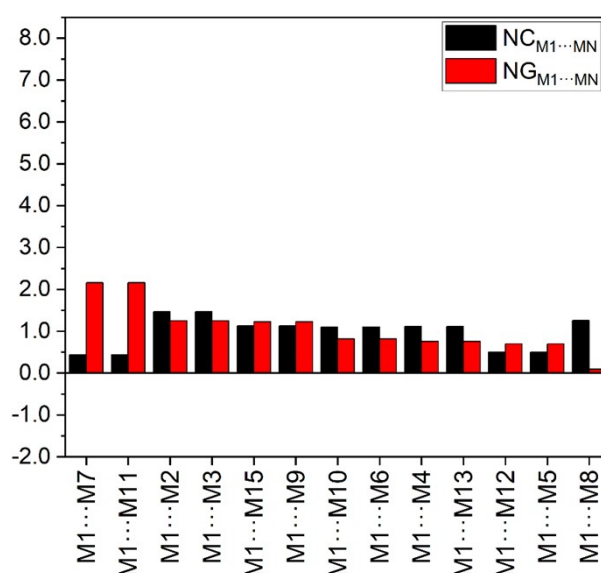


Figure S42- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **6**<sub>CA2</sub>.

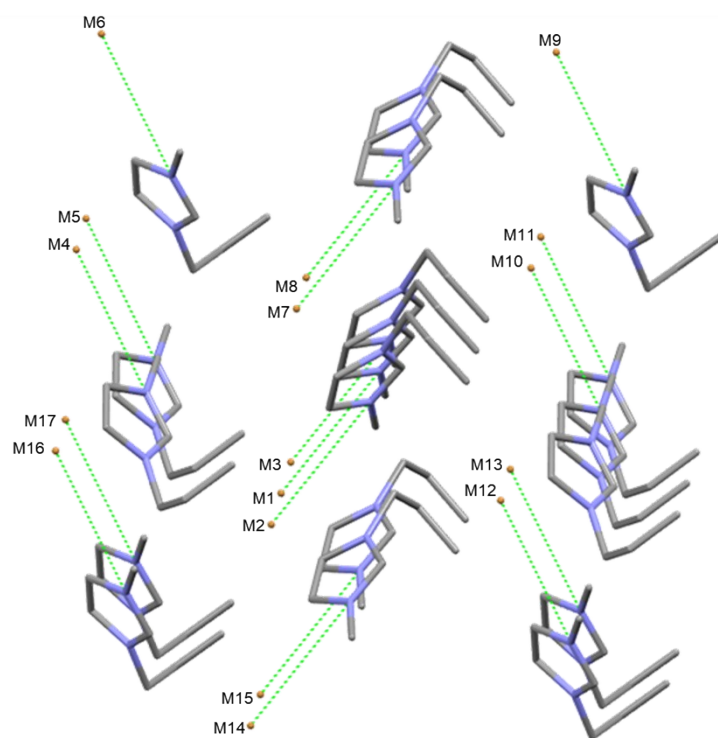


Figure S43- Supramolecular cluster of compound **6**<sub>CA3</sub>, based on the CA3 cation-anion pair.

Table S43- Symmetry codes for the monomers of compound **6**<sub>CA3</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1/2+x,1-y,z$
M2	$x,-1+y,z$	$1/2+x,-y,z$
M3	$x,1+y,z$	$1/2+x,2-y,z$
M4	$1/2-x,-1+y,-1/2+z$	$1/2-x,y,-1/2+z$
M5	$1/2-x,y,-1/2+z$	$-x,1-y,-1/2+z$
M6	$-x,1-y,-1/2+z$	$-1/2-x,y,-1/2+z$
M7	$-1/2+x,1-y,z$	$x,y,z$
M8	$-1/2+x,2-y,z$	$x,1+y,z$
M9	$-x,2-y,1/2+z$	$-1/2-x,1+y,1/2+z$
M10	$1/2-x,y,1/2+z$	$-x,1-y,1/2+z$
M11	$1/2-x,1+y,1/2+z$	$-x,2-y,1/2+z$
M12	$1-x,1-y,1/2+z$	$1/2-x,y,1/2+z$
M13	$1-x,2-y,1/2+z$	$1/2-x,1+y,1/2+z$
M14	$1/2+x,1-y,z$	$1+x,y,z$
M15	$1/2+x,2-y,z$	$1+x,1+y,z$

M16	1-x,1-y,-1/2+z	1/2-x,y,-1/2+z
M17	1-x,2-y,-1/2+z	1/2-x,1+y,-1/2+z

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S44- Contact area ( $C_{M_1 \dots M_N}$ ) and stabilization energy ( $G_{M_1 \dots M_N}$ ) and normalized contact area and stabilization energy data area ( $N_{C_{M_1 \dots M_N}}$  and  $N_{G_{M_1 \dots M_N}}$ ) between the dimers of the supramolecular cluster for **6**<sub>CA3</sub>.

Dímer	$C_{M_1 \dots M_N}$ (Å <sup>2</sup> )	$G_{M_1 \dots M_N}$ (kcal mol <sup>-1</sup> )	$N_{C_{M_1 \dots M_N}}$	$N_{G_{M_1 \dots M_N}}$
M1...M5	12.17	-24.32	0.78	4.09
M1...M10	12.17	-24.32	0.78	4.09
M1...M7	28.59	-10.09	1.84	1.7
M1...M14	28.59	-10.09	1.84	1.7
M1...M13	4.06	-9.45	0.26	1.59
M1... M17	4.06	-9.45	0.26	1.59
M1...M12	1.74	-7.37	0.11	1.24
M1... M16	1.74	-7.37	0.11	1.24
M1...M8	20.7	-3.43	1.33	0.58
M1... M15	20.7	-3.43	1.33	0.58
M1...M4	23.36	-2.44	1.5	0.41
M1...M11	23.36	-2.44	1.5	0.41
M1...M9	14.4	-0.28	0.93	0.05
M1...M6	14.4	0.29	0.93	-0.05
M1...M2	19.39	9.57	1.25	-1.61
M1...M3	19.39	9.57	1.25	-1.61
TOTAL	248.82	-95.05	16.00	16.00

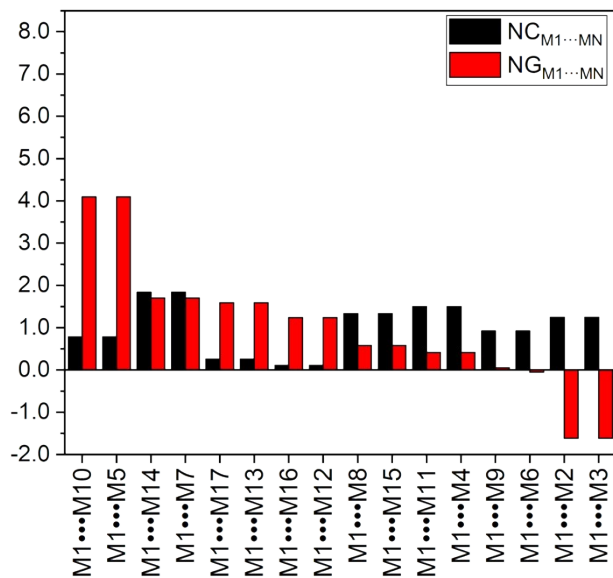


Figure S44- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **6**<sub>CA3</sub>.

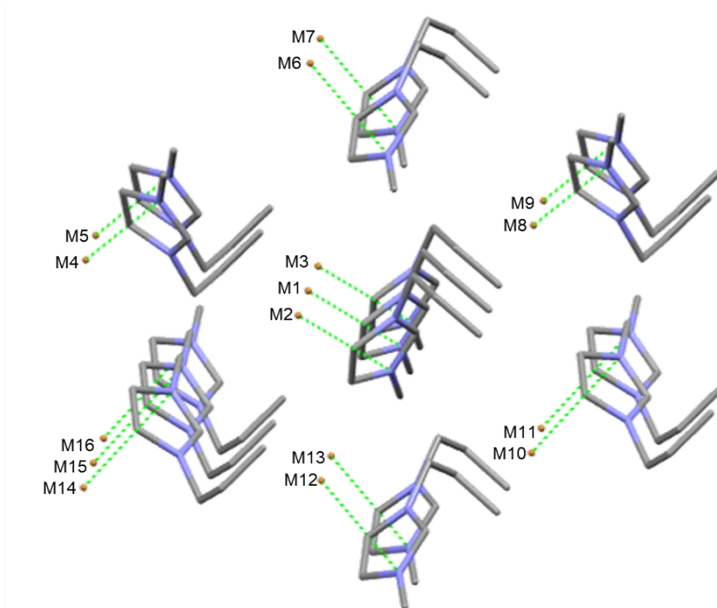


Figure S45- Supramolecular cluster of compound **6**<sub>CA4</sub>, based on the CA4 cation-anion pair.

Table S45- Symmetry codes for the monomers of compound **6**<sub>CA4</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$x,y,z$
M2	$x,-1+y,z$	$x,-1+y,z$
M3	$x,1+y,z$	$x,1+y,z$
M4	$-x,-y,-1/2+z$	$-x,-y,-1/2+z$
M5	$-x,1-y,-1/2+z$	$-x,1-y,-1/2+z$
M6	$-1/2+x,2-y,z$	$-1/2+x,2-y,z$
M7	$-x,1-y,1/2+z$	$-x,1-y,1/2+z$
M8	$-x,2-y,1/2+z$	$-x,2-y,1/2+z$
M9	$1/2-x,y,1/2+z$	$1/2-x,y,1/2+z$
M10	$1/2-x,1+y,1/2+z$	$1/2-x,1+y,1/2+z$
M11	$1/2+x,1-y,z$	$1/2+x,1-y,z$
M12	$1/2+x,2-y,z$	$1/2+x,2-y,z$
M13	$1/2-x,-1+y,-1/2+z$	$1/2-x,-1+y,-1/2+z$
M14	$1/2-x,y,-1/2+z$	$1/2-x,y,-1/2+z$
M15	$1/2-x,1+y,-1/2+z$	$1/2-x,1+y,-1/2+z$
M16	$x,y,z$	$x,y,z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S46- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **6**<sub>CA4</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M5	22.1	-24.41	1.32	3.04
M1...M9	22.1	-24.41	1.32	3.04
M1...M6	29.33	-22.12	1.76	2.75
M1...M12	29.33	-22.12	1.76	2.75
M1...M11	19.71	-13.89	1.18	1.73
M1...M14	4.06	-13.89	0.24	1.73
M1...M2	27.42	-9.88	1.64	1.23
M1...M3	27.42	-9.88	1.64	1.23
M1...M8	5.08	-0.71	0.30	0.09
M1...M4	5.08	0.01	0.30	0.00

M1... M16	7.09	2.95	0.42	-0.37
M1...M7	12.68	3.58	0.76	-0.44
M1...M13	12.68	3.58	0.76	-0.44
M1...M10	8.83	5.31	0.53	-0.66
M1... M15	17.4	5.31	1.04	-0.66
TOTAL	250.31	-120.57	15.00	15.00

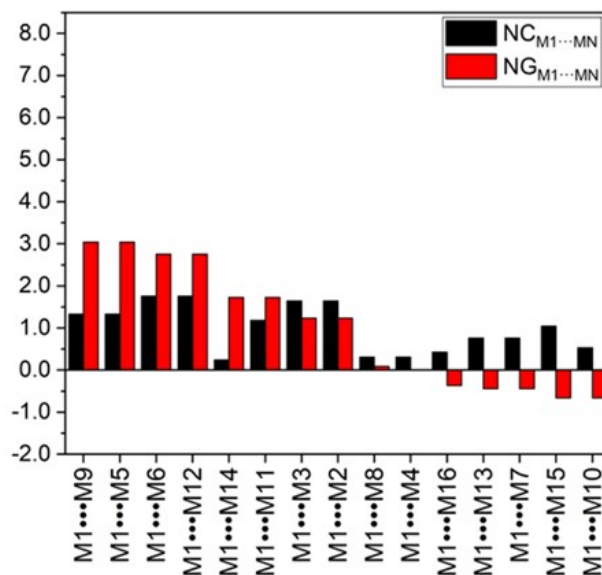


Figure S46- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **6**<sub>CA4</sub>.

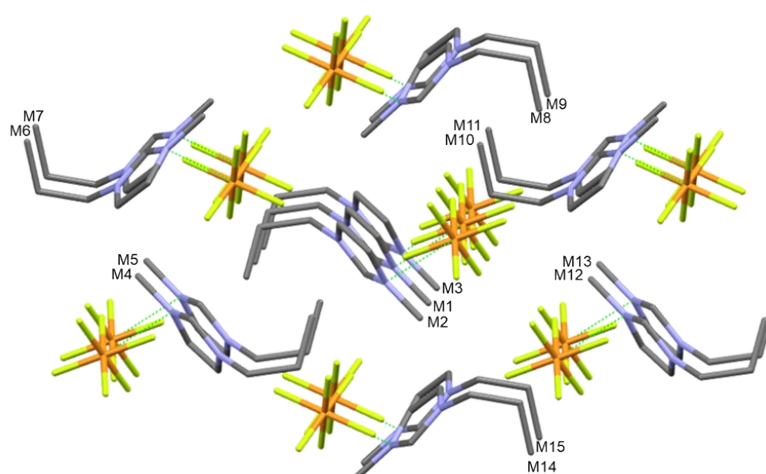


Figure S47- Supramolecular cluster of compound **7**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S47- Symmetry codes for the monomers of compound **7**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1+x,y,z$
M2	$-1+x,y,z$	$x,y,z$
M3	$1+x,y,z$	$2+x,y,z$
M4	$1-x,-y,-z$	$-x,-y,-z$
M5	$2-x,-y,-z$	$1-x,-y,-z$
M6	$-1+x,1/2-y,-1/2+z$	$x,1/2-y,-1/2+z$
M7	$x,1/2-y,-1/2+z$	$1+x,1/2-y,-1/2+z$
M8	$1-x,1/2+y,1/2-z$	$-x,1/2+y,1/2-z$
M9	$2-x,1/2+y,1/2-z$	$1-x,1/2+y,1/2-z$
M10	$x,1/2-y,1/2+z$	$1+x,1/2-y,1/2+z$
M11	$1+x,1/2-y,1/2+z$	$2+x,1/2-y,1/2+z$
M12	$2-x,-y,1-z$	$1-x,-y,1-z$
M13	$3-x,-y,1-z$	$2-x,-y,1-z$
M14	$1-x,-1/2+y,1/2-z$	$-x,-1/2+y,1/2-z$
M15	$2-x,-1/2+y,1/2-z$	$1-x,-1/2+y,1/2-z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P1 atom of the anion as reference.

Table S48- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **7**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M9	42.11	-29.65	2.01	3.4
M1... M15	42.11	-29.65	2.01	3.4
M1...M12	20.96	-21.87	1	2.51
M1...M6	17.31	-13.91	0.83	1.6
M1...M11	17.31	-13.91	0.83	1.6
M1...M2	9.96	-8.83	0.47	1.01
M1...M3	9.96	-8.83	0.47	1.01
M1...M5	26.4	-6.92	1.26	0.79
M1...M7	31.96	-0.98	1.52	0.11
M1...M10	31.96	-0.98	1.52	0.11
M1...M8	8.53	1.59	0.41	-0.18

M1...M14	8.53	1.59	0.41	-0.18
M1...M4	23.77	2.01	1.13	-0.23
M1...M13	2.86	8.4	0.14	-0.96
TOTAL	263.73	-121.94	14.00	14.00

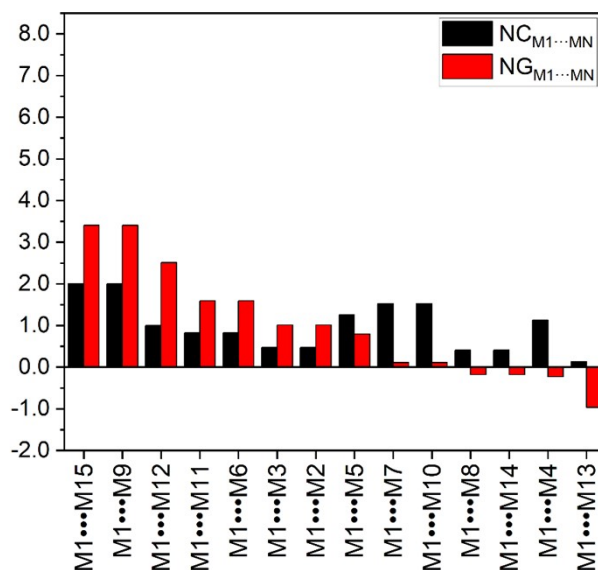


Figure S48- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **7**<sub>CA1</sub>.

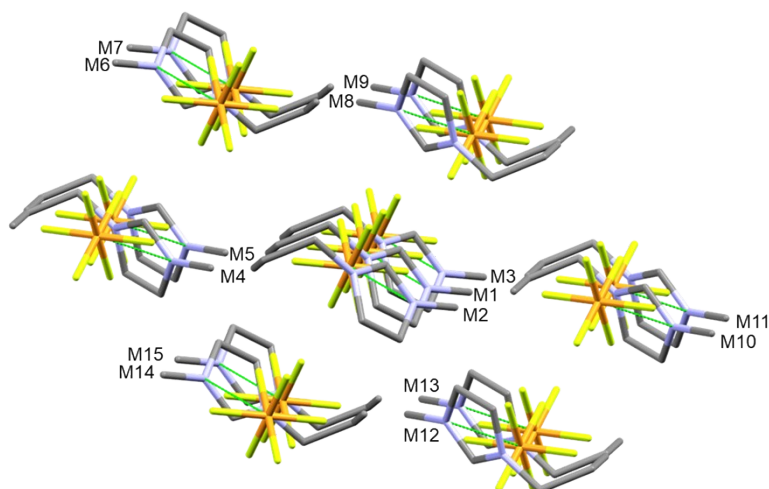


Figure S49- Supramolecular cluster of compound **7**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S49- Symmetry codes for the monomers of compound **7**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1-x,-1/2+y,1/2-z$
M2	$x,1+y,z$	$1-x,1/2+y,1/2-z$
M3	$x,-1+y,z$	$1-x,-1.5+y,1/2-z$
M4	$1-x,-y,-z$	$x,1/2-y,-1/2+z$
M5	$1-x,-1-y,-z$	$x,-1/2-y,-1/2+z$
M6	$x,1/2-y,-1/2+z$	$1-x,1-y,-z$
M7	$x,-1/2-y,-1/2+z$	$1-x,-y,-z$
M8	$2-x,-y,-z$	$1+x,1/2-y,-1/2+z$
M9	$2-x,-1-y,-z$	$1+x,-1/2-y,-1/2+z$
M10	$2-x,1/2+y,1/2-z$	$1+x,y,z$
M11	$2-x,-1/2+y,1/2-z$	$1+x,-1+y,z$
M12	$x,1/2-y,1/2+z$	$1-x,1-y,1-z$
M13	$x,-1/2-y,1/2+z$	$1-x,-y,1-z$
M14	$1-x,1/2+y,1/2-z$	$x,y,z$
M15	$1-x,-1/2+y,1/2-z$	$x,-1+y,z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P1 atom of the anion as reference.

Table S50- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **7**<sub>CA2</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M4	58.4	-32.19	2.88	3.50
M1...M8	44.16	-24.73	2.18	2.69
M1...M7	15.83	-14.28	0.78	1.55
M1...M13	15.83	-14.28	0.78	1.55
M1...M2	11.55	-13.83	0.57	1.50
M1...M3	11.55	-13.83	0.57	1.50
M1...M10	25.65	-9.24	1.26	1.00
M1...M11	25.65	-9.24	1.26	1.00
M1...M14	8.53	-5.84	0.42	0.63
M1... M15	28.46	-5.84	1.4	0.63
M1...M6	17.66	-0.43	0.87	0.05

M1...M12	17.66	-0.43	0.87	0.05
M1...M9	0.14	6.58	0.01	-0.72
M1...M5	2.86	8.71	0.14	-0.95
TOTAL	283.93	-128.86	14.00	14.00

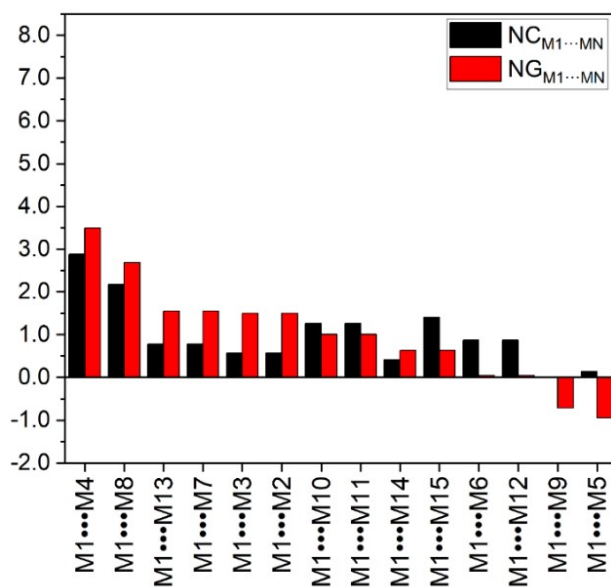


Figure S50- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **7**<sub>CA2</sub>.

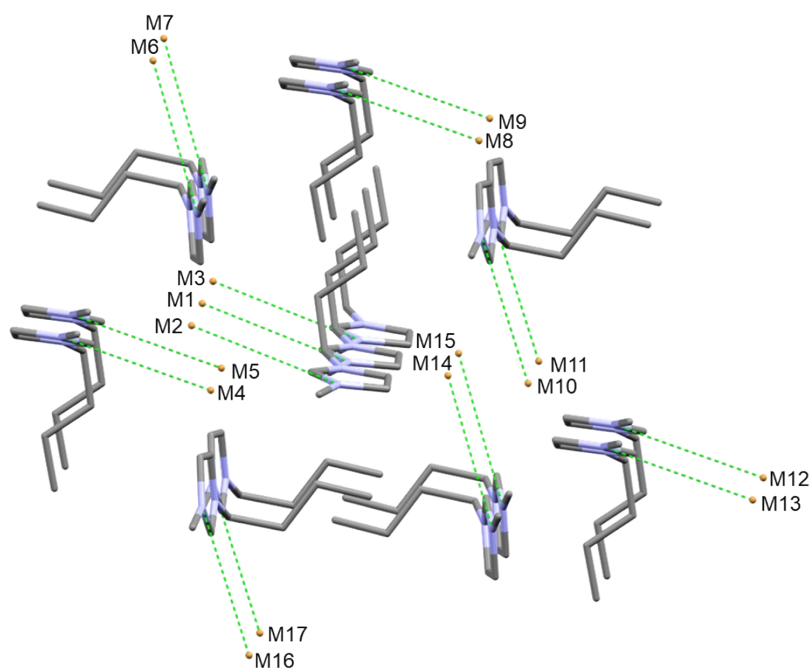


Figure S51- Supramolecular cluster of compound **8**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S51- Symmetry codes for the monomers of compound **8**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$1/2-x,1/2+y,1/2+z$
M2	$x,y,1+z$	$1/2-x,1/2+y,1.5+z$
M3	$x,y,-1+z$	$1/2-x,1/2+y,-1/2+z$
M4	$-x,1-y,1/2+z$	$-1/2+x,1/2-y,1+z$
M5	$-1/2+x,1/2-y,z$	$-x,1-y,-1/2+z$
M6	$1/2-x,1/2+y,1/2+z$	$x,1+y,1+z$
M7	$1/2-x,1/2+y,-1/2+z$	$x,1+y,z$
M8	$1-x,1-y,1/2+z$	$1/2+x,1/2-y,1+z$
M9	$1/2+x,1/2-y,z$	$1-x,1-y,-1/2+z$
M10	$1/2+x,1/2-y,z$	$1-x,-y,1/2+z$
M11	$1/2+x,1/2-y,-1+z$	$1-x,-y,-1/2+z$
M12	$1-x,-y,1/2+z$	$1/2+x,-1/2-y,1+z$
M13	$1-x,-y,-1/2+z$	$1/2+x,-1/2-y,z$
M14	$1/2-x,-1/2+y,1/2+z$	$x,y,1+z$
M15	$1/2-x,-1/2+y,-1/2+z$	$x,y,z$
M16	$-1/2+x,1/2-y,1+z$	$-1/2+x,1/2-y,1+z$
M17	$-1/2+x,1/2-y,z$	$-x,-y,1/2+z$

<sup>a</sup>Symmetry codes were taken using the N2 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S52- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $NC_{M1...MN}$  and  $NG_{M1...MN}$ ) between the dimers of the supramolecular cluster for **8**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$NC_{M1...MN}$	$NG_{M1...MN}$
M1...M4	9.04	-16.18	0.53	2.08
M1...M5	9.04	-16.18	0.53	2.08
M1...M10	39.15	-15.21	2.27	1.96
M1... M17	39.15	-15.21	2.27	1.96

M1...M7	28.35	-13.81	1.65	1.78
M1...M14	28.35	-13.81	1.65	1.78
M1...M6	10.37	-13.46	0.6	1.73
M1...M15	10.37	-13.46	0.6	1.73
M1...M8	33.02	-9.84	1.92	1.27
M1...M9	33.02	-9.84	1.92	1.27
M1...M11	5.28	-1.22	0.31	0.16
M1...M16	5.28	-1.22	0.31	0.16
M1...M12	0.63	2.77	0.04	-0.36
M1...M13	0.63	2.77	0.04	-0.36
M1...M2	11.9	4.86	0.69	-0.63
M1...M3	11.9	4.86	0.69	-0.63
TOTAL	275.48	-124.19	16.00	16.00

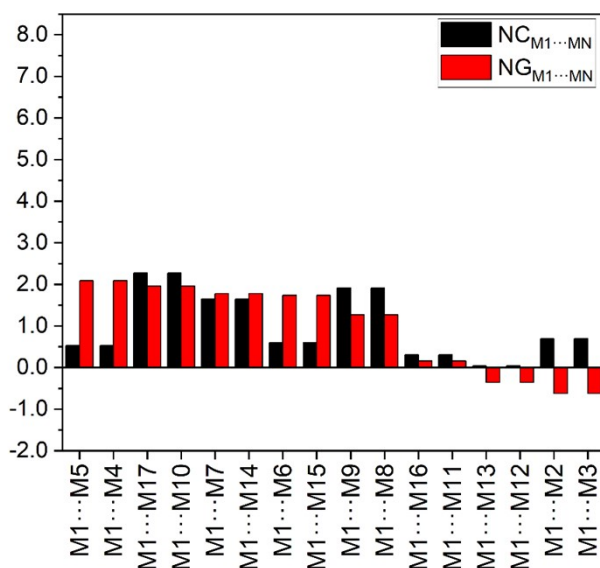


Figure S52- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **8**<sub>CA1</sub>.

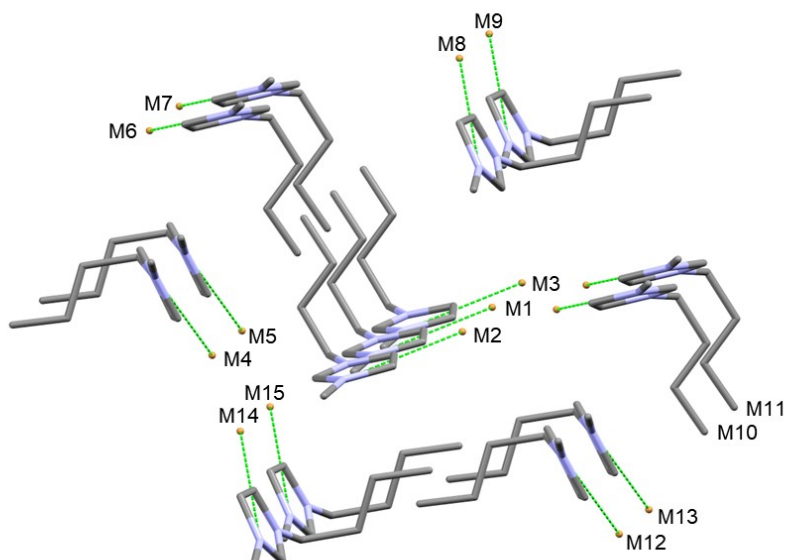


Figure S53- Supramolecular cluster of compound **8**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S53- Symmetry codes for the monomers of compound **8**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$x,y,z$
M2	$x,y,1+z$	$x,y,1+z$
M3	$x,y,-1+z$	$x,y,-1+z$
M4	$1/2-x,1/2+y,1/2+z$	$1/2-x,1/2+y,1/2+z$
M5	$1/2-x,1/2+y,-1/2+z$	$1/2-x,1/2+y,-1/2+z$
M6	$1-x,1-y,1/2+z$	$1-x,1-y,1/2+z$
M7	$1-x,1-y,-1/2+z$	$1-x,1-y,-1/2+z$
M8	$1/2+x,1/2-y,-1+z$	$1/2+x,1/2-y,-1+z$
M9	$1/2+x,1/2-y,-2+z$	$1/2+x,1/2-y,-2+z$
M10	$1-x,-y,1/2+z$	$1-x,-y,1/2+z$
M11	$1-x,-y,-1/2+z$	$1-x,-y,-1/2+z$
M12	$1/2-x,-1/2+y,1/2+z$	$1/2-x,-1/2+y,1/2+z$
M13	$1/2-x,-1/2+y,-1/2+z$	$1/2-x,-1/2+y,-1/2+z$
M14	$-1/2+x,1/2-y,1+z$	$-1/2+x,1/2-y,1+z$
M15	$-1/2+x,1/2-y,z$	$-1/2+x,1/2-y,z$

<sup>a</sup>Symmetry codes were taken using the N2 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S54- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $NC_{M1...MN}$  and  $NG_{M1...MN}$ ) between the dimers of the supramolecular cluster for **8**<sub>CA2</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$NC_{M1...MN}$	$NG_{M1...MN}$
M1...M4	9.08	-16.83	0.47	2.69
M1...M13	9.08	-16.83	0.47	2.69
M1...M8	39.27	-15.23	2.01	2.43
M1...M15	39.27	-15.23	2.01	2.43
M1...M2	18.94	-11.57	0.97	1.85
M1...M3	18.94	-11.57	0.97	1.85
M1...M6	30.48	-3.69	1.56	0.59
M1...M7	30.48	-3.69	1.56	0.59
M1...M9	10.34	-2.13	0.53	0.34
M1...M14	10.34	-2.13	0.53	0.34
M1...M10	7.03	0.96	0.36	-0.15
M1...M11	7.03	0.96	0.36	-0.15
M1...M5	21.3	4.63	1.09	-0.74
M1...M12	21.3	4.63	1.09	-0.74
TOTAL	272.88	-87.70	14.00	14.00

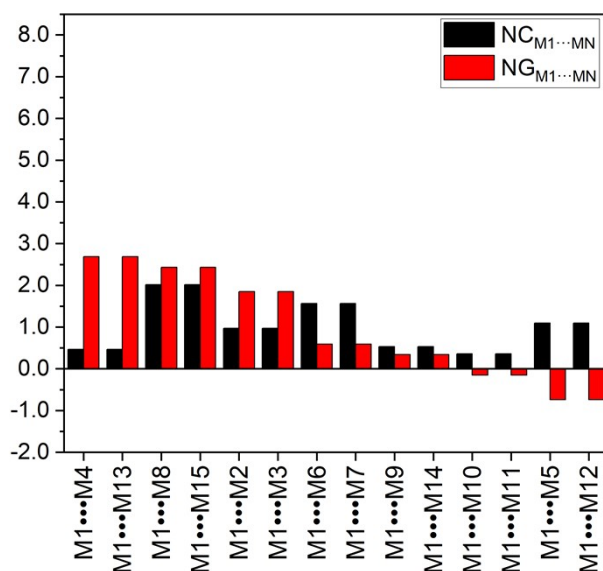


Figure S54- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **8**<sub>CA2</sub>.

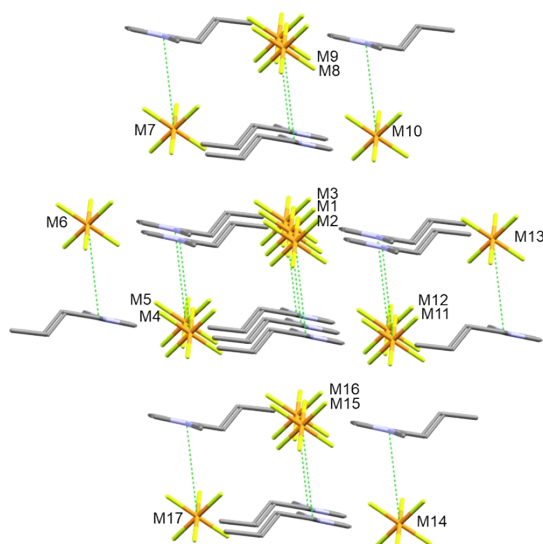


Figure S55- Supramolecular cluster of compound **9**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S55- Symmetry codes for the monomers of compound **9**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x,y,z$	$-x,1-y,1-z$
M2	$x,-1+y,z$	$-x,-y,1-z$
M3	$x,1+y,z$	$-x,2-y,1-z$
M4	$-x,-y,-z$	$x,-1+y,-1+z$
M5	$-x,1-y,-z$	$x,y,-1+z$
M6	$x,y,-1+z$	$-x,1-y,-z$
M7	$-1-x,1-y,-z$	$-1+x,y,-1+z$
M8	$-1+x,y,z$	$-1-x,1-y,1-z$
M9	$-1+x,1+y,z$	$-1-x,2-y,1-z$
M10	$-1-x,1-y,1-z$	$-1+x,y,z$
M11	$-x,-y,1-z$	$-x,1-y,2-z$
M12	$-x,1-y,1-z$	$x,-1+y,z$
M13	$x,y,1+z$	$x,y,z$
M14	$1-x,-y,1-z$	$1+x,-1+y,z$
M15	$1+x,-1+y,z$	$1-x,-y,1-z$
M16	$1+x,y,z$	$1-x,1-y,1-z$
M17	$1-x,-y,-z$	$1+x,-1+y,-1+z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P1 atom of the anion as reference.

Table S56- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $NC_{M1...MN}$  and  $NG_{M1...MN}$ ) between the dimers of the supramolecular cluster for **9**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$NC_{M1...MN}$	$NG_{M1...MN}$
M1...M5	9.04	-31.83	3.03	4.77
M1...M11	5.28	-28.3	2.2	4.24
M1...M12	0.63	-25.19	1.60	3.77
M1...M4	9.04	-11.6	1.50	1.74
M1...M8	33.02	-10.99	0.71	1.65
M1...M16	5.28	-10.99	0.71	1.65
M1...M9	33.02	-8.73	0.52	1.31
M1...M15	10.37	-8.7	0.52	1.30
M1... M17	39.15	-2.1	1.74	0.31
M1...M14	28.35	2.79	0.33	-0.42
M1...M6	10.37	3.79	0.64	-0.57
M1...M13	0.63	3.78	0.64	-0.57
M1...M2	11.9	4.02	0.77	-0.6
M1...M3	11.9	4.00	0.77	-0.6
M1...M7	28.35	4.53	0.07	-0.68
M1...M10	39.15	8.69	0.26	-1.30
TOTAL	306.23	-106.83	16.00	16.00

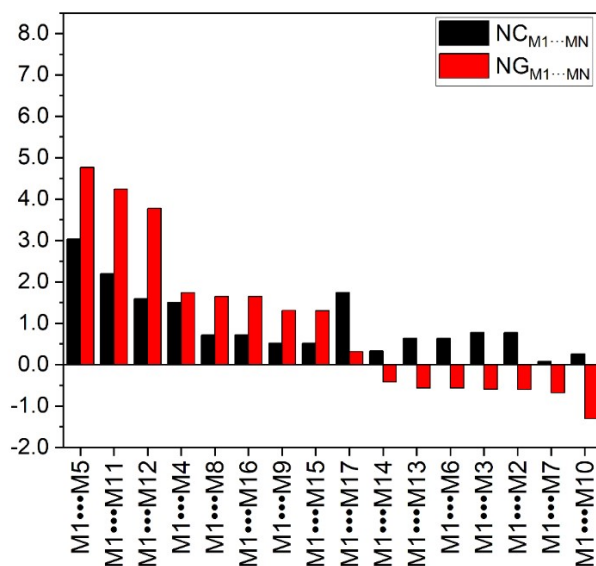


Figure S56- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **9**<sub>CA1</sub>.

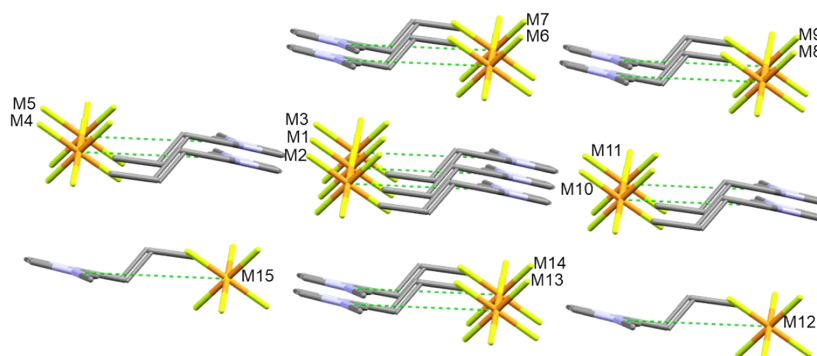


Figure S57- Supramolecular cluster of compound **9**<sub>CA2</sub>, based on the CA2 cation-anion pair.

Table S57- Symmetry codes for the monomers of compound **9**<sub>CA2</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x, y, z$	$x, y, -1+z$
M2	$x, -1+y, z$	$x, -1+y, -1+z$
M3	$x, 1+y, z$	$x, 1+y, -1+z$
M4	$x, y, -1+z$	$x, y, -2+z$
M5	$x, 1+y, -1+z$	$x, y, -2+z$
M6	$-x, -y, -z$	$-x, -y, 1-z$
M7	$-x, 1-y, -z$	$-x, 1-y, 1-z$

M8	-x,-y,1-z	-x,-y,2-z
M9	-x,1-y,1-z	-x,1-y,2-z
M10	x,-1+y,1+z	x,-1+y,z
M11	x,y,1+z	x,y,z
M12	1-x,-y,1-z	1-x,-y,2-z
M13	1-x,-y,-z	1-x,-y,1-z
M14	1-x,1-y,-z	1-x,1-y,1-z
M15	1-x,1-y,-1-z	1-x,1-y,-z

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P1 atom of the anion as reference.

Table S58- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **9**<sub>CA2</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M7	63.78	-39.12	2.86	4.09
M1...M14	28.7	-28.42	1.29	2.97
M1...M13	53.1	-24.83	2.38	2.6
M1...M5	15.8	-14.64	0.71	1.53
M1...M10	15.8	-14.64	0.71	1.53
M1...M4	24.76	-11.72	1.11	1.23
M1...M11	24.76	-11.72	1.11	1.23
M1...M6	13.42	-7.29	0.6	0.76
M1...M9	5.35	1.19	0.24	-0.12
M1...M8	10.42	1.78	0.47	-0.19
M1...M12	6.34	2.08	0.28	-0.22
M1...M2	22.44	2.2	1.01	-0.23
M1...M3	22.44	2.2	1.01	-0.23
M1... M15	4.92	9	0.22	-0.94
TOTAL	312.03	-133.95	14.00	14.00

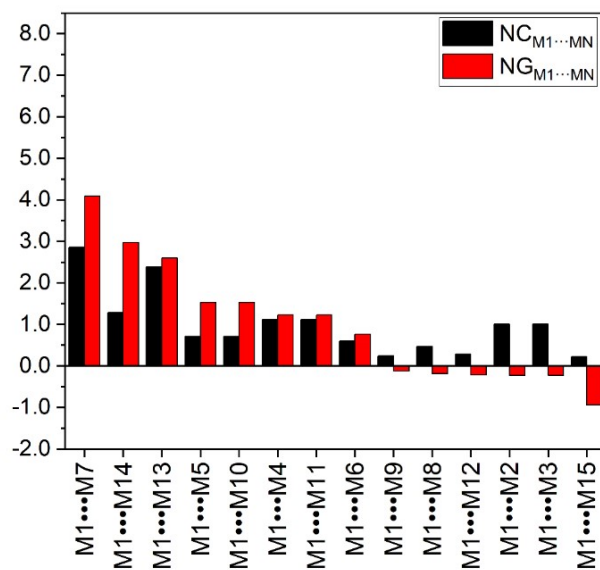


Figure S58- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **9**<sub>CA2</sub>.

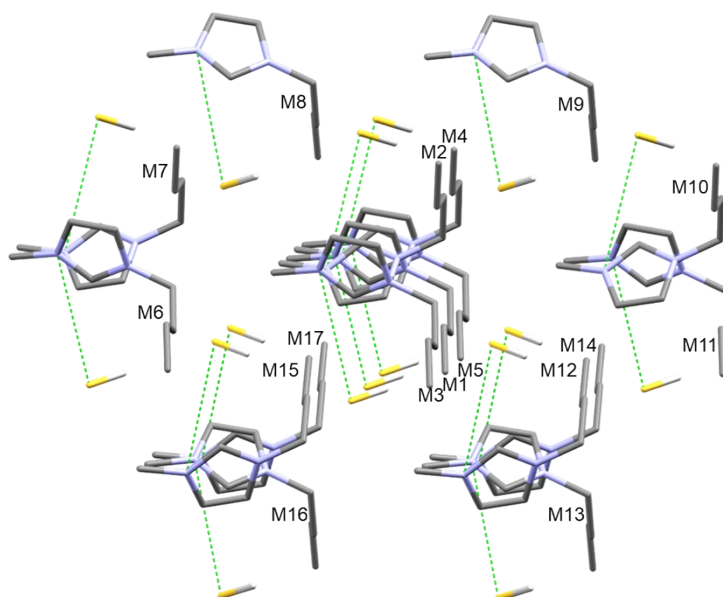


Figure S59- Supramolecular cluster of compound **10**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S59- Symmetry codes for the monomers of compound **10**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x, y, z$	$x, y, z$
M2	$-1/2+x, 1.5-y, z$	$-1/2+x, 1.5-y, z$
M3	$-1+x, y, z$	$-1+x, y, z$

M4	$1/2+x, 1.5-y, z$	$1/2+x, 1.5-y, z$
M5	$1+x, y, z$	$1+x, y, z$
M6	$x, y, -1+z$	$1/2-x, -1/2+y, -1.5+z$
M7	$1/2+x, 1.5-y, -1+z$	$1-x, 2-y, -1.5+z$
M8	$1/2-x, 1/2+y, -1/2+z$	$x, y, -1+z$
M9	$1/2-x, 1/2+y, 1/2+z$	$1/2-x, 1/2+y, 1/2+z$
M10	$-1/2+x, 1.5-y, 1+z$	$-x, 2-y, 1/2+z$
M11	$x, y, 1+z$	$1/2-x, -1/2+y, 1/2+z$
M12	$-x, 1-y, 1/2+z$	$-1/2+x, 1.5-y, z$
M13	$1/2-x, -1/2+y, 1/2+z$	$x, -1+y, z$
M14	$1-x, 1-y, 1/2+z$	$1/2+x, 1.5-y, z$
M15	$-x, 1-y, -1/2+z$	$-1/2+x, 1.5-y, -1+z$
M16	$1/2-x, -1/2+y, -1/2+z$	$x, -1+y, -1+z$
M17	$1-x, 1-y, -1/2+z$	$1/2-x, 1/2+y, 1/2+z$

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the S1 atom of the anion as reference.

Table S60- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **10**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M2	39.31	-14.02	2.26	1.98
M1...M4	39.31	-14.02	2.26	1.98
M1...M14	13.34	-12.82	0.77	1.81
M1... M17	13.34	-12.82	0.77	1.81
M1...M9	7.02	-12.19	0.4	1.72
M1...M16	7.02	-12.19	0.4	1.72
M1...M8	29.01	-12.14	1.67	1.71
M1...M13	29.01	-12.14	1.67	1.71
M1...M12	34.05	-9.77	1.96	1.38
M1...M15	34.05	-9.77	1.96	1.38
M1...M7	5.69	-1.46	0.33	0.21
M1...M10	5.69	-1.46	0.33	0.21
M1...M3	0.57	1.29	0.03	-0.18
M1...M5	0.57	1.29	0.03	-0.18

M1...M6	10.21	4.47	0.59	-0.63
M1...M11	10.21	4.47	0.59	-0.63
TOTAL	278.40	-113.29	16.00	16.00

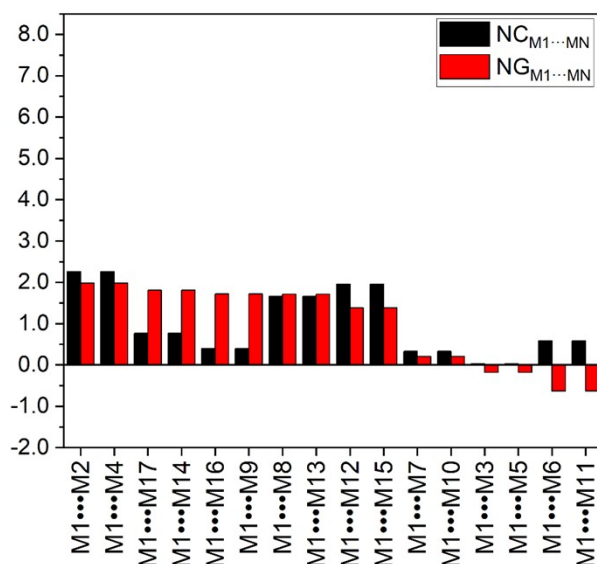


Figure S60- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **10**<sub>CA1</sub>.

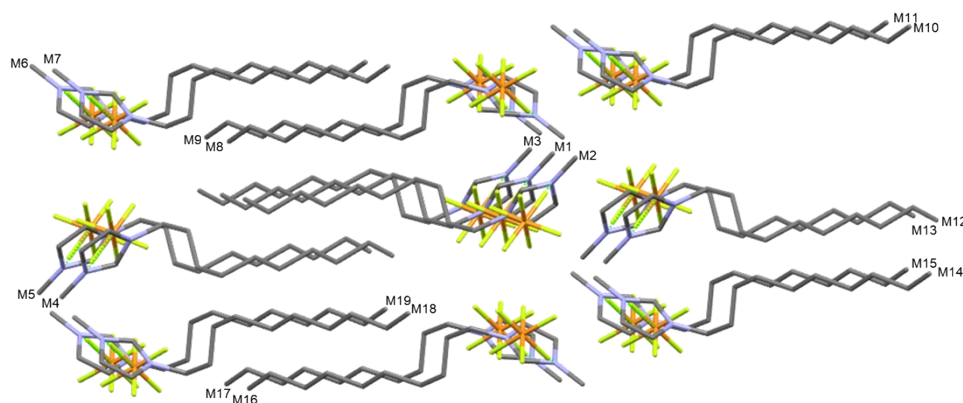


Figure S61- Supramolecular cluster of compound **11**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S61- Symmetry codes for the monomers of compound **11**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	$x, y, z$	$x, 1/2-y, 1/2+z$
M2	$x, y, 1+z$	$x, 1/2-y, 1.5+z$
M3	$x, y, -1+z$	$x, 1/2-y, -1/2+z$

M4	-x,-y,-z	-x,-1/2+y,-1/2-z
M5	-x,-y,-1-z	-x,-1/2+y,-1.5-z
M6	-x,1/2+y,1/2-z	-x,1-y,-z
M7	-x,1/2+y,-1/2-z	-x,1-y,-1-z
M8	x,1/2-y,1/2+z	x,y,1+z
M9	x,1/2-y,-1/2+z	x,y,z
M10	1-x,1/2+y,1.5-z	1-x,1-y,1-z
M11	1-x,1/2+y,1/2-z	1-x,1-y,-z
M12	1-x,-y,2-z	1-x,-1/2+y,1.5-z
M13	1-x,-y,1-z	1-x,-1/2+y,1/2-z
M14	1-x,-1/2+y,1.5-z	1-x,-y,1-z
M15	1-x,-1/2+y,1/2-z	1-x,-y,-z
M16	x,-1/2-y,1/2+z	x,-1+y,1+z
M17	x,-1/2-y,-1/2+z	x,-1+y,z
M18	-x,-1/2+y,1/2-z	-x,-y,-z
M19	-x,-1/2+y,-1/2-z	-x,-y,-1-z

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P1 atom of the anion as reference.

Table S62- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **11**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M13	47.34	-30.89	1.84	4.13
M1...M2	25.94	-14.58	1.01	1.95
M1...M3	25.94	-14.51	1.01	1.94
M1...M8	69.39	-13.42	2.70	1.79
M1...M9	69.39	-13.4	2.70	1.79
M1...M10	7.09	-11.21	0.28	1.50
M1...M14	7.09	-11.21	0.28	1.50
M1...M4	60.12	-8.09	2.34	1.08
M1...M5	38.69	-5.16	1.5	0.69
M1...M7	31.28	-3.71	1.22	0.50
M1... M19	31.28	-3.71	1.22	0.50
M1...M16	17.35	-3.22	0.67	0.43

M1... M17	17.35	-3.2	0.67	0.43
M1...M6	0.1	-2.01	0.00	0.27
M1... M18	0.1	-2.01	0.00	0.27
M1...M11	6.98	1.37	0.27	-0.18
M1...M15	6.98	1.37	0.27	-0.18
M1...M12	0.33	2.92	0.01	-0.39
TOTAL	462.74	-134.66	18.00	18.00

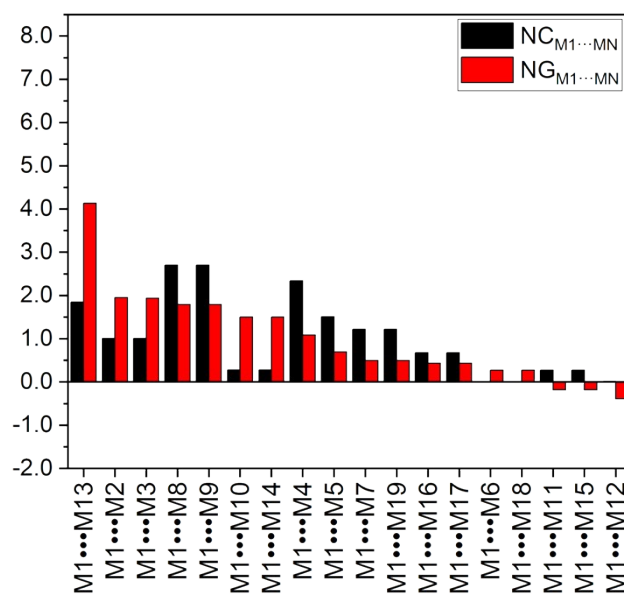


Figure S62- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **11**<sub>CA1</sub>.

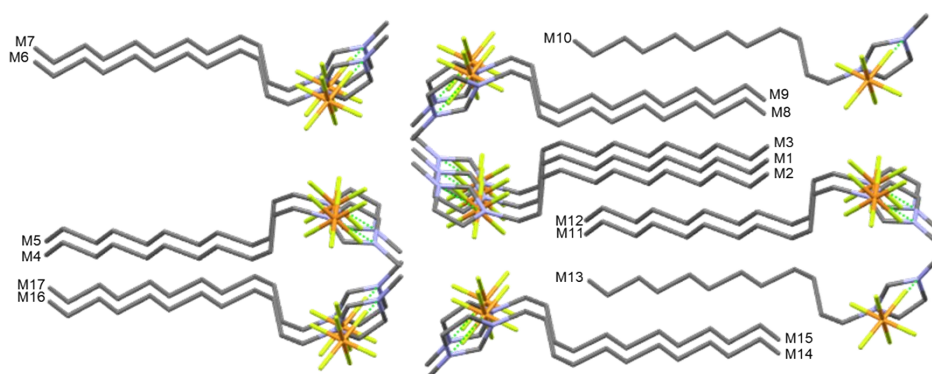


Figure S63- Supramolecular cluster of compound **12**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S63- Symmetry codes for the monomers of compound **12**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	x,y,z	1+x,y,z
M2	-1+x,y,z	x,y,z
M3	1+x,y,z	2+x,y,z
M4	2-x,-y,1-z	1-x,-y,1-z
M5	3-x,-y,1-z	2-x,-y,1-z
M6	1.5-x,-1/2+y,1-z	1/2-x,-1/2+y,1-z
M7	2.5-x,-1/2+y,1-z	1.5-x,-1/2+y,1-z
M8	-1/2+x,-1/2-y,z	1/2+x,-1/2-y,z
M9	1/2+x,-1/2-y,z	1.5+x,-1/2-y,z
M10	1/2-x,-1/2+y,-z	-1/2-x,-1/2+y,-z
M11	-x,-y,-z	-1-x,-y,-z
M12	1-x,-y,-z	-x,-y,-z
M13	1/2-x,1/2+y,-z	-1/2-x,1/2+y,-z
M14	-1/2+x,1/2-y,z	1/2+x,1/2-y,z
M15	1/2+x,1/2-y,z	1.5+x,1/2-y,z
M16	1.5-x,1/2+y,1-z	1/2-x,1/2+y,1-z
M17	2.5-x,1/2+y,1-z	1.5-x,1/2+y,1-z

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the P1 atom of the anion as reference.

Table S64- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **12**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M4	46.37	-29.55	1.47	3.42
M1...M8	80.2	-15.36	2.54	1.78
M1...M9	80.2	-15.36	2.54	1.78
M1...M2	26.14	-14.82	0.83	1.72
M1...M3	26.14	-14.82	0.83	1.72
M1...M7	6.68	-10.41	0.21	1.21
M1... M17	6.68	-10.41	0.21	1.21
M1...M12	64.54	-9.11	2.05	1.05
M1...M11	50.68	-7.7	1.61	0.89
M1...M10	34.14	-4.49	1.08	0.52

M1...M13	34.14	-4.49	1.08	0.52
M1...M14	17.51	-3.11	0.56	0.36
M1...M15	17.51	-3.11	0.56	0.36
M1...M6	6.67	1.12	0.21	-0.13
M1...M16	6.67	1.12	0.21	-0.13
M1...M5	0.17	2.29	0.01	-0.27
TOTAL	504.44	-138.19	16.00	16.00

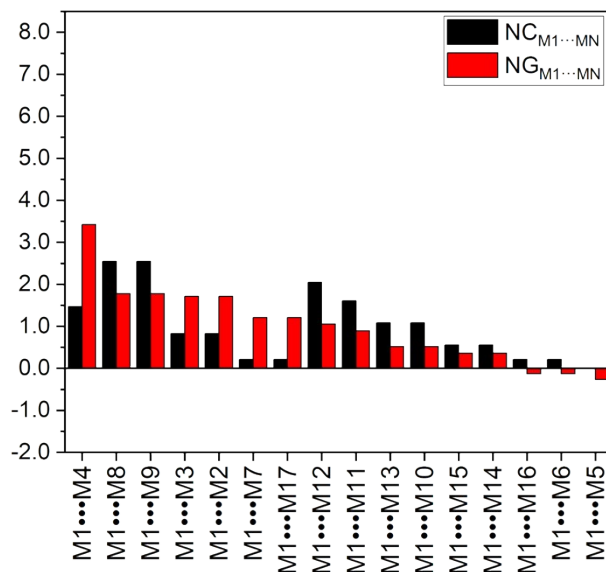


Figure S64- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **12**<sub>CA1</sub>.

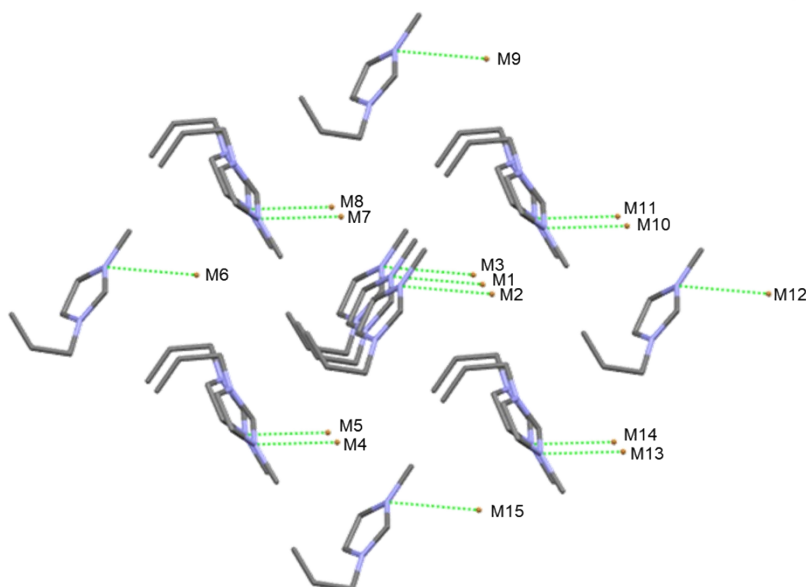


Figure S65- Supramolecular cluster of compound **13**<sub>CA1</sub>, based on the CA1 cation-anion pair.

Table S65- Symmetry codes for the monomers of compound **13**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
M1	x,y,z	x,1+y,z
M2	-1+x,y,z	-1+x,1+y,z
M3	1+x,y,z	1+x,1+y,z
M4	1-x,-1/2+y,2-z	1-x,1/2+y,2-z
M5	2-x,-1/2+y,2-z	2-x,1/2+y,2-z
M6	x,-1+y,z	x,y,z
M7	1-x,-1/2+y,1-z	1-x,1/2+y,1-z
M8	2-x,-1/2+y,1-z	2-x,1/2+y,1-z
M9	x,y,-1+z	x,1+y,-1+z
M10	1-x,1/2+y,1-z	1-x,1.5+y,1-z
M11	2-x,1/2+y,1-z	2-x,1.5+y,1-z
M12	x,1+y,z	x,2+y,z
M13	1-x,1/2+y,2-z	1-x,1.5+y,2-z
M14	2-x,1/2+y,2-z	2-x,1.5+y,2-z
M15	x,y,1+z	x,1+y,1+z

<sup>a</sup>Symmetry codes were taken using the N1 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S66- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **13**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M5	33.17	-14.59	1.93	2.47
M1...M14	33.17	-14.59	1.93	2.47
M1...M8	22.67	-10.86	1.32	1.84
M1...M11	22.67	-10.86	1.32	1.84
M1...M7	16.49	-9.01	0.96	1.53
M1...M10	16.49	-9.01	0.96	1.53
M1...M4	10.81	-7.10	0.63	1.2
M1...M13	10.81	-7.10	0.63	1.2
M1...M6	4.10	-4.94	0.24	0.84
M1...M12	4.10	-4.94	0.24	0.84
M1...M2	24.62	-0.87	1.43	0.15

M1...M3	24.62	-0.87	1.43	0.15
M1...M9	8.71	6.02	0.51	-1.02
M1... M15	8.71	6.05	0.51	-1.02
TOTAL	241.14	-82.67	14.00	14.00

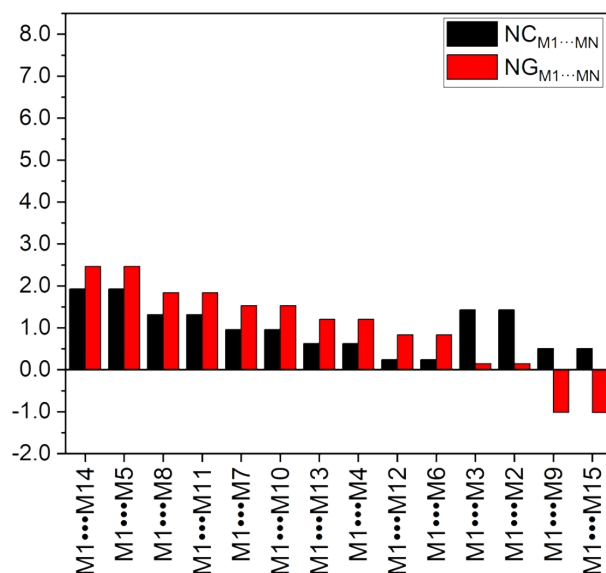


Figure S66- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **13**<sub>CA1</sub>.

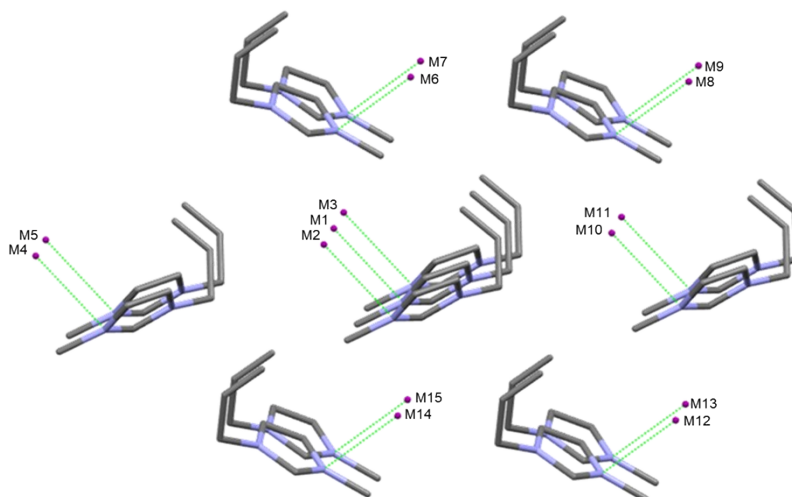


Figure S67- Supramolecular cluster of compound **14**<sub>CA1r</sub> based on the CA1 cation-anion pair.

Table S67- Symmetry codes for the monomers of compound **14**<sub>CA1</sub>.

Monomer	Cation symmetry code <sup>a</sup>	Anion symmetry code <sup>b</sup>
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M1	x,y,z	-1+x,y,-1+z
M2	1+x,y,z	x,y,-1+z
M3	-1+x,y,z	-2+x,y,-1+z
M4	x,y,-1+z	-1+x,y,-2+z
M5	-1+x,y,-1+z	-2+x,y,-2+z
M6	1-x,-1/2+y,-z	2-x,-1/2+y,1-z
M7	-x,-1/2+y,-z	1-x,-1/2+y,1-z
M8	1-x,-1/2+y,1-z	2-x,-1/2+y,2-z
M9	-x,-1/2+y,1-z	1-x,-1/2+y,2-z
M10	1+x,y,1+z	x,y,z
M11	x,y,1+z	-1+x,y,z
M12	1-x,1/2+y,1-z	2-x,1/2+y,2-z
M13	-x,1/2+y,1-z	1-x,1/2+y,2-z
M14	1-x,1/2+y,-z	2-x,1/2+y,1-z
M15	-x,1/2+y,-z	1-x,1/2+y,1-z

<sup>a</sup>Symmetry codes were taken using the N2 atom of the cation as reference. <sup>b</sup>Symmetry codes were taken using the Br1 atom of the anion as reference.

Table S68- Contact area ( $C_{M1...MN}$ ) and stabilization energy ( $G_{M1...MN}$ ) and normalized contact area and stabilization energy data area ( $N_{CM1...MN}$  and  $N_{GM1...MN}$ ) between the dimers of the supramolecular cluster for **14**<sub>CA1</sub>.

Dímer	$C_{M1...MN}$ (Å <sup>2</sup> )	$G_{M1...MN}$ (kcal mol <sup>-1</sup> )	$N_{CM1...MN}$	$N_{GM1...MN}$
M1...M7	18.81	-16.92	1.02	2.18
M1... M15	18.81	-16.92	1.02	2.18
M1...M6	25.5	-14.23	1.39	1.84
M1...M14	25.5	-14.23	1.39	1.84
M1...M10	7.28	-13.05	0.4	1.69
M1...M5	7.28	-12.2	0.4	1.57
M1...M2	29.3	-3.75	1.6	0.48
M1...M3	29.3	-3.75	1.6	0.48
M1...M9	4.88	-2.77	0.27	0.36
M1...M13	4.88	-2.77	0.27	0.36
M1...M8	27.64	-2.64	1.5	0.34
M1...M12	27.64	-2.64	1.5	0.34
M1...M4	15.17	-1.28	0.83	0.17

M1...M11	15.17	-1.28	0.83	0.17
TOTAL	257.16	-108.42	14.00	14.00

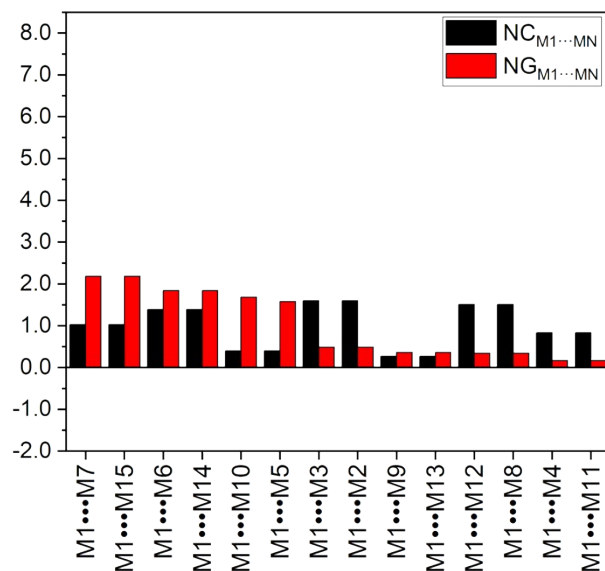


Figure S68- Normalized contact ( $NC_{M1...MN}$ ) area and stabilization energy ( $NG_{M1...MN}$ ) data of each dimer from the supramolecular cluster of compound **1**<sub>CA1</sub>.

### 3. Crystallization Mechanisms Proposals

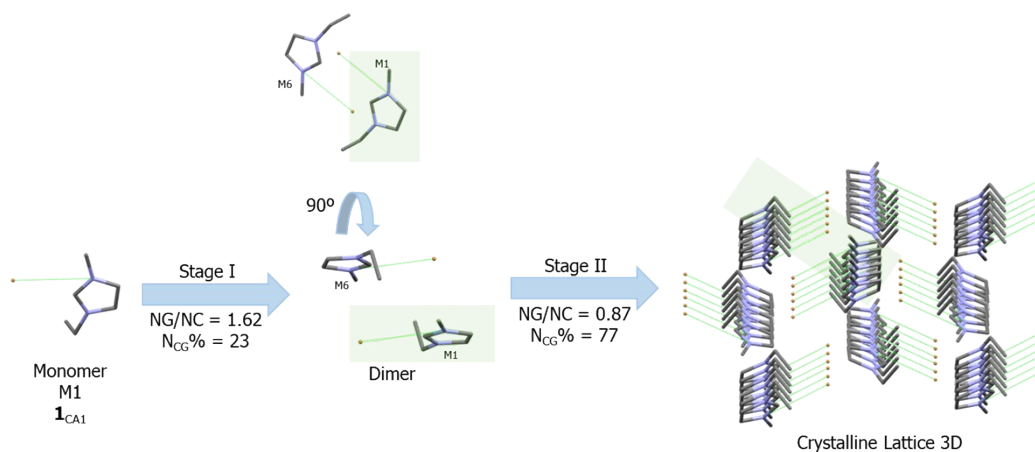


Figure S69- Proposed crystallization mechanism for compound **1**<sub>CA1</sub>.

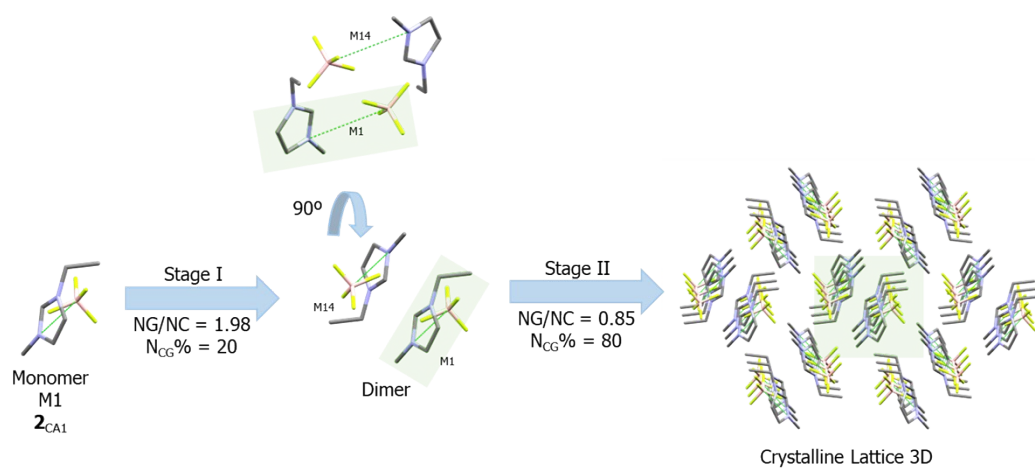


Figure S70- Proposed crystallization mechanism for compound  $2_{CA1}$ .

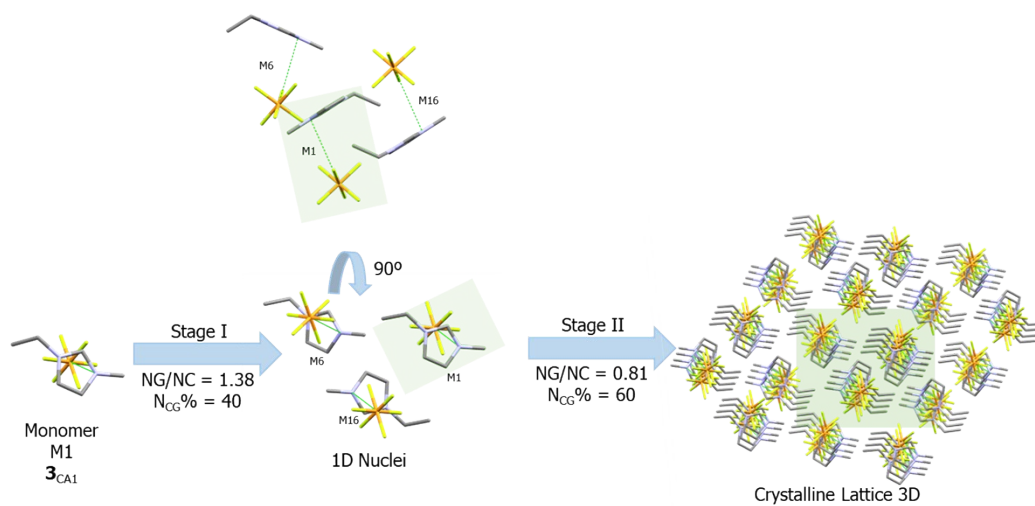


Figure S71- Proposed crystallization mechanism for compound  $3_{CA1}$ .

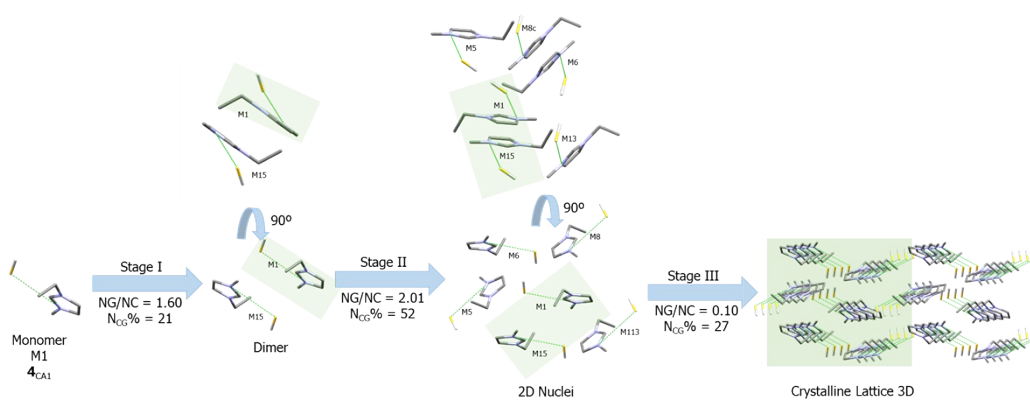


Figure S72- Proposed crystallization mechanism for compound  $4_{CA1}$ .

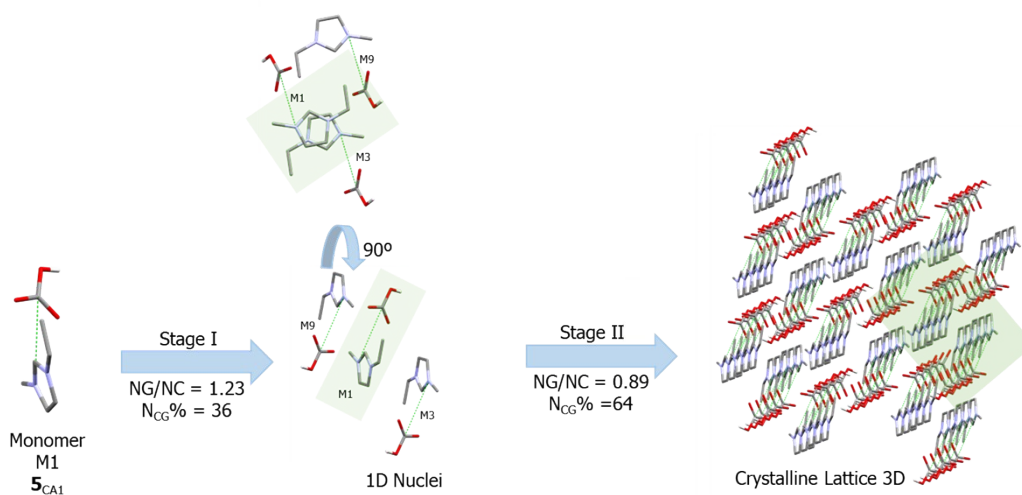


Figure S73- Proposed crystallization mechanism for compound **5<sub>CA1</sub>**.

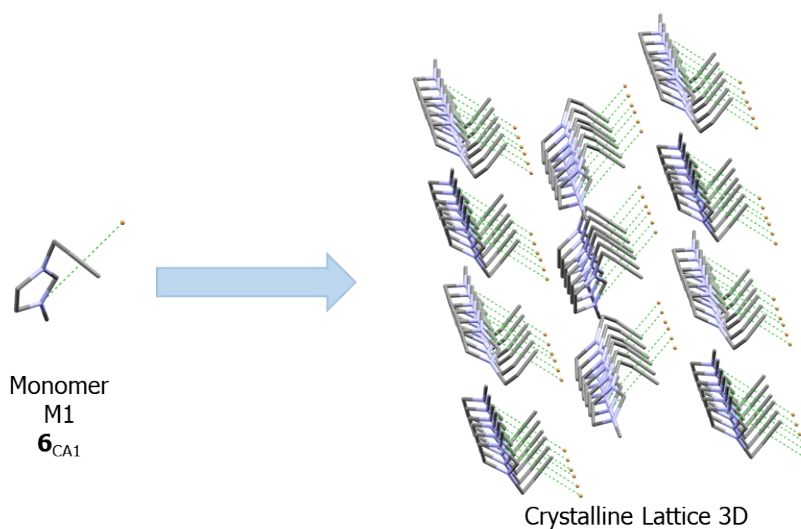


Figure S74- Proposed crystallization mechanism for compound **6<sub>CA1</sub>**.

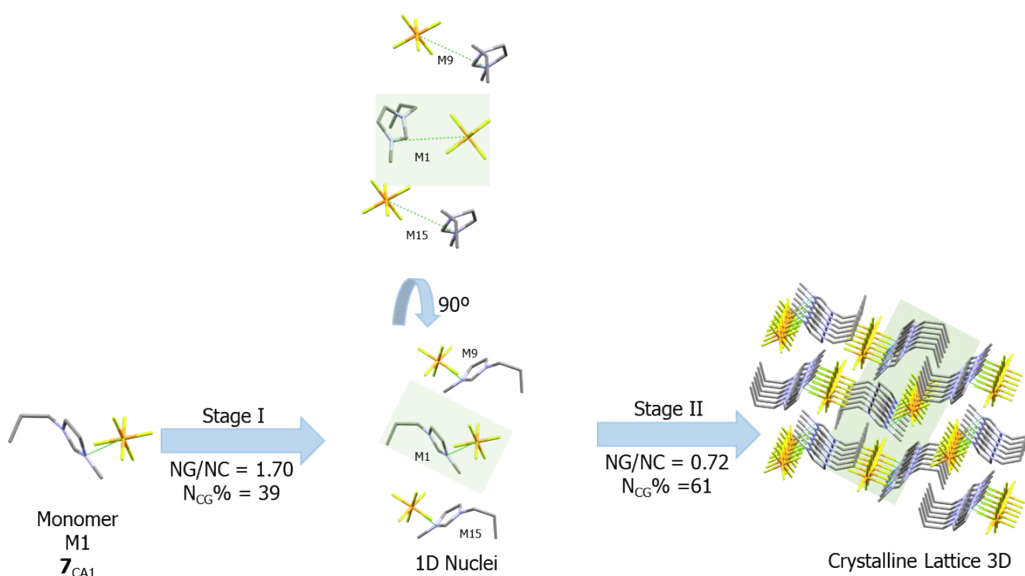


Figure S75- Proposed crystallization mechanism for compound **7**<sub>CA1</sub>.

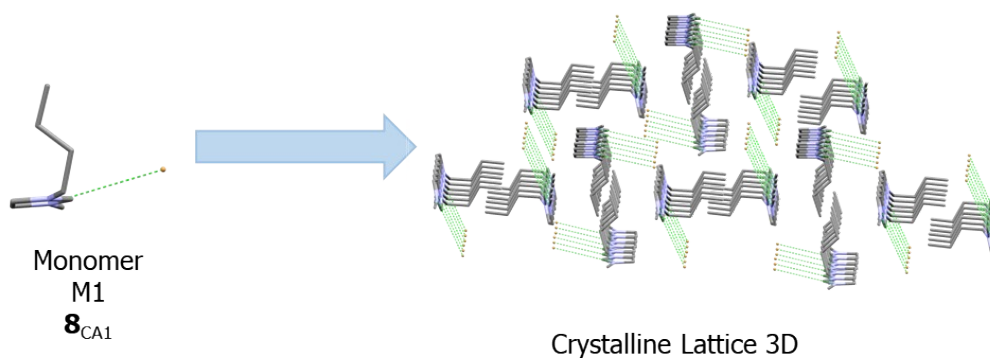


Figure S76- Proposed crystallization mechanism for compound **8**<sub>CA1</sub>.

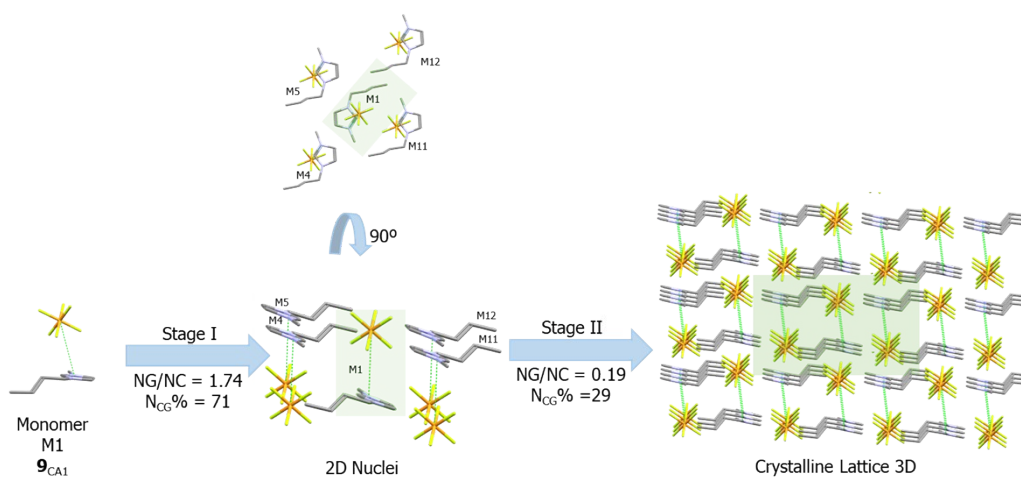


Figure S77- Proposed crystallization mechanism for compound **9**<sub>CA1</sub>.

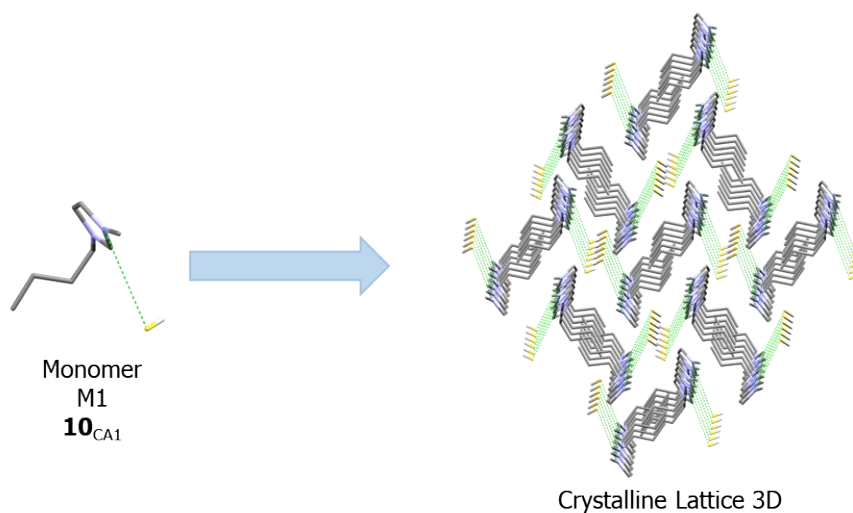


Figure S78- Proposed crystallization mechanism for compound **10**<sub>CA1</sub>.

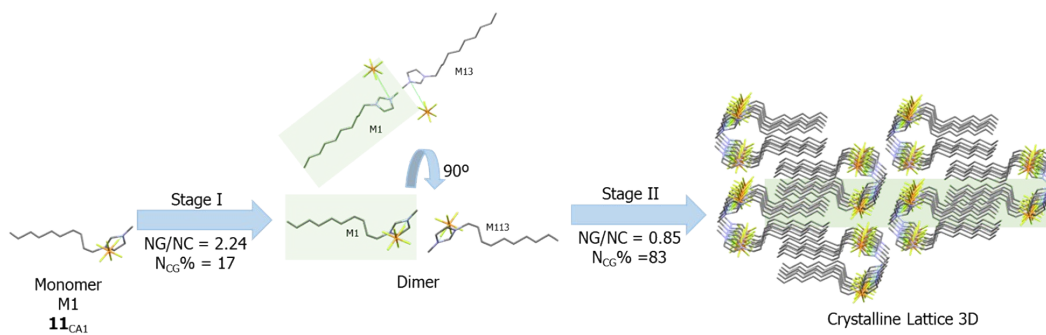


Figure S79- Proposed crystallization mechanism for compound **11**<sub>CA1</sub>.

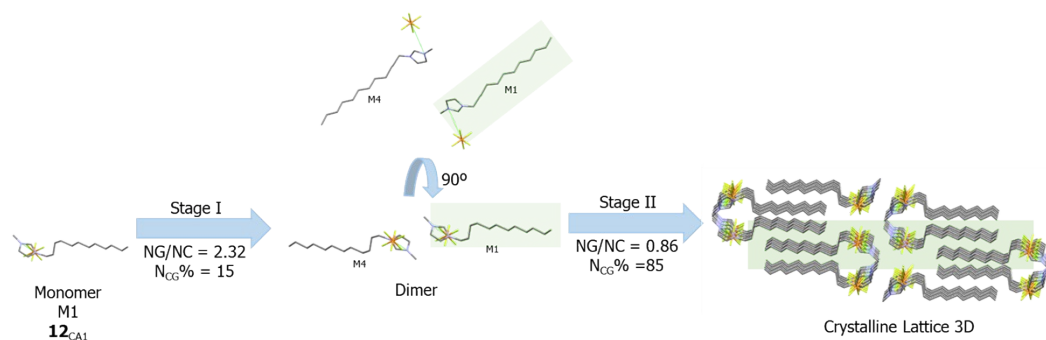


Figure S80- Proposed crystallization mechanism for compound **12**<sub>CA1</sub>.

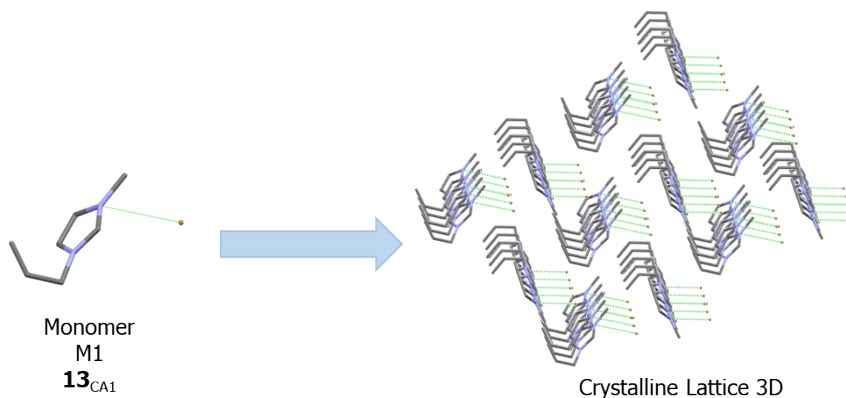


Figure S81- Proposed crystallization mechanism for compound **13**<sub>CA1</sub>.

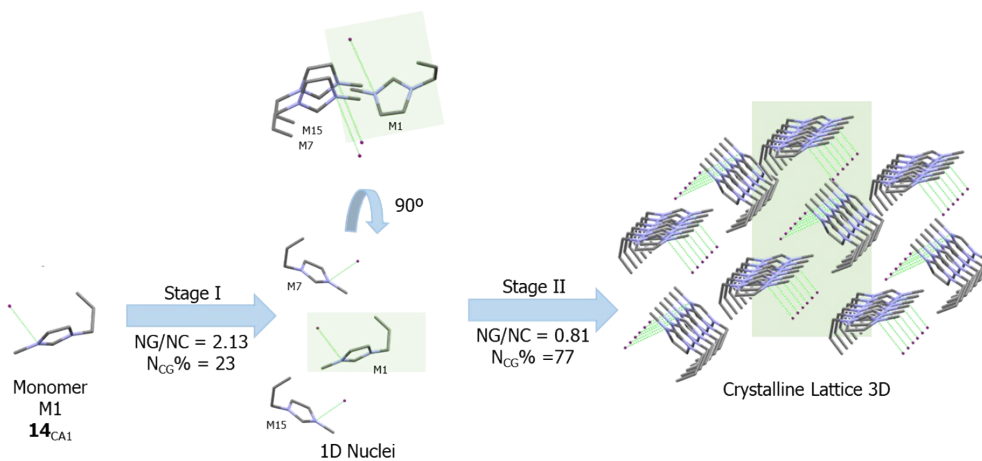


Figure S82-Proposed crystallization mechanism for compound **14**<sub>CA1</sub>.

4. Graphic of cluster energy efficiency (CEE)

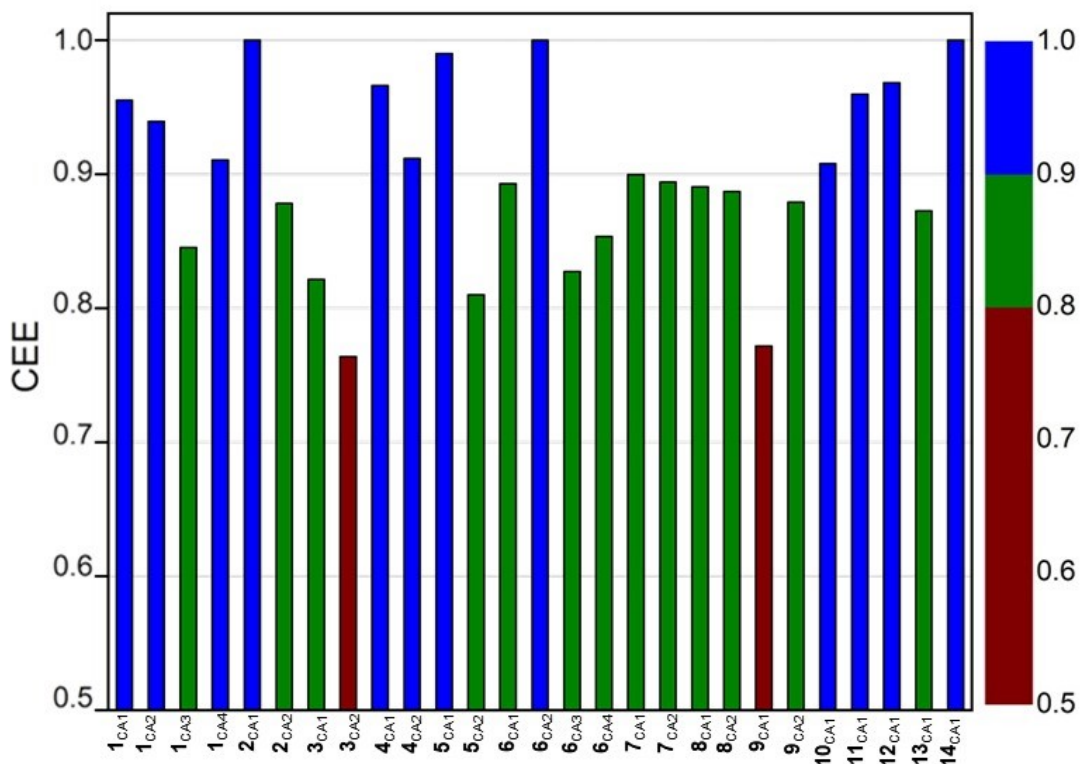


Figure S83- Range values of cluster energy efficiency (CEE) for the studied compounds. Regions: (A)  $1.0 \geq \text{CEE} \geq 0.9$  (high), (B)  $0.9 > \text{CEE} \geq 0.8$  (mean), (C)  $0.8 > \text{CEE}$  (low).