SUPPORTING INFORMATION

The Role of Attractive and Repulsive Interactions in the Stabilization of Ammonium Salts Structures

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

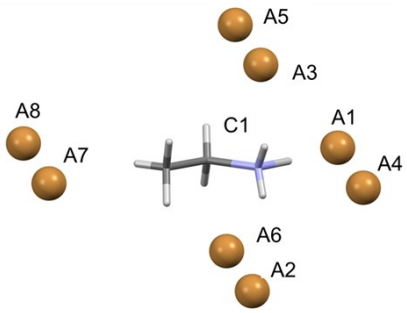


Figure S1. Anions that present contact area with C1 cation of salt **1a**.

Table S1. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **1a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	1-x,-1/2+y,2-z	6.15	-1700358.03	0.00	3.35
C1···A2	x,-1+y,z	7.24	-1700339.84	18.19	3.38
C1···A3	x,y,z	7.24	-1700339.84	18.19	3.38
C1···A4	-x,-1/2+y,2-z	6.87	-1700335.21	22.82	3.41
C1···A5	1+x,y,z	3.23	-1700316.90	41.13	4.60
C1···A6	1+x,-1+y,z	3.23	-1700316.90	41.13	4.60
C1···A7	-x,-1/2+y,1-z	3.47	-1700299.50	58.53	6.17
C1···A8	1-x,-1/2+y,1-z	2.52	-1700297.78	60.25	6.45

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

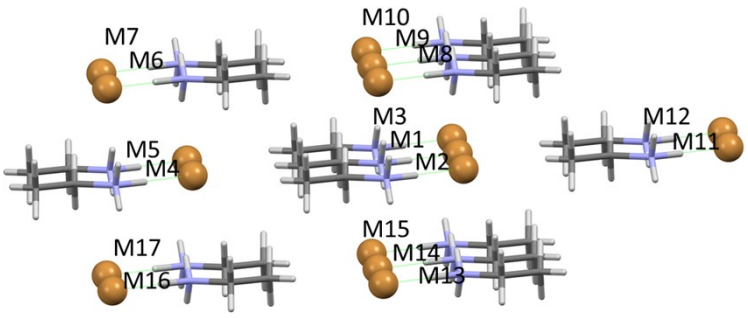


Figure S2. Supramolecular cluster of salt **1a**.

Table S2. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **1a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1-x,-0.5+y,2-z				
M1···M2	-1+x,y,z	-x,-0.5+y,2-z	19.53	-1.03	2.03	0.16
M1···M3	1+x,y,z	2-x,-0.5+y,2-z	19.53	-1.03	2.03	0.16
M1···M4	-1+x,y,-1+z	-x,-0.5+y,1-z	3.47	-5.09	0.36	0.82
M1···M5	x,y,-1+z	1-x,-0.5+y,1-z	2.7	-2.99	0.28	0.48
M1···M6	-x,0.5+y,1-z	-1+x,y,-1+z	5.21	2.69	0.54	-0.43
M1···M7	1-x,0.5+y,1-z	x,y,-1+z	15.48	1.03	1.61	-0.16
M1···M8	-x,0.5+y,2-z	-1+x,y,z	0.61	-1.87	0.06	0.30
M1···M9	1-x,0.5+y,2-z	x,y,z	23.65	-33.36	2.45	5.34
M1···M10	2-x,0.5+y,2-z	1+x,y,z	6.47	-9.36	0.67	1.50
M1···M11	x,y,1+z	1-x,-0.5+y,3-z	2.70	-2.99	0.28	0.48
M1···M12	1+x,y,1+z	2-x,-0.5+y,3-z	3.47	-5.09	0.36	0.82
M1···M13	-x,-0.5+y,2-z	-1+x,-1+y,z	0.61	-1.87	0.06	0.30
M1···M14	1-x,-0.5+y,2-z	x,-1+y,z	23.65	-33.36	2.45	5.34
M1···M15	2-x,-0.5+y,2-z	1+x,-1+y,z	6.47	-9.36	0.67	1.50
M1···M16	-x,-0.5+y,1-z	-1+x,-1+y,-1+z	5.21	2.69	0.54	-0.43
M1···M17	1-x,-0.5+y,1-z	x,-1+y,-1+z	15.48	1.03	1.61	-0.16
Total			154.24	-99.97	16.00	16.00

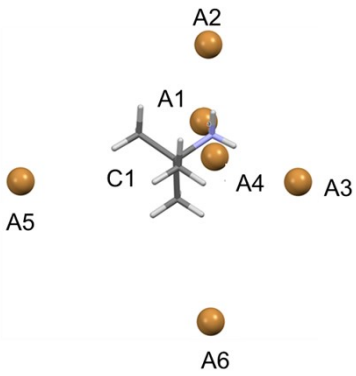


Figure S3. Anions that present contact area with C1 cation of salt **2a**.

Table S3. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **2a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$[d]	N···X[e]
C1···A1	x,y,z	11.21	-1749697.49	0.00	3.36
C1···A2	1/2-x,-1/2+y,z	10.34	-1749693.94	3.55	3.34
C1···A3	1-x,-1/2+y,1.5-z	9.89	-1749692.77	4.72	3.33
C1···A4	x,-1+y,z	4.41	-1749655.10	42.39	5.66
C1···A5	1-x,1-y,1-z	3.89	-1749653.44	44.05	6.49
C1···A6	1.5-x,-1/2+y,z	2.80	-1749651.87	45.62	6.13

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

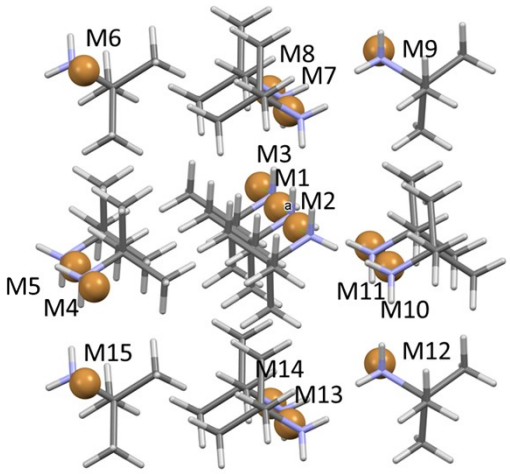


Figure S4. Supramolecular cluster of salt **2a**.

Table S4. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **2a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	x,-1+y,z	x,-1+y,z	4.41	-6.86	0.32	1.56
M1···M3	x,1+y,z	x,1+y,z	4.41	-6.86	0.32	1.56
M1···M4	1-x,-y,1-z	1-x,-y,1-z	12.13	1.35	0.87	-0.31
M1···M5	1-x,1-y,1-z	1-x,1-y,1-z	25.46	-13.46	1.82	3.06
M1···M6	-1/2+x,1/2-y,1-z	-1/2+x,1/2-y,1-z	12.8	-1.97	0.92	0.45
M1···M7	1/2-x,-1/2+y,z	1/2-x,-1/2+y,z	20.37	-12.42	1.46	2.82
M1···M8	1/2-x,1/2+y,z	1/2-x,1/2+y,z	20.37	-12.42	1.46	2.82
M1···M9	-1/2+x,y,1.5-z	-1/2+x,y,1.5-z	7.42	9.81	0.53	-2.23
M1···M10	1-x,-1/2+y,1.5-z	1-x,-1/2+y,1.5-z	17.28	-12.03	1.24	2.73
M1···M11	1-x,1/2+y,1.5-z	1-x,1/2+y,1.5-z	17.28	-12.03	1.24	2.73
M1···M12	1/2+x,y,1.5-z	1/2+x,y,1.5-z	7.42	9.81	0.53	-2.23
M1···M13	1.5-x,-1/2+y,z	1.5-x,-1/2+y,z	16.83	-1.28	1.20	0.29
M1···M14	1.5-x,1/2+y,z	1.5-x,1/2+y,z	16.83	-1.28	1.20	0.29
M1···M15	1/2+x,1/2-y,1-z	1/2+x,1/2-y,1-z	12.8	-1.97	0.92	0.45
Total			195.81	-61.61	14.00	14.00

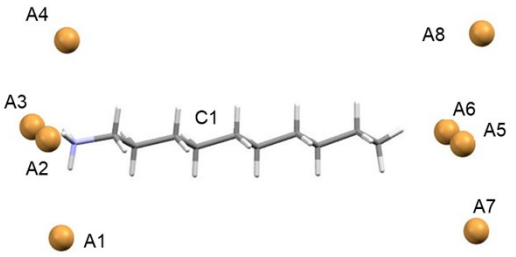


Figure S5. Anions that present contact area with C1 cation of salt **3a.**

Table S5. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **3a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	1-x,-y,1-z	8.97	-1897578.12	0.00	3.38
C1···A2	1+x,y,z	8.02	-1897577.99	0.14	3.30
C1···A3	x,y,z	9.8	-1897577.49	0.63	3.35
C1···A4	1-x,1-y,1-z	8.95	-1897570.55	7.57	3.58
C1···A5	x,1/2-y,-1/2+z	3.89	-1897504.91	73.21	14.48
C1···A6	-1+x,1/2-y,-1/2+z	2.74	-1897499.78	78.34	16.62
C1···A7	-x,-1/2+y,1/2-z	1.17	-1897499.62	78.51	16.46
C1···A8	-x,1/2+y,1/2-z	0.04	-1897499.18	78.95	16.59

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

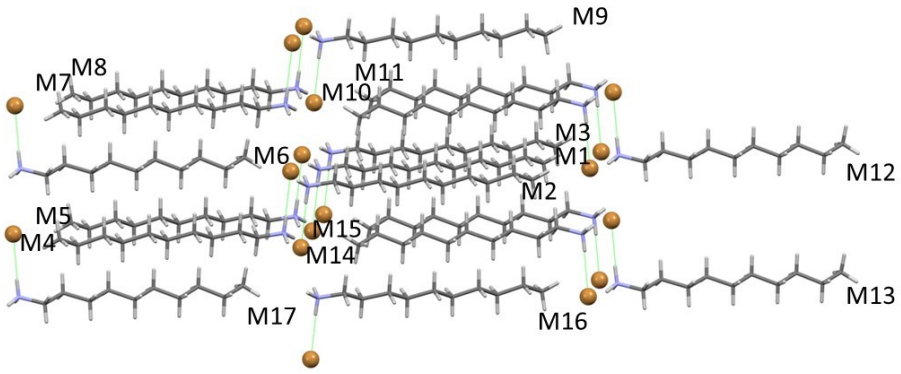


Figure S6. Supramolecular cluster of **3a**.

Table S6. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **3a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1-x,-y,1-z				
M1···M2	1+x,y,z	2-x,-y,1-z	18.03	5.89	0.83	-0.67
M1···M3	-1+x,y,z	-x,-y,1-z	18.03	5.89	0.83	-0.67
M1···M4	2-x,-y,1-z	1+x,y,z	19.93	-47.63	0.92	5.43
M1···M5	1-x,-y,1-z	x,y,z	22.67	-46.29	1.05	5.28
M1···M6	1+x,1/2-y,1/2+z	2-x,1/2+y,1.5-z	10.29	-1.64	0.48	0.19
M1···M7	2-x,1-y,1-z	1+x,1+y,z	2.69	5.41	0.12	-0.62
M1···M8	1-x,1-y,1-z	x,1+y,z	1.83	4.16	0.08	-0.47
M1···M9	x,1+y,z	1-x,1-y,1-z	8.95	-18.06	0.41	2.06
M1···M10	1-x,1/2+y,1/2-z	x,1/2-y,-1/2+z	57.27	-7.28	2.65	0.83
M1···M11	-x,1/2+y,1/2-z	-1+x,1/2-y,-1/2+z	53.89	-6.02	2.49	0.69
M1···M12	-1+x,1/2-y,-1/2+z	-x,1/2+y,1/2-z	10.25	-1.64	0.47	0.19
M1···M13	-1+x,-1/2-y,-1/2+z	-x,-1/2+y,1/2-z	1.17	-0.89	0.05	0.10
M1···M14	1-x,-1/2+y,1/2-z	x,-1/2-y,-1/2+z	57.27	-7.28	2.65	0.83
M1···M15	-x,-1/2+y,1/2-z	-1+x,-1/2-y,-1/2+z	53.89	-6.02	2.49	0.69
M1···M16	x,-1+y,z	1-x,-1-y,1-z	8.95	-18.06	0.41	2.06
M1···M17	1+x,-1/2-y,1/2+z	2-x,-1/2+y,1.5-z	1.17	-0.89	0.05	0.10
Total			346.28	-140.37	16.00	16.00

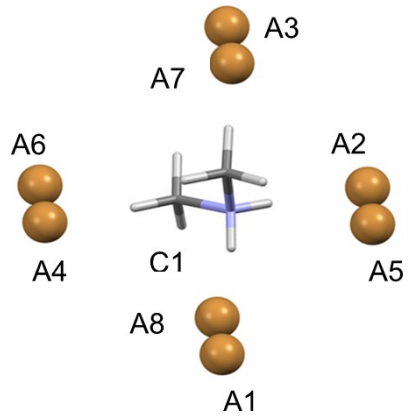


Figure S7. Anions that present contact area with C1 cation of salt **4a**.

Table S7. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **4a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	1/2-x,1/2-y,1-z	7.90	-1700420.23	0.00	3.266
C1···A2	x,1-y,-1/2+z	7.03	-1700420.17	0.06	3.284
C1···A3	1-x,1-y,1-z	6.7	-1700404.05	16.18	4.191
C1···A4	x,-1+y,z	6.92	-1700402.17	18.06	4.320
C1···A5	x,-y,-1/2+z	4.55	-1700391.33	28.90	4.757
C1···A6	x,y,z	4.76	-1700389.01	31.22	5.182
C1···A7	1-x,-y,1-z	2.77	-1700385.10	35.13	5.424
C1···A8	1/2-x,1.5-y,1-z	1.63	-1700381.60	38.63	5.350

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

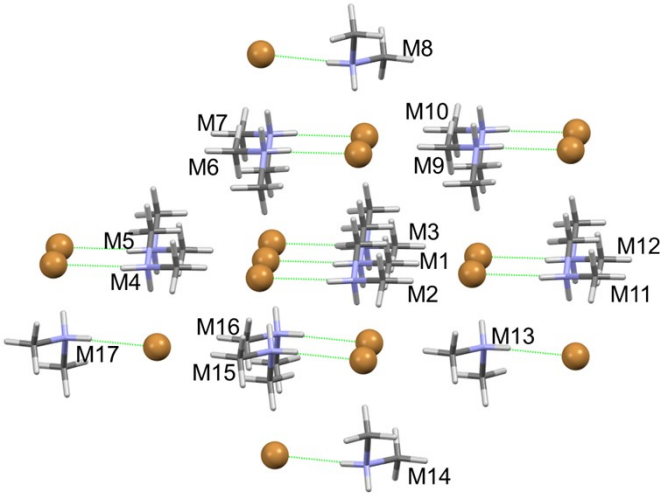


Figure S8. Supramolecular cluster of **4a**.

Table S8. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **4a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1/2-x,1/2-y,1-z				
M1···M2	x,-1+y,z	1/2-x,-1/2-y,1-z	14.69	8.06	1.51	-1.32
M1···M3	x,1+y,z	1/2-x,1.5-y,1-z	14.69	8.06	1.51	-1.32
M1···M4	-1/2+x,-1/2+y,z	-x,-y,1-z	6.7	-14.03	0.69	2.29
M1···M5	-1/2+x,1/2+y,z	-x,1-y,1-z	2.77	-5.29	0.28	0.87
M1···M6	1/2-x,-1/2-y,1-z	x,-1+y,z	13.86	-26.47	1.42	4.33
M1···M7	1/2-x,1/2-y,1-z	x,y,z	22.91	-19.76	2.35	3.23
M1···M8	x,-y,1/2+z	1/2-x,-1/2+y,1.5-z	0.49	5.43	0.05	-0.89
M1···M9	1-x,-y,1-z	1/2+x,-1/2+y,z	18.77	4.03	1.93	-0.66
M1···M10	1-x,1-y,1-z	1/2+x,1/2+y,z	0.85	2.91	0.09	-0.48
M1···M11	1/2+x,-1/2+y,z	1-x,-y,1-z	2.77	-5.29	0.28	0.87
M1···M12	1/2+x,1/2+y,z	1-x,1-y,1-z	6.7	-14.03	0.69	2.29
M1···M13	1-x,y,1/2-z	1/2+x,1/2-y,-1/2+z	14.26	6.37	1.46	-1.04
M1···M14	x,-y,-1/2+z	1/2-x,-1/2+y,1/2-z	0.49	5.43	0.05	-0.89
M1···M15	1/2-x,-1/2+y,1/2-z	x,-y,-1/2+z	17.86	-31.34	1.83	5.13
M1···M16	1/2-x,1/2+y,1/2-z	x,1-y,-1/2+z	17.86	-31.34	1.83	5.13
M1···M17	-x,y,1/2-z	-1/2+x,1/2-y,-1/2+z	0.09	9.43	0.01	-1.54
Total			155.76	-97.82	16.00	16.00

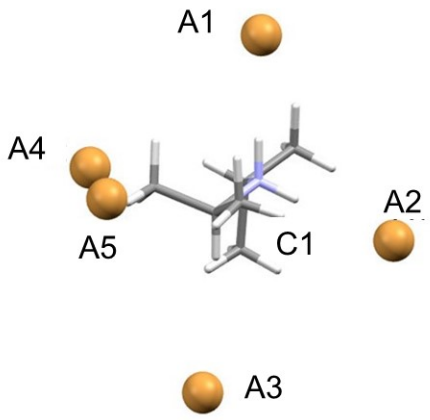


Figure S9. Anions that present contact area with C1 cation of salt **5a.**

Table S9. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **5a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	10.12	1799005.68	0.00	3.3380
C1···A2	-1/2+x,1/2-y,1-z	10.19	1799005.59	0.09	3.3230
C1···A3	-1+x,y,z	7.17	1798981.33	24.35	4.8140
C1···A4	1-x,-1/2+y,1/2-z	7.18	1798981.17	24.51	4.9760
C1···A5	1-x,1/2+y,1/2-z	5.74	1798968.51	37.17	6.0050

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

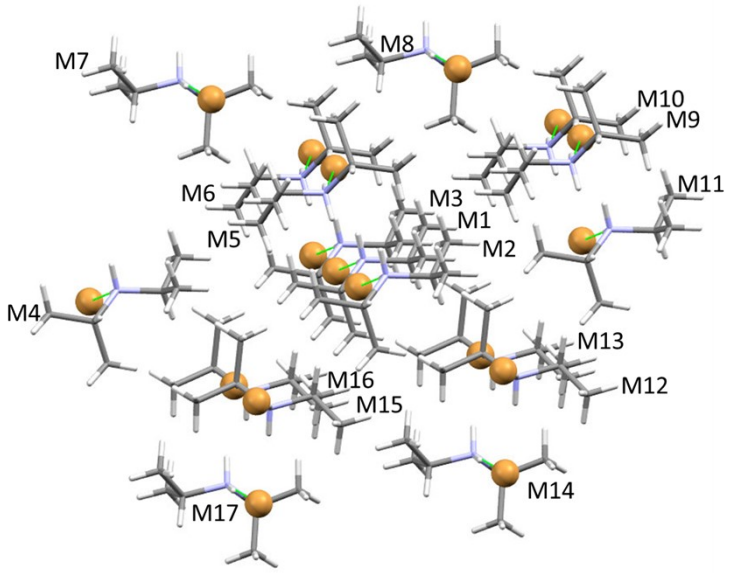


Figure S10. Supramolecular cluster of **5a**.

Table S10. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **5a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	-1+x,y,z	-1+x,y,z	7.17	-9.55	0.51	1.87
M1···M3	1+x,y,z	1+x,y,z	7.17	-9.55	0.51	1.87
M1···M4	x,1+y,z	x,1+y,z	11.09	2.23	0.79	-0.44
M1···M5	-1/2+x,1/2-y,1-z	-1/2+x,1/2-y,1-z	29.71	-12.66	2.12	2.48
M1···M6	1/2+x,1/2-y,1-z	1/2+x,1/2-y,1-z	29.71	-12.66	2.12	2.48
M1···M7	1/2-x,1-y,1/2+z	1/2-x,1-y,1/2+z	0.77	-1.96	0.05	0.38
M1···M8	1/2-x,-y,1/2+z	1/2-x,-y,1/2+z	8.35	-1.64	0.60	0.32
M1···M9	-1/2+x,-1/2-y,1-z	-1/2+x,-1/2-y,1-z	9.02	0.44	0.64	-0.09
M1···M10	1/2+x,-1/2-y,1-z	1/2+x,-1/2-y,1-z	9.02	0.44	0.64	-0.09
M1···M11	x,-1+y,z	x,-1+y,z	11.09	2.23	0.79	-0.44
M1···M12	-x,-1/2+y,1/2-z	-x,-1/2+y,1/2-z	13.69	0.69	0.98	-0.13
M1···M13	1-x,-1/2+y,1/2-z	1-x,-1/2+y,1/2-z	32.27	-18.45	2.30	3.61
M1···M14	1/2-x,-y,-1/2+z	1/2-x,-y,-1/2+z	8.35	-1.64	0.60	0.32
M1···M15	-x,1/2+y,1/2-z	-x,1/2+y,1/2-z	13.69	0.69	0.98	-0.13
M1···M16	1-x,1/2+y,1/2-z	1-x,1/2+y,1/2-z	32.27	-18.45	2.30	3.61
M1···M17	1/2-x,1-y,-1/2+z	1/2-x,1-y,-1/2+z	0.77	-1.96	0.05	0.38
Total			224.14	-81.84	16.00	16.00

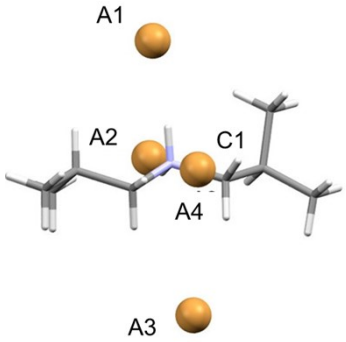


Figure S11. Anions that present contact area with C1 cation of salt **6a**.

Table S11. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **6a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	1/2+x,1/2-y,z	10.93	1848352.31	0.00	3.280
C1···A2	x,y,z	13.61	1848350.72	1.59	3.346
C1···A3	1-x,-y,z	9.33	1848338.11	14.21	4.021
C1···A4	1+x,y,z	5.87	1848331.08	21.23	4.430

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

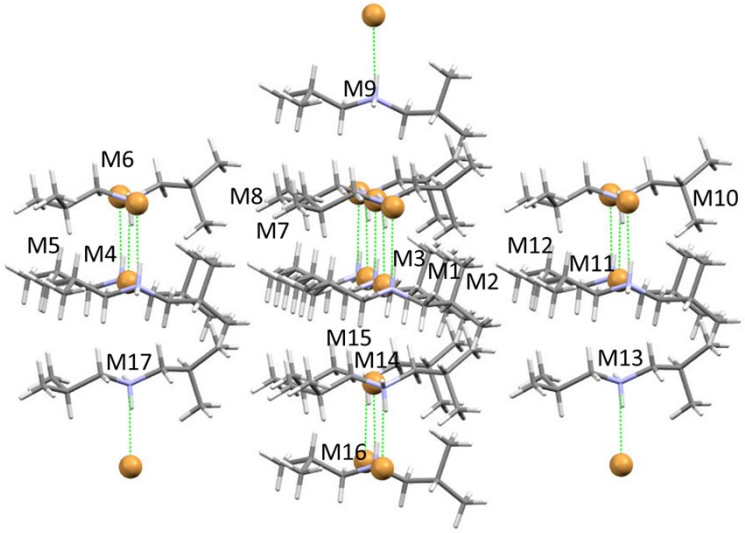


Figure S12. Supramolecular cluster of **6a**.

Table S12. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **6a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1/2+x,1/2-y,z				
M1···M2	1+x,y,z	1.5+x,1/2-y,z	1.39	3.17	0.08	-0.55
M1···M3	-1+x,y,z	-1/2+x,1/2-y,z	1.39	3.17	0.08	-0.55
M1···M4	2-x,y,1/2+z	1.5-x,1/2-y,1/2+z	10.35	0.66	0.61	-0.12
M1···M5	1-x,y,1/2+z	1/2-x,1/2-y,1/2+z	8.23	0.79	0.48	-0.14
M1···M6	1.5-x,1/2-y,1/2+z	1-x,y,1/2+z	8.69	-3.52	0.51	0.62
M1···M7	1/2+x,1/2-y,z	1+x,y,z	50.17	-32.71	2.95	5.72
M1···M8	-1/2+x,1/2-y,z	x,y,z	50.17	-32.71	2.95	5.72
M1···M9	1.5-x,1/2+y,z	1-x,1-y,z	12.46	-12.63	0.73	2.21
M1···M10	1.5-x,1/2-y,-1/2+z	1-x,y,-1/2+z	8.69	-3.52	0.51	0.62
M1···M11	2-x,y,-1/2+z	1.5-x,1/2-y,-1/2+z	10.35	0.66	0.61	-0.12
M1···M12	1-x,y,-1/2+z	1/2-x,1/2-y,-1/2+z	8.23	0.79	0.48	-0.14
M1···M13	x,-y,-1/2+z	1/2+x,-1/2+y,-1/2+z	11.87	-0.88	0.70	0.15
M1···M14	2-x,-y,z	1.5-x,-1/2+y,z	35.99	-1.38	2.12	0.24
M1···M15	1-x,-y,z	1/2-x,-1/2+y,z	29.86	0.17	1.76	-0.03
M1···M16	1.5-x,-1/2+y,z	1-x,-y,z	12.46	-12.63	0.73	2.21
M1···M17	x,-y,1/2+z	1/2+x,-1/2+y,1/2+z	11.87	-0.88	0.70	0.15
Total			272.17	-91.48	16.00	16.00

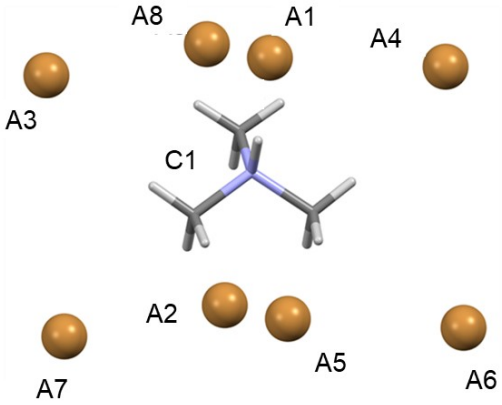


Figure S13. Anions that present contact area with C1 cation of salt **7a**.

Table S13. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **7a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	-x,1/2+y,1-z	7.98	1725117.51	0.00	3.237
C1···A2	1-x,1/2+y,2-z	7.67	1725100.13	17.39	4.222
C1···A3	x,1+y,z	5.17	1725091.14	26.37	4.571
C1···A4	x,y,z	5.17	1725091.14	26.37	4.571
C1···A5	1-x,1/2+y,1-z	5.07	1725088.89	28.62	4.697
C1···A6	1+x,y,z	3.84	1725080.39	37.13	5.286
C1···A7	1+x,1+y,z	3.84	1725080.39	37.13	5.286
C1···A8	-x,1/2+y,2-z	3.52	1725079.98	37.53	5.304

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

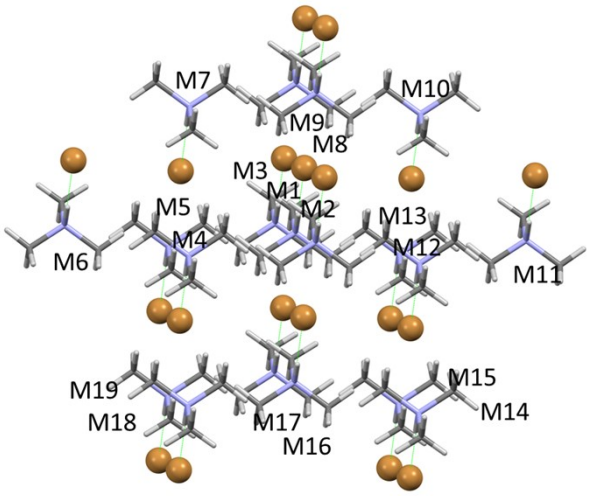


Figure S14. Anions that present contact area with C1 cation of salt **7a**.

Table S14. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **7a.**

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	-x,0.5+y,1-z				
M1···M2	x,y,-1+z	-x,0.5+y,-z	3.6	-2.99	0.37	0.63
M1···M3	x,y,1+z	-x,0.5+y,2-z	3.6	-2.99	0.37	0.63
M1···M4	1-x,0.5+y,1-z	1+x,1+y,z	22.7	-15.93	2.36	3.35
M1···M5	1-x,0.5+y,2-z	1+x,1+y,1+z	19.72	1.71	2.05	-0.36
M1···M6	x,1+y,z	-x,1.5+y,1-z	0.21	3.69	0.02	-0.78
M1···M7	-x,0.5+y,1-z	x,1+y,z	10.34	-19.41	1.07	4.08
M1···M8	-1+x,y,-1+z	-1-x,0.5+y,-z	7.67	-12.46	0.80	2.62
M1···M9	-1+x,y,z	-1-x,0.5+y,1-z	21.37	1.43	2.22	-0.30
M1···M10	-x,-0.5+y,1-z	x,y,z	10.34	-19.41	1.07	4.08
M1···M11	x,-1+y,z	-x,-0.5+y,1-z	0.21	3.69	0.02	-0.78
M1···M12	1-x,-0.5+y,1-z	1+x,y,z	22.7	-15.93	2.36	3.35
M1···M13	1-x,-0.5+y,2-z	1+x,y,1+z	19.72	1.71	2.05	-0.36
M1···M14	2-x,-0.5+y,1-z	2+x,y,z	0.07	-1.34	0.01	0.28
M1···M15	2-x,-0.5+y,2-z	2+x,y,1+z	0.9	2.52	0.09	-0.53
M1···M16	1+x,y,z	1-x,0.5+y,1-z	21.37	1.43	2.22	-0.30
M1···M17	1+x,y,1+z	1-x,0.5+y,2-z	7.67	-12.46	0.80	2.62
M1···M18	2-x,0.5+y,1-z	2+x,1+y,z	0.07	-1.34	0.01	0.28
M1···M19	2-x,0.5+y,2-z	2+x,1+y,1+z	0.9	2.52	0.09	-0.53
Total			173.16	-85.55	18.00	18.00

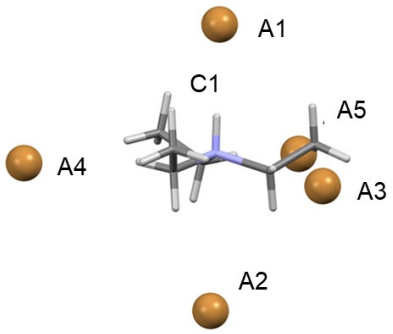


Figure S15. Anions that present contact area with C1 cation of salt **8a**.

Table S15. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **8a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	11.23	1798990.28	0.00	3.282
C1···A2	x,y,1+z	8.68	1798972.67	17.61	4.031
C1···A3	y,1+x,1/2+z	6.30	1798964.36	25.92	4.841
C1···A4	-1+y,x,1/2+z	6.30	1798964.35	25.93	4.840
C1···A5	y,x,1/2+z	6.30	1798964.35	25.94	4.841

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

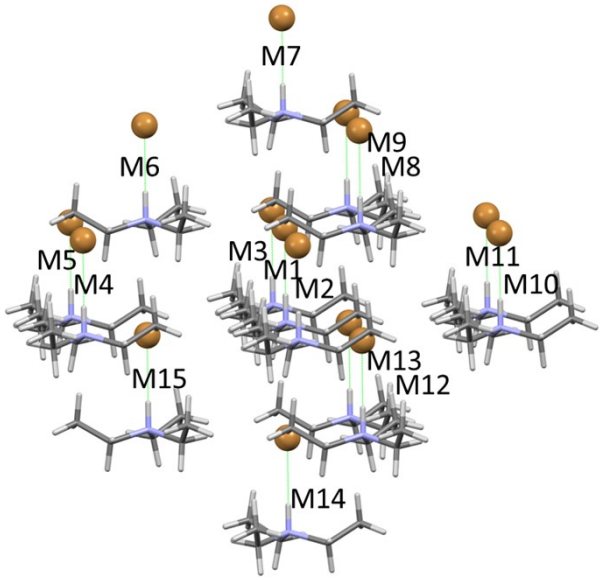


Figure S16. Supramolecular cluster of **8a**.

Table S16. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **8a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	x,1+y,z	x,1+y,z	7.47	2.46	0.47	-1.20
M1···M3	x,-1+y,z	x,-1+y,z	7.47	2.46	0.47	-1.20
M1···M4	-1+x,y,z	-1+x,y,z	7.47	2.45	0.47	-1.19
M1···M5	-1+x,-1+y,z	-1+x,-1+y,z	7.47	2.47	0.47	-1.20
M1···M6	-1+y,x,-0.5+z	-1+y,x,-0.5+z	26.73	-3.81	1.68	1.86
M1···M7	x,y,-1+z	x,y,-1+z	8.68	-10.33	0.55	5.03
M1···M8	y,1+x,-0.5+z	y,1+x,-0.5+z	26.73	-3.81	1.68	1.85
M1···M9	y,x,-0.5+z	y,x,-0.5+z	26.73	-3.81	1.68	1.86
M1···M10	1+x,1+y,z	1+x,1+y,z	7.47	2.45	0.47	-1.19
M1···M11	1+x,y,z	1+x,y,z	7.47	2.46	0.47	-1.20
M1···M12	y,1+x,0.5+z	y,1+x,0.5+z	26.73	-3.81	1.68	1.85
M1···M13	y,x,0.5+z	y,x,0.5+z	26.73	-3.81	1.68	1.86
M1···M14	x,y,1+z	x,y,1+z	8.68	-10.33	0.55	5.03
M1···M15	-1+y,x,0.5+z	-1+y,x,0.5+z	26.73	-3.81	1.68	1.86
Total			222.56	-28.76	14.00	14.00

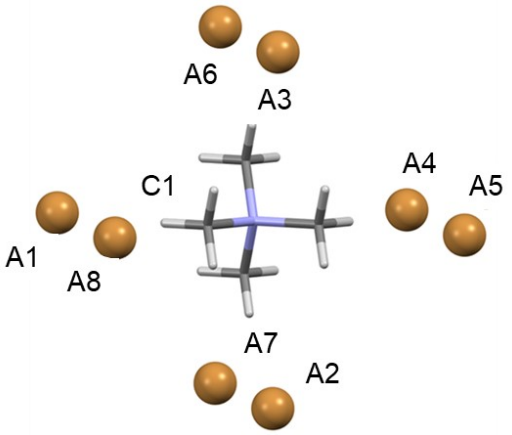


Figure S17. Anions that present contact area with C1 cation of salt **9a**.

Table S17. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **9a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	½+x,1-y,1-z	5.88	1749720.01	0.00	4.345
C1···A2	1+x,y,-1+z	5.88	1749720.01	0.00	4.345
C1···A3	x,y,-1+z	5.88	1749720.01	0.00	4.345
C1···A4	½+x,-y,1-z	5.88	1749720.01	0.00	4.345
C1···A5	½+x,-y,-z	4.04	1749706.63	13.38	5.125
C1···A6	x,y,z	4.04	1749706.63	13.38	5.125
C1···A7	1+x,y,z	4.04	1749706.63	13.38	5.125
C1···A8	½+x,1-y,-z	4.04	1749706.63	13.38	5.125

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

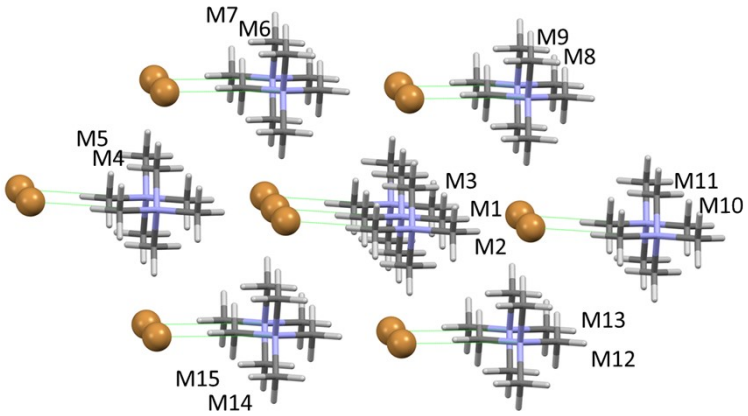


Figure S18. Supramolecular cluster of **9a**.

Table S18. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **9a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	0.5+x,1-y,1-z				
M1···M2	x,y,-1+z	0.5+x,1-y,-z	23.44	6.60	1.80	-1.09
M1···M3	x,y,1+z	0.5+x,1-y,2-z	23.44	6.60	1.80	-1.09
M1···M4	x,1+y,z	0.5+x,2-y,1-z	5.88	-14.74	0.45	2.42
M1···M5	x,1+y,1+z	0.5+x,2-y,2-z	4.04	-13.82	0.31	2.27
M1···M6	0.5-y,x,z	x,1+y,-1+z	24.82	-8.86	1.91	1.46
M1···M7	0.5-y,x,1+z	x,1+y,z	4.04	-1.44	0.31	0.24
M1···M8	0.5-y,-1+x,z	x,y,-1+z	24.82	-8.86	1.91	1.46
M1···M9	0.5-y,-1+x,1+z	x,y,z	4.04	-1.44	0.31	0.24
M1···M10	x,-1+y,-1+z	0.5+x,-y,-z	4.04	-13.82	0.31	2.27
M1···M11	x,-1+y,z	0.5+x,-y,1-z	5.88	-14.74	0.45	2.42
M1···M12	1.5-y,-1+x,z	1+x,y,-1+z	24.82	-8.86	1.91	1.46
M1···M13	1.5-y,-1+x,1+z	1+x,y,z	4.04	-1.44	0.31	0.24
M1···M14	1.5-y,x,z	1+x,1+y,-1+z	24.82	-8.86	1.91	1.46
M1···M15	1.5-y,x,1+z	1+x,1+y,z	4.04	-1.44	0.31	0.24
Total			182.16	-85.12	14.00	14.00

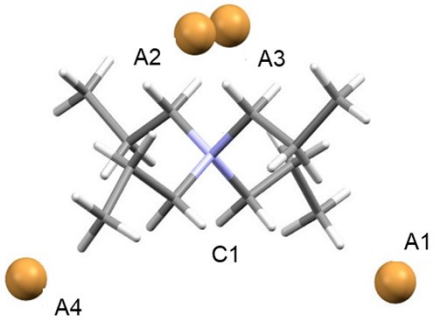


Figure S19. Anions that present contact area with C1 cation of salt **11a**.

Table S19. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **11a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$[d]	N···X[e]
C1···A1	x,y,z	9.84	-1946939.89	0.00	4.9034
C1···A2	1/2+x,1/2+y,1/2+z	9.84	-1946939.89	0.00	4.9034
C1···A3	1/2+x,-1/2+y,1/2+z	9.84	-1946939.89	0.00	4.9034
C1···A4	1+x,y,z	9.84	-1946939.89	0.00	4.9034

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

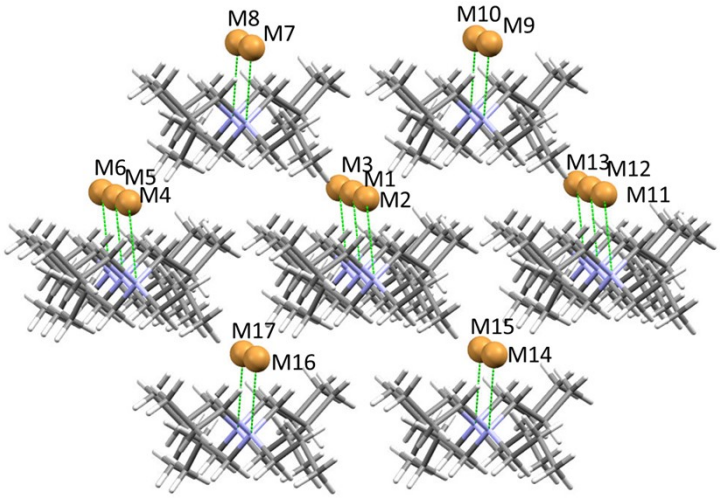


Figure S20. Supramolecular cluster of **11a**.

Table S20. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) the supramolecular cluster of salt **11a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	1+x,y,z	1+x,y,z	40.37	-15.29	1.89	2.34
M1···M3	-1+x,y,z	-1+x,y,z	40.37	-15.29	1.89	2.34
M1···M4	1+x,1+y,z	1+x,1+y,z	4.07	-0.80	0.19	0.12
M1···M5	x,1+y,z	x,1+y,z	30.53	3.37	1.43	-0.52
M1···M6	-1+x,1+y,z	-1+x,1+y,z	4.07	0.01	0.19	0.00
M1···M7	1.5+x,1/2+y,-1/2+z	1.5+x,1/2+y,-1/2+z	18	-0.88	0.84	0.13
M1···M8	1/2+x,1/2+y,-1/2+z	1/2+x,1/2+y,-1/2+z	27.84	-19.08	1.30	2.92
M1···M9	1.5+x,-1/2+y,-1/2+z	1.5+x,-1/2+y,-1/2+z	18	-1.38	0.84	0.21
M1···M10	1/2+x,-1/2+y,-1/2+z	1/2+x,-1/2+y,-1/2+z	27.84	-18.24	1.30	2.79
M1···M11	1+x,-1+y,z	1+x,-1+y,z	4.07	0.01	0.19	0.00
M1···M12	x,-1+y,z	x,-1+y,z	30.53	3.37	1.43	-0.52
M1···M13	-1+x,-1+y,z	-1+x,-1+y,z	4.07	-0.80	0.19	0.12
M1···M14	1.5+x,-1/2+y,1/2+z	1.5+x,-1/2+y,1/2+z	18	-1.38	0.84	0.21
M1···M15	1/2+x,-1/2+y,1/2+z	1/2+x,-1/2+y,1/2+z	27.84	-18.24	1.30	2.79
M1···M16	1.5+x,1/2+y,1/2+z	1.5+x,1/2+y,1/2+z	18	-0.88	0.84	0.13
M1···M17	1/2+x,1/2+y,1/2+z	1/2+x,1/2+y,1/2+z	27.84	-19.08	1.30	2.92
Total			341.44	-104.59	16.00	16.00

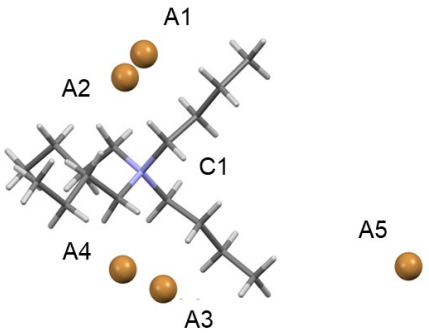


Figure S21. Anions that present contact area with C1 cation of salt **12a**.

Table S21. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **12a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	11.04	-2045544.9669543	0.00	4.935
C1···A2	1-x,1-y,1-z	11.07	-2045544.5928721	0.37	4.963
C1···A3	-1/2+x,-1/2+y,z	10.78	-2045544.5029734	0.46	4.973
C1···A4	1.5-x,1/2-y,1-z	10.87	-2045544.3072543	0.66	4.983
C1···A5	1.5-x,-1/2+y,1.5-z	0.71	-2045509.3120784	35.65	9.426

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

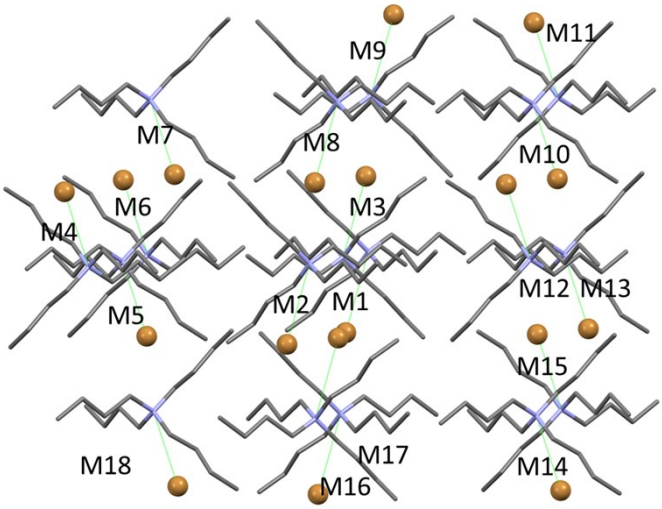


Figure S22. Supramolecular cluster of **12a.** Hydrogens were omitted for clarity.

Table S22. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **12a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	½-x,1/2-y,1-z	½-x,1/2-y,1-z	52.66	-3.20	2.05	0.38
M1···M3	1.5-x,1/2-y,1-z	1.5-x,1/2-y,1-z	74.90	-41.09	2.92	4.90
M1···M4	-x,y,1/2-z	-x,y,1/2-z	4.14	0.72	0.16	-0.09
M1···M5	-1/2+x,1/2-y,-1/2+z	-1/2+x,1/2-y,-1/2+z	24.23	-3.54	0.94	0.42
M1···M6	1-x,y,1/2-z	1-x,y,1/2-z	29.04	-4.73	1.13	0.56
M1···M7	x,1-y,-1/2+z	x,1-y,-1/2+z	7.59	-1.06	0.30	0.13
M1···M8	1-x,1-y,1-z	1-x,1-y,1-z	75.57	-41.31	2.94	4.92
M1···M9	½+x,1/2+y,z	½+x,1/2+y,z	10.82	-16.30	0.42	1.94
M1···M10	x,1-y,1/2+z	x,1-y,1/2+z	7.59	-1.06	0.30	0.13
M1···M11	1.5-x,1/2+y,1.5-z	1.5-x,1/2+y,1.5-z	11.39	-3.75	0.44	0.45
M1···M12	1-x,y,1.5-z	1-x,y,1.5-z	21.5	-1.34	0.84	0.16
M1···M13	½+x,1/2-y,1/2+z	½+x,1/2-y,1/2+z	24.23	-3.54	0.94	0.42
M1···M14	x,-y,1/2+z	x,-y,1/2+z	8.49	0.28	0.33	-0.03
M1···M15	1.5-x,-1/2+y,1.5-z	1.5-x,-1/2+y,1.5-z	11.39	-3.75	0.44	0.45
M1···M16	-1/2+x,-1/2+y,z	-1/2+x,-1/2+y,z	10.78	-16.30	0.42	1.94
M1···M17	1-x,-y,1-z	1-x,-y,1-z	53.96	-2.90	2.10	0.35
M1···M18	x,-y,-1/2+z	x,-y,-1/2+z	8.49	0.28	0.33	-0.03
Total			436.77	-142.60	17.00	17.00

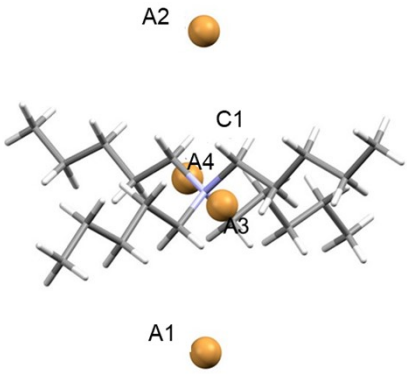


Figure S23. Anions that present contact area with C1 cation of salt **13a**.

Table S23. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **13a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	7.75	2144149.79	0.00	4.6171
C1···A2	1.5-x,1/2-y,1-z	7.75	2144149.79	0.00	4.6171
C1···A3	x,y,1+z	14.50	2144149.68	0.10	5.2517
C1···A4	½-x,1/2-y,1-z	14.50	2144149.68	0.10	5.2517

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

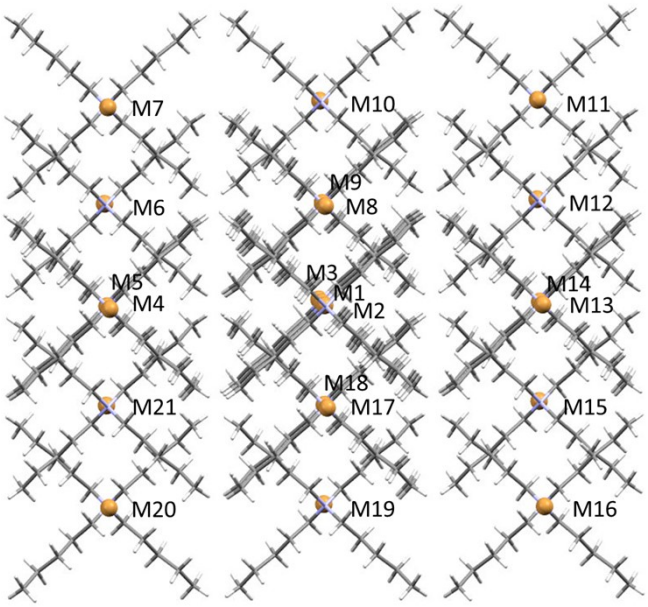


Figure S24. Supramolecular cluster of **13a**.

Table S24. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **13a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	x,y,1+z	x,y,1+z	7.75	-16.03	0.28	2.14
M1···M3	x,y,-1+z	x,y,-1+z	7.75	-16.03	0.28	2.14
M1···M4	1-x,-y,2-z	1-x,-y,2-z	2.99	-0.71	0.11	0.09
M1···M5	1-x,-y,1-z	1-x,-y,1-z	2.99	-4.22	0.11	0.56
M1···M6	-1/2+x,-1/2+y,z	-1/2+x,-1/2+y,z	19.23	0.00	0.71	0.00
M1···M7	-x,-y,2-z	-x,-y,2-z	12.84	-0.82	0.47	0.11
M1···M8	1/2-x,1/2-y,2-z	1/2-x,1/2-y,2-z	65.21	-5.89	2.39	0.79
M1···M9	1/2-x,1/2-y,1-z	1/2-x,1/2-y,1-z	94.21	-43.27	3.46	5.78
M1···M10	-1+x,y,z	-1+x,y,z	35.34	-0.74	1.30	0.10
M1···M11	-x,1-y,1-z	-x,1-y,1-z	12.84	-2.00	0.47	0.27
M1···M12	-1/2+x,1/2+y,z	-1/2+x,1/2+y,z	19.23	-2.00	0.71	0.27
M1···M13	1-x,1-y,2-z	1-x,1-y,2-z	2.99	-0.71	0.11	0.09
M1···M14	1-x,1-y,1-z	1-x,1-y,1-z	2.99	-4.22	0.11	0.56
M1···M15	1/2+x,1/2+y,z	1/2+x,1/2+y,z	19.23	0.00	0.71	0.00
M1···M16	2-x,1-y,2-z	2-x,1-y,2-z	12.84	-0.82	0.47	0.11
M1···M17	1.5-x,1/2-y,2-z	1.5-x,1/2-y,2-z	65.21	-5.89	2.39	0.79
M1···M18	1.5-x,1/2-y,1-z	1.5-x,1/2-y,1-z	94.21	-43.27	3.46	5.78
M1···M19	1+x,y,z	1+x,y,z	35.34	-0.74	1.30	0.10
M1···M20	2-x,-y,1-z	2-x,-y,1-z	12.84	-2.00	0.47	0.27
M1···M21	1/2+x,-1/2+y,z	1/2+x,-1/2+y,z	19.23	-0.31	0.71	0.04
Total			545.26	-149.65	20.00	20.00

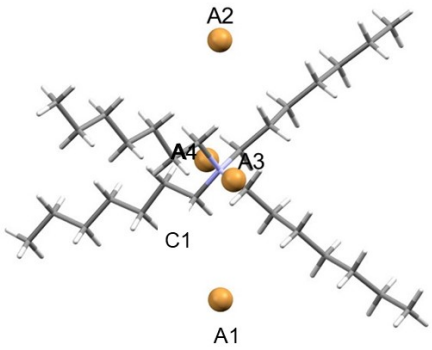


Figure S25. Anions that present contact area with C1 cation of salt **15a**.

Table S25. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **15a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$[d]	N···X[e]
C1···A1	½+x,1/2-y,z	11.35	2341360.99	0.00	4.8996
C1···A2	½+x,1.5-y,z	11.35	2341360.99	0.00	4.8996
C1···A3	1+x,y,z	11.32	2341360.94	0.05	4.9045
C1···A4	x,y,z	11.32	2341360.94	0.05	4.9045

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

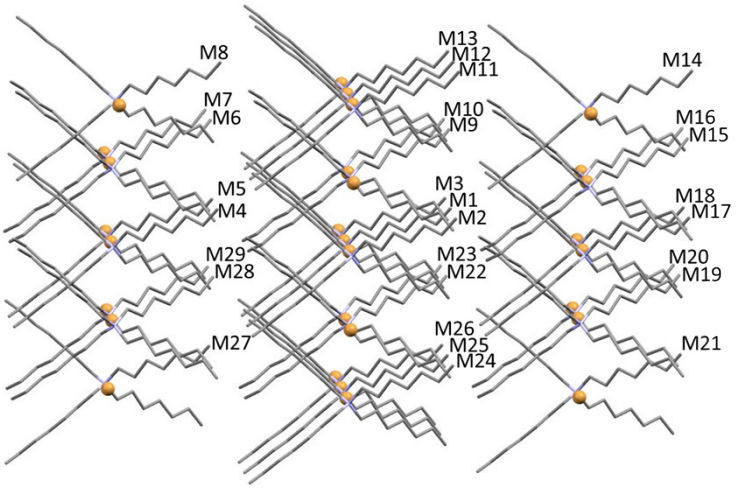


Figure S26. Supramolecular cluster of **15a.** Hydrogens were omitted for clarity.

Table S26. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **15a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1/2+x,1/2-y,z				
M1⋯M2	x,1+y,z	1/2+x,1.5-y,z	31.14	-19.35	1.19	3.05
M1⋯M3	x,-1+y,z	1/2+x,-1/2-y,z	31.14	-19.35	1.19	3.05
M1⋯M4	x,1/2+y,1/2+z	1/2+x,1-y,1/2+z	9.28	-0.47	0.35	0.07
M1⋯M5	x,-1/2+y,1/2+z	1/2+x,-y,1/2+z	9.28	-0.18	0.35	0.03
M1⋯M6	-1/2+x,1-y,1/2+z	x,-1/2+y,1/2+z	9.95	-0.06	0.38	0.01
M1⋯M7	-1/2+x,-y,1/2+z	x,-1.5+y,1/2+z	8.42	-0.61	0.32	0.10
M1⋯M8	-1+x,1/2+y,1/2+z	-1/2+x,2-y,1/2+z	8.56	-1.27	0.33	0.20
M1⋯M9	-1/2+x,1.5-y,z	x,1+y,z	98.23	-12.21	3.75	1.92
M1⋯M10	-1/2+x,1/2-y,z	x,y,z	120.87	-48.49	4.62	7.64
M1⋯M11	-1+x,1+y,z	-1/2+x,1.5-y,z	12.16	-2.05	0.46	0.32
M1⋯M12	-1+x,y,z	-1/2+x,1/2-y,z	19.72	0.80	0.75	-0.13
M1⋯M13	-1+x,-1+y,z	-1/2+x,-1/2-y,z	12.02	-2.25	0.46	0.35
M1⋯M14	-1+x,1/2+y,-1/2+z	-1/2+x,2-y,-1/2+z	8.56	-1.27	0.33	0.20
M1⋯M15	-1/2+x,2-y,-1/2+z	x,1/2+y,-1/2+z	8.42	-0.61	0.32	0.10
M1⋯M16	-1/2+x,1-y,-1/2+z	x,-1/2+y,-1/2+z	9.95	-0.06	0.38	0.01
M1⋯M17	x,1/2+y,-1/2+z	1/2+x,1-y,-1/2+z	9.28	-0.18	0.35	0.03
M1⋯M18	x,-1/2+y,-1/2+z	1/2+x,-y,-1/2+z	9.28	-0.47	0.35	0.07
M1⋯M19	1/2+x,1-y,-1/2+z	1+x,-1/2+y,-1/2+z	9.95	-0.03	0.38	0.00
M1⋯M20	1/2+x,-y,-1/2+z	1+x,-1.5+y,-1/2+z	8.42	-0.82	0.32	0.13
M1⋯M21	1+x,-1/2+y,-1/2+z	1.5+x,1-y,-1/2+z	8.56	-1.92	0.33	0.30
M1⋯M22	1/2+x,1.5-y,z	1+x,1+y,z	98.23	-12.21	3.75	1.92
M1⋯M23	1/2+x,1/2-y,z	1+x,y,z	120.87	-48.49	4.62	7.64
M1⋯M24	1+x,1+y,z	1.5+x,1.5-y,z	12.02	-2.25	0.46	0.35
M1⋯M25	1+x,y,z	1.5+x,1/2-y,z	19.72	0.80	0.75	-0.13
M1⋯M26	1+x,-1+y,z	1.5+x,-1/2-y,z	12.16	-2.05	0.46	0.32
M1⋯M27	1+x,-1/2+y,1/2+z	1.5+x,1-y,1/2+z	8.56	-1.92	0.33	0.30
M1⋯M28	1/2+x,2-y,1/2+z	1+x,1/2+y,1/2+z	8.42	-0.82	0.32	0.13
M1⋯M29	1/2+x,1-y,1/2+z	1+x,-1/2+y,1/2+z	9.95	-0.03	0.38	0.00
Total			733.12	-177.83	28.00	28.00

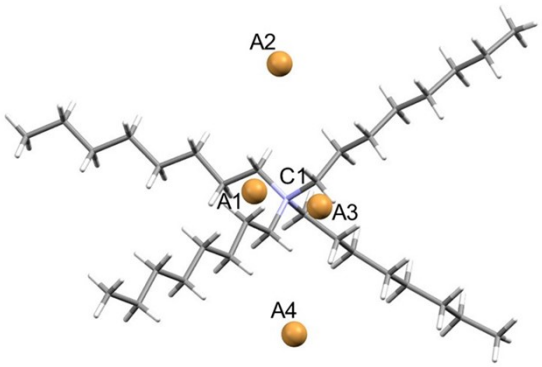


Figure S27. Anions that present contact area with C1 cation of salt **16a**.

Table S27. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **16a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	11.34	-3888.33859574	0.00	4.8521
C1···A2	1+y,1-x,1-z	11.34	-3888.33859574	0.00	4.8521
C1···A3	1+x,y,z	11.34	-3888.33859574	0.00	4.8521
C1···A4	1+y,-x,1-z	11.34	-3888.33859574	0.00	4.8521

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

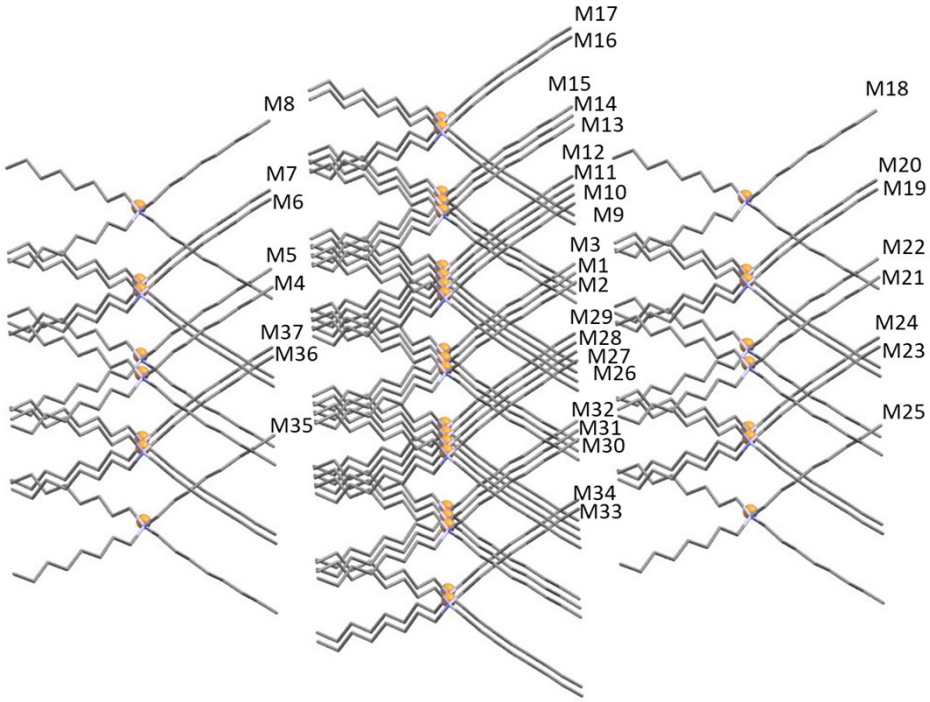


Figure S28. Supramolecular cluster of **16a**. Hydrogens were omitted for clarity.

Table S28. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **16a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	1+x,y,z	1+x,y,z	36.21	-19.57	1.54	4.96
M1···M3	-1+x,y,z	-1+x,y,z	36.21	-19.57	1.54	4.96
M1···M4	1+x,y,1+z	1+x,y,1+z	8.79	-0.31	0.37	0.08
M1···M5	-1+x,y,1+z	-1+x,y,1+z	8.79	-0.44	0.37	0.11
M1···M6	1.5+y,-1/2+x,2-z	1+y,1-x,2-z	12.8	-0.13	0.54	0.03
M1···M7	1/2+y,-1/2+x,2-z	y,1-x,2-z	6.25	0.04	0.27	-0.01
M1···M8	x,1+y,1+z	x,1+y,1+z	8.79	-0.11	0.37	0.03
M1···M9	2.5+y,-1/2+x,1-z	2+y,1-x,1-z	0.01	-2.34	0.00	0.59
M1···M10	1.5+y,-1/2+x,1-z	1+y,1-x,1-z	128.46	-22.59	5.46	5.72
M1···M11	1/2+y,-1/2+x,1-z	y,1-x,1-z	128.46	-22.59	5.46	5.72
M1···M12	-1/2+y,-1/2+x,1-z	-1+y,1-x,1-z	0.01	-2.34	0.00	0.59
M1···M13	1+x,1+y,z	1+x,1+y,z	16.06	-1.89	0.68	0.48
M1···M14	x,1+y,z	x,1+y,z	24.87	0.50	1.06	-0.13
M1···M15	-1+x,1+y,z	-1+x,1+y,z	16.06	-1.91	0.68	0.48
M1···M16	1.5+y,1/2+x,1-z	1+y,2-x,1-z	0.01	1.09	0.00	-0.28
M1···M17	1/2+y,1/2+x,1-z	y,2-x,1-z	0.01	1.09	0.00	-0.28
M1···M18	x,1+y,-1+z	x,1+y,-1+z	8.79	-0.01	0.37	0.00
M1···M19	1.5+y,-1/2+x,-z	1+y,1-x,-z	6.25	0.04	0.27	-0.01
M1···M20	1/2+y,-1/2+x,-z	y,1-x,-z	12.8	-0.13	0.54	0.03
M1···M21	1+x,y,-1+z	1+x,y,-1+z	8.79	-0.31	0.37	0.08
M1···M22	-1+x,y,-1+z	-1+x,y,-1+z	8.79	-0.44	0.37	0.11
M1···M23	1.5+y,-1.5+x,-z	1+y,-x,-z	12.8	-0.22	0.54	0.06
M1···M24	1/2+y,-1.5+x,-z	y,-x,-z	6.25	0.14	0.27	-0.04
M1···M25	x,-1+y,-1+z	x,-1+y,-1+z	8.79	-0.11	0.37	0.03
M1···M26	2.5+y,-1.5+x,1-z	2+y,-x,1-z	0.01	-2.43	0.00	0.61
M1···M27	1.5+y,-1.5+x,1-z	1+y,-x,1-z	128.46	-21.95	5.46	5.56
M1···M28	1/2+y,-1.5+x,1-z	y,-x,1-z	128.46	-21.95	5.46	5.56
M1···M29	-1/2+y,-1.5+x,1-z	-1+y,-x,1-z	0.01	-2.43	0.00	0.61
M1···M30	1+x,-1+y,z	1+x,-1+y,z	16.06	-1.91	0.68	0.48
M1···M31	x,-1+y,z	x,-1+y,z	24.87	0.50	1.06	-0.13
M1···M32	-1+x,-1+y,z	-1+x,-1+y,z	16.06	-1.89	0.68	0.48
M1···M33	1.5+y,-2.5+x,1-z	1+y,-1-x,1-z	0.01	1.06	0.00	-0.27
M1···M34	1/2+y,-2.5+x,1-z	y,-1-x,1-z	0.01	1.06	0.00	-0.27
M1···M35	x,-1+y,1+z	x,-1+y,1+z	8.79	-0.01	0.37	0.00
M1···M36	1.5+y,-1.5+x,2-z	1+y,-x,2-z	6.25	0.14	0.27	-0.04
M1···M37	1/2+y,-1.5+x,2-z	y,-x,2-z	12.8	-0.22	0.54	0.06
Total			846.84	-142.17	36.00	36.00

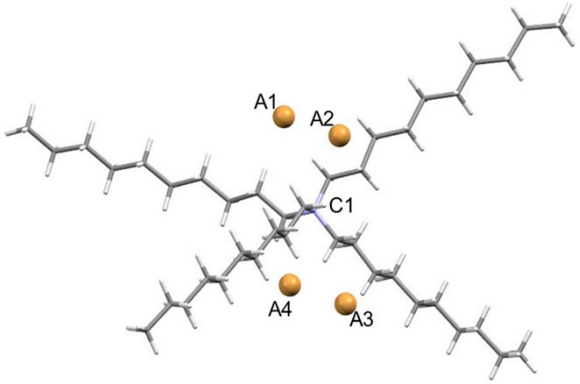


Figure S29. Anions that present contact area with C1 cation of salt **17a**.

Table S29. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **17a**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	½+x,1/2+y,z	11.16	-2637173.74	0.00	4.827
C1···A2	½+x,1/2+y,z	11.06	-2637173.71	0.03	4.820
C1···A3	1+x,y,z	11.10	-2637173.69	0.05	4.831
C1···A4	x,y,z	11.04	-2637173.70	0.05	4.838

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

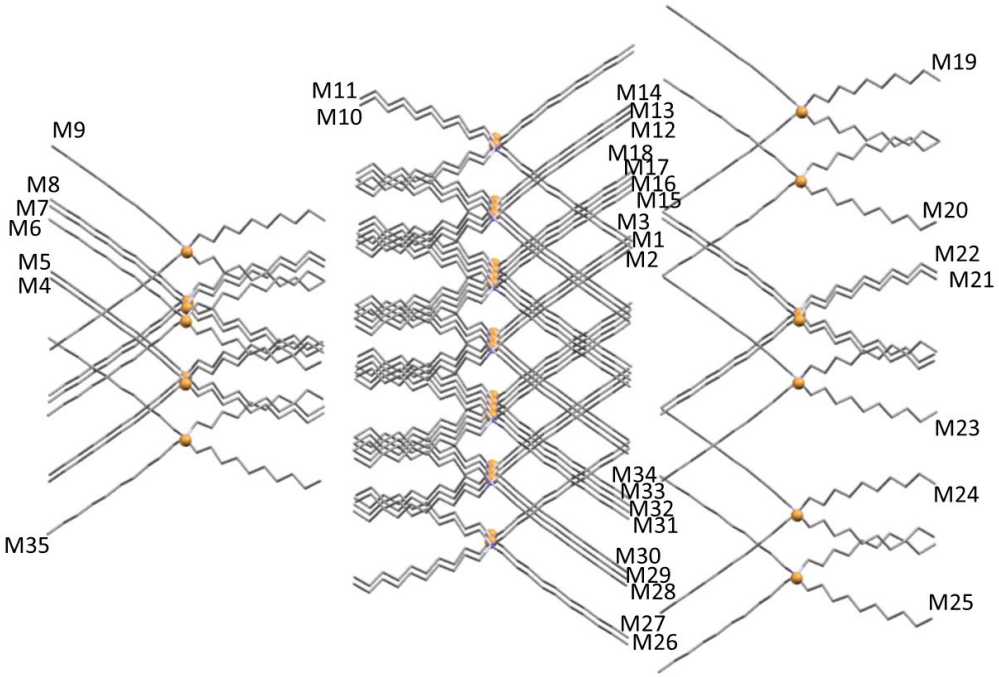


Figure S30. Supramolecular cluster of **17a.** Hydrogens were omitted for clarity.

Table S30. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **17a**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1/2+x,1/2+y,z				
M1···M2	1/2+x,-1/2+y,z	1+x,y,z	36.45	-20.66	1.21	3.61
M1···M3	-1/2+x,1/2+y,z	x,1+y,z	36.45	-20.66	1.21	3.61
M1···M4	2-x,-y,1-z	1.5-x,-1/2-y,1-z	17.71	-0.10	0.59	0.02
M1···M5	1.5-x,1/2-y,1-z	1-x,-y,1-z	4.61	-2.27	0.15	0.40
M1···M6	1+x,-y,1/2+z	2.5-x,-1/2-y,1-z	7.84	-0.47	0.26	0.08
M1···M7	x,1-y,1/2+z	1.5-x,1/2-y,1-z	6.3	-1.17	0.21	0.20
M1···M8	-1/2+x,1.5-y,1/2+z	1-x,1-y,1-z	10.71	-1.31	0.36	0.23
M1···M9	2.5-x,1/2-y,1-z	2-x,-y,1-z	12.58	-1.43	0.42	0.25
M1···M10	2.5-x,1/2+y,1/2-z	1+x,1+y,z	10.47	-0.36	0.35	0.06
M1···M11	2-x,1+y,1/2-z	1/2+x,1.5+y,z	12.11	-0.50	0.40	0.09
M1···M12	1+x,y,z	1.5+x,1/2+y,z	19.22	-3.51	0.64	0.61
M1···M13	1/2+x,1/2+y,z	1+x,1+y,z	25.54	-0.57	0.85	0.10
M1···M14	x,1+y,z	1/2+x,1.5+y,z	19.61	-3.74	0.65	0.65
M1···M15	2.5-x,-1/2+y,1/2-z	1+x,y,z	10.47	-0.36	0.35	0.06
M1···M16	2-x,y,1/2-z	1/2+x,1/2+y,z	147.00	-27.40	4.89	4.79
M1···M17	1.5-x,1/2+y,1/2-z	x,1+y,z	147.11	-28.01	4.90	4.90
M1···M18	1-x,1+y,1/2-z	-1/2+x,1.5+y,z	10.98	-3.84	0.37	0.67
M1···M19	2-x,2-y,-z	1.5-x,1.5-y,-z	8.57	-0.66	0.29	0.12
M1···M20	1/2+x,1.5-y,-1/2+z	2-x,1-y,-z	10.71	-1.31	0.36	0.23
M1···M21	x,1-y,-1/2+z	1.5-x,1/2-y,-z	10.55	-1.05	0.35	0.18
M1···M22	1/2+x,1/2-y,-1/2+z	2-x,-y,-z	6.30	-1.17	0.21	0.20
M1···M23	1.5-x,1/2-y,-z	1-x,-y,-z	17.86	-1.43	0.59	0.25
M1···M24	1-x,-y,-z	1/2-x,-1/2-y,-z	8.95	-0.89	0.30	0.16
M1···M25	-1+x,-y,-1/2+z	1/2-x,-1/2-y,-z	7.84	-0.47	0.26	0.08
M1···M26	1-x,-1+y,1/2-z	-1/2+x,-1/2+y,z	10.98	-3.84	0.37	0.67
M1···M27	1/2-x,-1/2+y,1/2-z	-1+x,y,z	11.00	-0.40	0.37	0.07
M1···M28	x,-1+y,z	1/2+x,-1/2+y,z	19.61	-3.74	0.65	0.65
M1···M29	-1/2+x,-1/2+y,z	x,y,z	25.54	-0.57	0.85	0.10
M1···M30	-1+x,y,z	-1/2+x,1/2+y,z	19.22	-3.51	0.64	0.61
M1···M31	2-x,-1+y,1/2-z	1/2+x,-1/2+y,z	12.11	-0.50	0.40	0.09
M1···M32	1.5-x,-1/2+y,1/2-z	x,y,z	147.05	-28.77	4.90	5.03
M1···M33	1-x,y,1/2-z	-1/2+x,1/2+y,z	148.37	-28.28	4.94	4.95
M1···M34	1/2-x,1/2+y,1/2-z	-1+x,1+y,z	11.00	-0.40	0.37	0.07
M1···M35	-1/2+x,1/2-y,1/2+z	1-x,-y,1-z	10.55	-1.05	0.35	0.18
Total			1021.37	-194.41	34.00	34.00

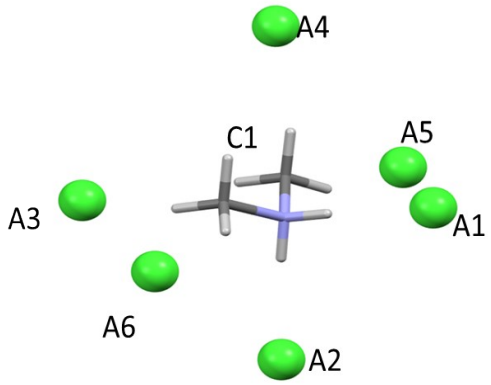


Figure S31. Anions that present contact area with C1 cation of salt **4b**.

Table S31. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **4b**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	8.38	-373880.05	0.00	3.10
C1···A2	½-x,1/2+y,-z	7.60	-373879.82	0.23	3.10
C1···A3	-1/2+x,1/2-y,-z	6.29	-373860.05	20.00	4.14
C1···A4	½-x,-1/2+y,-z	7.41	-373859.48	20.57	4.15
C1···A5	½-x,1/2-y,1/2+z	4.32	-373845.09	34.95	4.94
C1···A6	½-x,1/2-y,-1/2+z	4.32	-373845.09	34.95	4.94

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

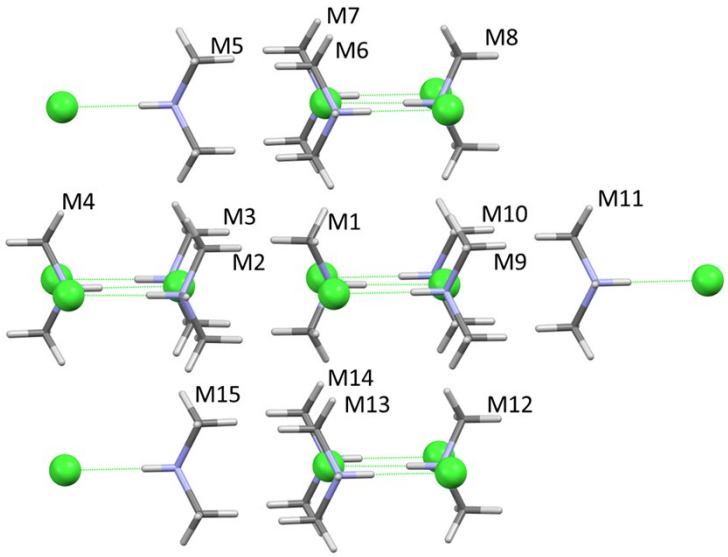


Figure S32. Supramolecular cluster of **4b**.

Table S32. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **4b**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	-x,-y,z	-x,-y,z	7.11	3.06	0.65	-0.44
M1···M3	-x,1-y,z	-x,1-y,z	12.24	5.72	1.12	-0.83
M1···M4	-0.5+x,0.5-y,-z	-0.5+x,0.5-y,-z	7.41	-13.65	0.68	1.98
M1···M5	-x,y,0.5-z	-x,y,0.5-z	8.49	3.11	0.78	-0.45
M1···M6	x,-y,0.5-z	x,-y,0.5-z	5.88	8.64	0.54	-1.25
M1···M7	x,1-y,0.5-z	x,1-y,0.5-z	8.76	7.73	0.80	-1.12
M1···M8	0.5-x,0.5-y,0.5+z	0.5-x,0.5-y,0.5+z	15.24	-20.07	1.40	2.91
M1···M9	0.5-x,-0.5+y,-z	0.5-x,-0.5+y,-z	21.01	-38.40	1.92	5.57
M1···M10	0.5-x,0.5+y,-z	0.5-x,0.5+y,-z	21.01	-38.40	1.92	5.57
M1···M11	0.5+x,0.5-y,-z	0.5+x,0.5-y,-z	7.41	-13.65	0.68	1.98
M1···M12	0.5-x,0.5-y,-0.5+z	0.5-x,0.5-y,-0.5+z	15.24	-20.07	1.40	2.91
M1···M13	x,-y,-0.5-z	x,-y,-0.5-z	5.88	8.64	0.54	-1.25
M1···M14	x,1-y,-0.5-z	x,1-y,-0.5-z	8.76	7.73	0.80	-1.12
M1···M15	-x,y,-0.5-z	-x,y,-0.5-z	8.49	3.11	0.78	-0.45
Total			152.93	-96.54	14.00	14.00

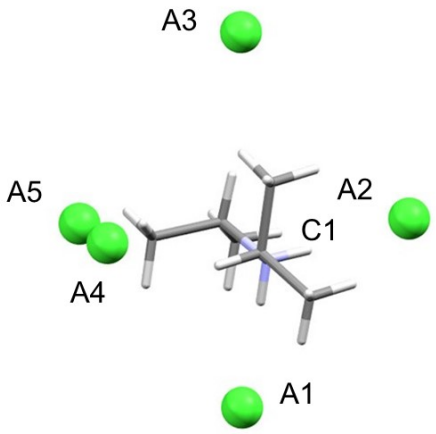


Figure S33. Anions that present contact area with C1 cation of salt **5b**.

Table S33. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **5b**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	10.14	-472462.44	0.00	3.1690
C1···A2	1.5-x,1/2+y,1/2-z	9.46	-472461.84	0.60	3.1759
C1···A3	x,1+y,z	6.72	-472434.57	27.87	4.7631
C1···A4	2-x,1-y,1-z	6.24	-472434.03	28.41	4.9022
C1···A5	1-x,1-y,1-z	5.15	-472419.99	42.45	6.0473

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

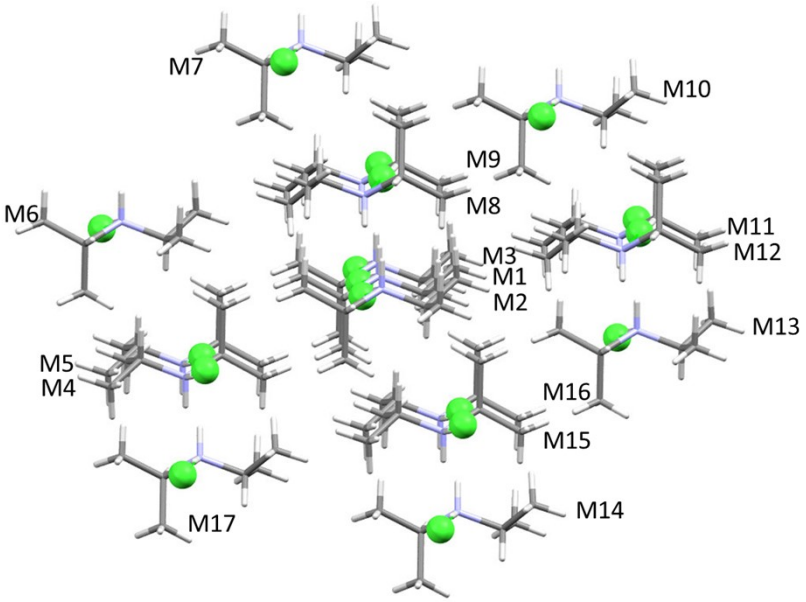


Figure S34. Supramolecular cluster of **5b**.

Table S34. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **5b**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	x,1+y,z	x,1+y,z	6.72	-9.34	0.49	1.84
M1···M3	x,-1+y,z	x,-1+y,z	6.72	-9.34	0.49	1.84
M1···M4	1-x,2-y,1-z	1-x,2-y,1-z	6.77	0.14	0.50	-0.03
M1···M5	1-x,1-y,1-z	1-x,1-y,1-z	24.04	-12.56	1.76	2.47
M1···M6	-1+x,y,z	-1+x,y,z	11.08	2.19	0.81	-0.43
M1···M7	-1/2+x,1.5-y,-1/2+z	-1/2+x,1.5-y,-1/2+z	0.64	-1.37	0.05	0.27
M1···M8	1.5-x,1/2+y,1/2-z	1.5-x,1/2+y,1/2-z	30.61	-13.31	2.24	2.62
M1···M9	1.5-x,-1/2+y,1/2-z	1.5-x,-1/2+y,1/2-z	30.61	-13.31	2.24	2.62
M1···M10	1/2+x,1.5-y,-1/2+z	1/2+x,1.5-y,-1/2+z	8.15	-1.95	0.60	0.38
M1···M11	2.5-x,1/2+y,1/2-z	2.5-x,1/2+y,1/2-z	7.62	0.33	0.56	-0.06
M1···M12	2.5-x,-1/2+y,1/2-z	2.5-x,-1/2+y,1/2-z	7.62	0.33	0.56	-0.06
M1···M13	1+x,y,z	1+x,y,z	11.08	2.19	0.81	-0.43
M1···M14	1/2+x,1.5-y,1/2+z	1/2+x,1.5-y,1/2+z	0.64	-1.37	0.05	0.27
M1···M15	2-x,2-y,1-z	2-x,2-y,1-z	20.53	0.33	1.50	-0.06
M1···M16	2-x,1-y,1-z	2-x,1-y,1-z	37.72	-22.42	2.76	4.41
M1···M17	-1/2+x,1.5-y,1/2+z	-1/2+x,1.5-y,1/2+z	8.15	-1.95	0.60	0.38
Total			218.7	-81.43	16.00	16.00

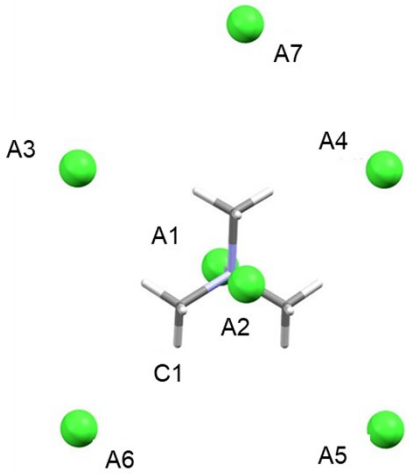


Figure S35. Anions that present contact area with C1 cation of salt **7b**.

Table S35. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **7b**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	8.66	398562.98	0.00	3.07
C1···A2	x,y,1+z	8.50	398542.85	20.13	4.084
C1···A3	1-x,1/2+y,1-z	6.56	398536.65	26.33	4.34
C1···A4	1-x,-1/2+y,1-z	6.56	398536.65	26.33	4.34
C1···A5	-x,-1/2+y,1-z	4.55	398523.89	39.09	5.10
C1···A6	-x,1/2+y,1-z	4.55	398523.89	39.09	5.10
C1···A7	1+x,y,1+z	0.01	398503.97	59.01	6.72

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

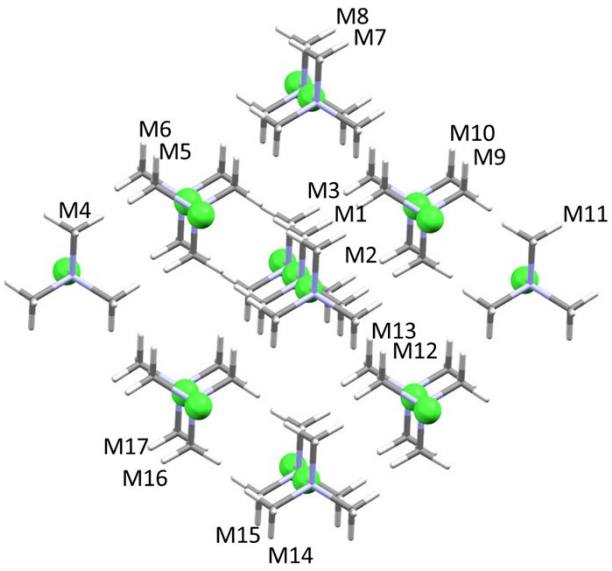


Figure S36. Supramolecular cluster of **7b**.

Table S36. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **7b**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	x,y,1+z	x,y,1+z	8.50	-11.92	0.79	2.51
M1···M3	x,y,-1+z	x,y,-1+z	8.50	-11.92	0.79	2.51
M1···M4	x,1+y,z	x,1+y,z	4.85	4.90	0.45	-1.03
M1···M5	1-x,1/2+y,2-z	1-x,1/2+y,2-z	16.98	2.38	1.58	-0.50
M1···M6	1-x,1/2+y,1-z	1-x,1/2+y,1-z	18.33	-23.67	1.70	4.99
M1···M7	1+x,y,1+z	1+x,y,1+z	0.01	-2.14	0.00	0.45
M1···M8	1+x,y,z	1+x,y,z	12.32	6.79	1.15	-1.43
M1···M9	1-x,-1/2+y,2-z	1-x,-1/2+y,2-z	16.98	2.38	1.58	-0.50
M1···M10	1-x,-1/2+y,1-z	1-x,-1/2+y,1-z	18.33	-23.67	1.70	4.99
M1···M11	x,-1+y,z	x,-1+y,z	4.85	4.90	0.45	-1.03
M1···M12	-x,-1/2+y,2-z	-x,-1/2+y,2-z	5.40	2.21	0.50	-0.47
M1···M13	-x,-1/2+y,1-z	-x,-1/2+y,1-z	19.65	-16.63	1.83	3.51
M1···M14	-1+x,y,1+z	-1+x,y,1+z	12.32	-1.85	1.15	0.39
M1···M15	-1+x,y,z	-1+x,y,z	0.01	6.79	0.00	-1.43
M1···M16	-x,1/2+y,2-z	-x,1/2+y,2-z	5.40	2.21	0.50	-0.47
M1···M17	-x,1/2+y,1-z	-x,1/2+y,1-z	19.65	-16.63	1.83	3.51
Total			172.08	-75.87	16.00	16.00

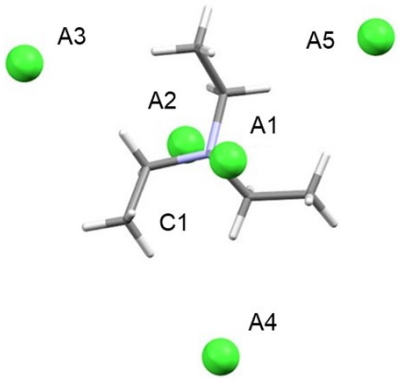


Figure S37. Anions that present contact area with C1 cation of salt **8b**.

Table S37. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **8b**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	10.21	472503.35	0.00	3.0980
C1···A2	x,y,1+z	8.06	472486.56	16.79	3.9000
C1···A3	-1+y,x,1/2+z	5.44	472474.83	28.52	4.7825
C1···A4	y,1+x,1/2+z	5.44	472474.83	28.52	4.7825
C1···A5	y,x,1/2+z	5.44	472474.82	28.53	4.7839

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

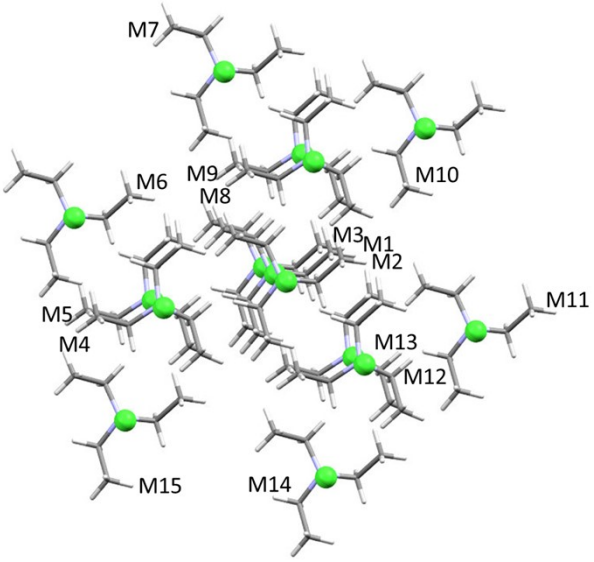


Figure S38. Supramolecular cluster of **8b**.

Table S38. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **8b**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	x,y,-1+z	x,y,-1+z	8.06	-10.69	0.52	4.82
M1···M3	x,y,1+z	x,y,1+z	8.06	-10.68	0.52	4.81
M1···M4	y,1+x,-1/2+z	y,1+x,-1/2+z	26.72	-3.92	1.74	1.77
M1···M5	y,1+x,1/2+z	y,1+x,1/2+z	26.72	-3.91	1.74	1.76
M1···M6	x,1+y,z	x,1+y,z	6.5	2.29	0.42	-1.03
M1···M7	-1+x,y,z	-1+x,y,z	6.5	2.30	0.42	-1.04
M1···M8	-1+y,x,-1/2+z	-1+y,x,-1/2+z	26.72	-3.93	1.74	1.77
M1···M9	-1+y,x,1/2+z	-1+y,x,1/2+z	26.72	-3.91	1.74	1.76
M1···M10	-1+x,-1+y,z	-1+x,-1+y,z	6.5	2.30	0.42	-1.04
M1···M11	x,-1+y,z	x,-1+y,z	6.50	2.30	0.42	-1.04
M1···M12	y,x,-1/2+z	y,x,-1/2+z	26.72	-3.91	1.74	1.76
M1···M13	y,x,1/2+z	y,x,1/2+z	26.72	-3.91	1.74	1.76
M1···M14	1+x,y,z	1+x,y,z	6.5	2.30	0.42	-1.04
M1···M15	1+x,1+y,z	1+x,1+y,z	6.5	2.31	0.42	-1.04
Total			215.44	-31.06	14.00	14.00

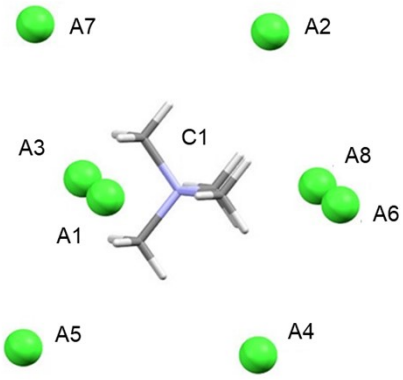


Figure S39. Anions that present contact area with C1 cation of salt **9b**.

Table S39. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **9b**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	-1/2+x,1-y,1-z	5.73	423152.70	0.00	4.25
C1···A2	x,y,-1+z	5.73	423152.70	0.00	4.25
C1···A3	½+x,1-y,1-z	5.73	423152.70	0.00	4.25
C1···A4	x,1+y,-1+z	5.73	423152.70	0.00	4.25
C1···A5	x,1+y,z	3.79	423138.26	14.45	5.09
C1···A6	½+x,1-y,-z	3.79	423138.26	14.45	5.09
C1···A7	x,y,z	3.79	423138.26	14.45	5.09
C1···A8	-1/2+x,1-y,-z	3.79	423138.26	14.45	5.09

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

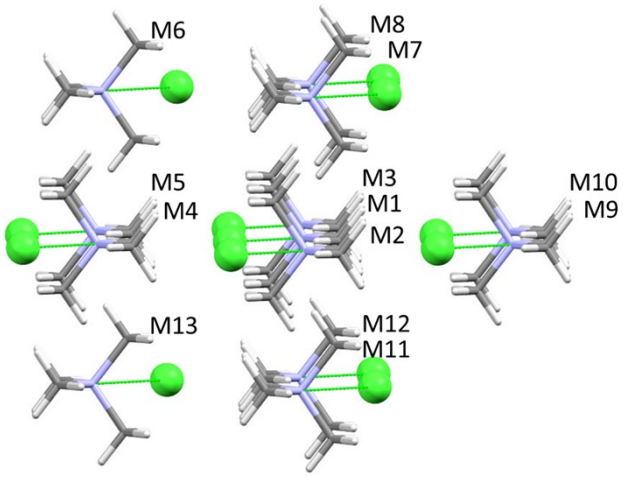


Figure S40. Supramolecular cluster of **9b**.

Table S40. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **9b**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	-1/2+x,1-y,1-z				
M1···M2	-1+x,y,z	-1.5+x,1-y,1-z	5.73	-15.45	0.39	1.13
M1···M3	1+x,y,z	1/2+x,1-y,1-z	5.73	-15.45	0.39	1.13
M1···M4	-1+x,y,1+z	-1.5+x,1-y,2-z	3.79	-14.01	0.26	1.02
M1···M5	x,y,1+z	-1/2+x,1-y,2-z	23	7.47	1.56	-0.54
M1···M6	1/2-y,x,1+z	x,y,z	7.59	-24.37	0.52	1.78
M1···M7	1/2-y,x,z	x,y,-1+z	29.88	-41.13	2.03	3.00
M1···M8	1.5-y,x,z	1+x,y,-1+z	18.42	5.23	1.25	-0.38
M1···M9	x,y,-1+z	-1/2+x,1-y,-z	23	7.47	1.56	-0.54
M1···M10	1+x,y,-1+z	1/2+x,1-y,-z	3.79	-14.01	0.26	1.02
M1···M11	1/2-y,1+x,z	x,1+y,-1+z	29.88	-41.13	2.03	3.00
M1···M12	1.5-y,1+x,z	x,1+y,-1+z	18.42	5.23	1.25	-0.38
M1···M13	1/2-y,1+x,1+z	x,1+y,z	7.59	-24.37	0.52	1.78
Total			176.82	-164.52	12.00	12.00

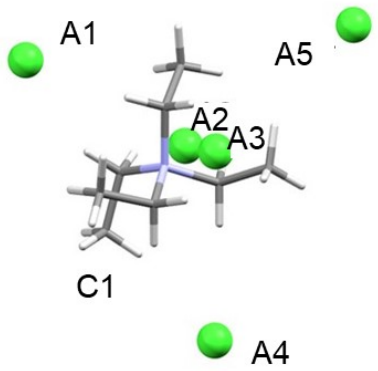


Figure S41. Anions that present contact area with C1 cation of salt **10b**.

Table S41. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **10b**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	x,y,z	9.39	521781.67	0.00	4.278
C1···A2	-x,-1/2+y,1.5-z	8.00	521781.06	0.62	4.320
C1···A3	1-x,-1/2+y,1.5-z	8.89	521780.90	0.77	4.335
C1···A4	x,1/2-y,1/2+z	7.82	521780.10	1.58	4.410
C1···A5	x,-1+y,z	4.08	521761.79	19.88	5.770

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

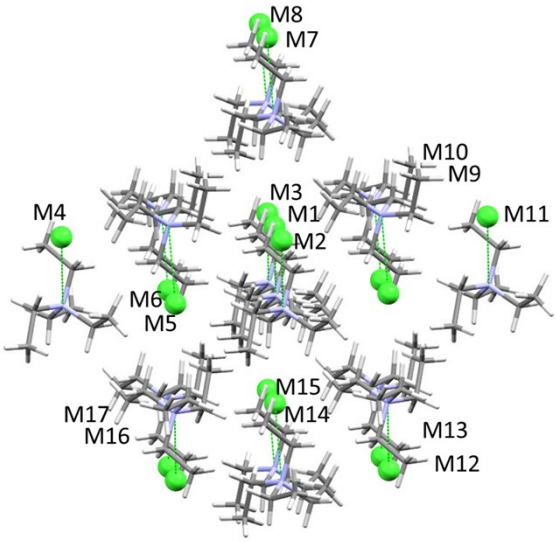


Figure S42. Supramolecular cluster of **10b**.

Table S42. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **10b**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	x,1+y,z	x,1+y,z	13.75	-5.69	0.90	0.86
M1···M3	x,-1+y,z	x,-1+y,z	13.75	-5.69	0.90	0.86
M1···M4	-1+x,y,z	-1+x,y,z	0.47	4.90	0.03	-0.74
M1···M5	-x,1/2+y,1.5-z	-x,1/2+y,1.5-z	28.28	-15.36	1.84	2.31
M1···M6	-x,-1/2+y,1.5-z	-x,-1/2+y,1.5-z	28.28	-15.36	1.84	2.31
M1···M7	x,1/2-y,-1/2+z	x,1/2-y,-1/2+z	16.83	-18.29	1.10	2.75
M1···M8	x,-1/2-y,-1/2+z	x,-1/2-y,-1/2+z	0.09	0.27	0.01	-0.04
M1···M9	1-x,1/2+y,1.5-z	1-x,1/2+y,1.5-z	30.07	-14.94	1.96	2.25
M1···M10	1-x,-1/2+y,1.5-z	1-x,-1/2+y,1.5-z	30.07	-14.94	1.96	2.25
M1···M11	1+x,y,z	1+x,y,z	0.47	4.90	0.03	-0.74
M1···M12	1-x,1-y,2-z	1-x,1-y,2-z	6.97	-5.16	0.45	0.78
M1···M13	1-x,-y,2-z	1-x,-y,2-z	28.53	0.98	1.86	-0.15
M1···M14	x,1/2-y,1/2+z	x,1/2-y,1/2+z	16.83	-18.29	1.10	2.75
M1···M15	x,-1/2-y,1/2+z	x,-1/2-y,1/2+z	0.09	0.27	0.01	-0.04
M1···M16	-x,1-y,2-z	-x,1-y,2-z	6.39	-4.73	0.42	0.71
M1···M17	-x,-y,2-z	-x,-y,2-z	24.48	0.86	1.60	-0.13
Total			245.35	-106.25	16.00	16.00

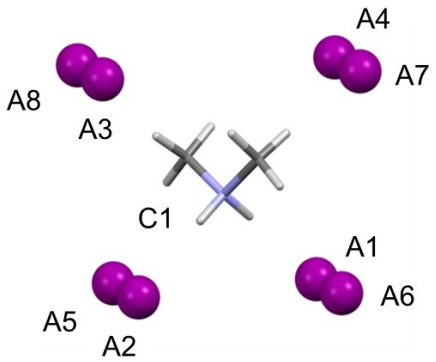


Figure S43. Anions that present contact area with C1 cation of salt **4c**.

Table S43. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **4c**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	1-x,y,1-z	7.05	-270743.92	0.00	3.526
C1···A2	x,y,z	7.05	-270743.92	0.00	3.526
C1···A3	1.5-x,-1/2+y,2-z	6.35	-270728.49	15.44	4.469
C1···A4	-1/2+x,-1/2+y,-1+z	6.35	-270728.49	15.44	4.469
C1···A5	x,y,-1+z	5.22	-270720.57	23.35	4.829
C1···A6	1-x,y,2-z	5.22	-270720.57	23.35	4.829
C1···A7	-1/2+x,-1/2+y,z	4.50	-270717.21	26.71	5.351
C1···A8	1.5-x,-1/2+y,1-z	4.50	-270717.21	26.71	5.351

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

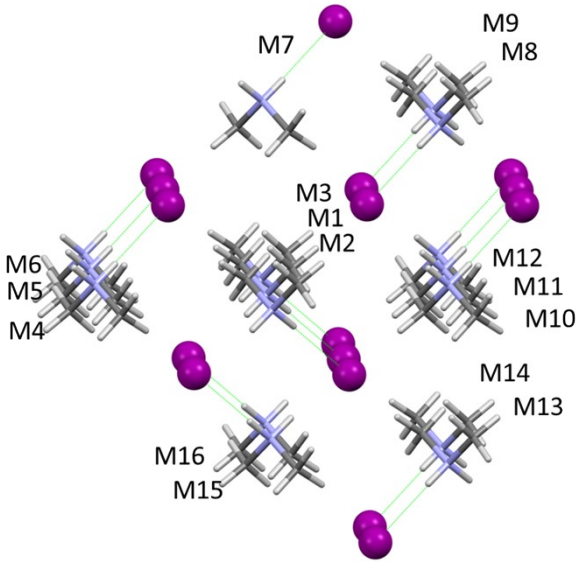


Figure S44. Supramolecular cluster of **4c**.

Table S44. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **4c.**

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1-x,y,1-z				
M1···M2	x,y,1+z	1-x,y,2-z	19.51	4.19	1.75	-0.61
M1···M3	x,y,-1+z	1-x,y,-z	19.51	4.19	1.75	-0.61
M1···M4	1.5-x,0.5-y,2-z	1.5-x,-0.5+y,2-z	6.35	-12.58	0.57	1.83
M1···M5	1.5-x,0.5-y,1-z	1.5-x,-0.5+y,1-z	19.83	-2.97	1.77	0.43
M1···M6	1.5-x,0.5-y,-z	1.5-x,-0.5+y,-z	0.05	0.99	0.00	-0.14
M1···M7	1-x,-y,1-z	1-x,-1+y,1-z	20.12	7.04	1.80	-1.02
M1···M8	-0.5+x,-0.5+y,z	-0.5+x,-0.5+y,z	4.5	-8.88	0.40	1.29
M1···M9	-0.5+x,-0.5+y,-1+z	-0.5+x,-0.5+y,-1+z	6.35	-5.62	0.57	0.82
M1···M10	0.5-x,0.5-y,2-z	0.5-x,-0.5+y,2-z	0.05	0.99	0.00	-0.14
M1···M11	0.5-x,0.5-y,1-z	0.5-x,-0.5+y,1-z	19.83	-2.97	1.77	0.43
M1···M12	0.5-x,0.5-y,-z	0.5-x,-0.5+y,-z	6.35	-12.58	0.57	1.83
M1···M13	-0.5+x,0.5+y,z	-0.5+x,0.5+y,z	4.5	-8.88	0.40	1.29
M1···M14	-0.5+x,0.5+y,-1+z	-0.5+x,0.5+y,-1+z	6.35	-5.62	0.57	0.82
M1···M15	1-x,1-y,1-z	x,y,z	23.36	-44.49	2.09	6.47
M1···M16	1-x,1-y,-z	x,y,-1+z	10.95	-15.91	0.98	2.32
Total			167.61	-103.09	15.00	15.00

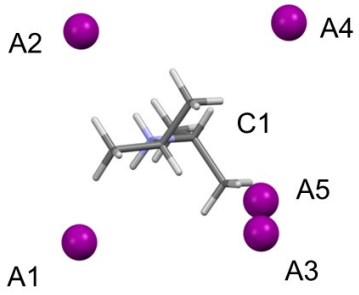


Figure S45. Anions that present contact area with C1 cation of salt **5c**.

Table S45. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **5c**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	1+x,y,z	11.4	-369220.35	0	3.586
C1···A2	1/2+x,1.5-y,-z	11.45	369217.25	3.10	3.578
C1···A3	1-x,-1/2+y,1/2-z	8.86	369199.44	20.91	5.058
C1···A4	x,y,z	8.26	369198.48	21.86	4.991
C1···A5	1-x,1/2+y,1/2-z	6.50	369186.69	33.66	6.215

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

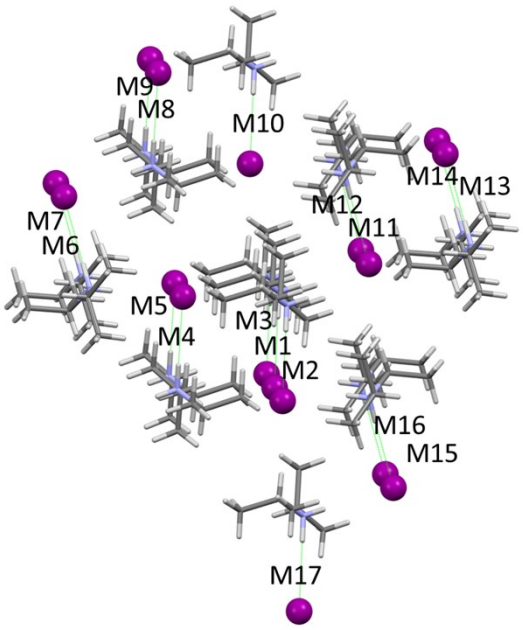


Figure S46. Supramolecular cluster of **5c**.

Table S46. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **5c**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1+x,y,z				
M1···M2	x,1+y,z	1+x,1+y,z	12.68	2.71	0.84	-0.56
M1···M3	x,-1+y,z	1+x,-1+y,z	12.68	2.71	0.84	-0.56
M1···M4	2-x,0.5+y,0.5-z	1-x,0.5+y,0.5-z	34.33	-18.87	2.28	3.93
M1···M5	2-x,-0.5+y,0.5-z	1-x,-0.5+y,0.5-z	34.33	-18.87	2.28	3.93
M1···M6	1.5-x,2-y,0.5+z	0.5-x,2-y,0.5+z	0.52	-1.97	0.03	0.41
M1···M7	1.5-x,1-y,0.5+z	0.5-x,1-y,0.5+z	8.61	-1.58	0.57	0.33
M1···M8	1-x,0.5+y,0.5-z	-x,0.5+y,0.5-z	14.14	1.11	0.94	-0.23
M1···M9	1-x,-0.5+y,0.5-z	-x,-0.5+y,0.5-z	14.14	1.11	0.94	-0.23
M1···M10	-1+x,y,z	x,y,z	8.26	-9.92	0.55	2.07
M1···M11	-0.5+x,1.5-y,-z	0.5+x,1.5-y,-z	31.52	-10.41	2.09	2.17
M1···M12	-0.5+x,0.5-y,-z	0.5+x,0.5-y,-z	10.39	0.51	0.69	-0.11
M1···M13	1.5-x,2-y,-0.5+z	0.5-x,2-y,-0.5+z	0.52	-1.97	0.03	0.41
M1···M14	1.5-x,1-y,-0.5+z	0.5-x,1-y,-0.5+z	8.61	-1.58	0.57	0.33
M1···M15	0.5+x,1.5-y,-z	1.5+x,1.5-y,-z	31.52	-10.41	2.09	2.17
M1···M16	0.5+x,0.5-y,-z	1.5+x,0.5-y,-z	10.39	0.51	0.69	-0.11
M1···M17	1+x,y,z	2+x,y,z	8.26	-9.92	0.55	2.07
Total			240.90	-76.86	16.00	16.00

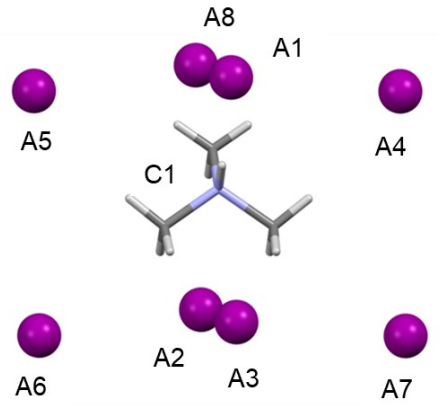


Figure S47. Anions that present contact area with C1 cation of salt **7c**.

Table S47. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **7c**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$[d]	N···X[e]
C1···A1	1+x,y,1+z	7.15	295318.51	0.00	3.500
C1···A2	x,y,z	7.43	295308.49	10.02	4.405
C1···A3	x,y,1+z	6.43	295302.14	16.37	4.663
C1···A4	1-x,-1/2+y,1-z	5.51	295301.89	16.62	4.675
C1···A5	1-x,1/2+y,1-z	5.51	295301.89	16.62	4.675
C1···A6	-x,1/2+y,1-z	4.82	295293.21	25.30	5.329
C1···A7	-x,-1/2+y,1-z	4.82	295293.21	25.30	5.329
C1···A8	1+x,y,z	4.24	295293.08	25.43	5.353

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

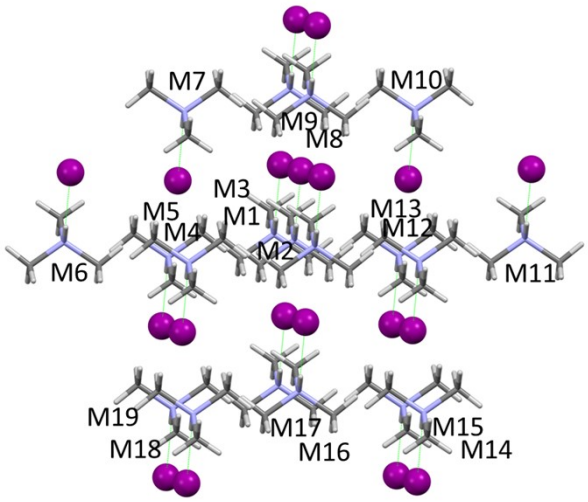


Figure S48. Supramolecular cluster of **7c**.

Table S48. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **7c**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	1+x,y,1+z	3.6			
M1···M2	x,y,1+z	1+x,y,2+z	4.24	-4.06	0.42	0.72
M1···M3	x,y,-1+z	1+x,y,z	4.24	-4.06	0.42	0.72
M1···M4	1-x,0.5+y,2-z	-x,0.5+y,1-z	24.84	-19.78	2.43	3.53
M1···M5	1-x,0.5+y,1-z	-x,0.5+y,-z	20.21	2.70	1.98	-0.48
M1···M6	x,1+y,z	1+x,1+y,1+z	0.35	4.68	0.03	-0.83
M1···M7	2-x,0.5+y,2-z	1-x,0.5+y,1-z	11.01	-22.24	1.08	3.96
M1···M8	1+x,y,1+z	2+x,y,2+z	7.43	-14.53	0.73	2.59
M1···M9	1+x,y,z	2+x,y,1+z	22.94	0.86	2.25	-0.15
M1···M10	2-x,-0.5+y,2-z	1-x,-0.5+y,1-z	11.01	-22.28	1.08	3.97
M1···M11	x,-1+y,z	1+x,-1+y,1+z	0.35	4.68	0.03	-0.83
M1···M12	1-x,-0.5+y,2-z	-x,-0.5+y,1-z	24.84	-19.79	2.43	3.53
M1···M13	1-x,-0.5+y,1-z	-x,-0.5+y,-z	20.21	2.71	1.98	-0.48
M1···M14	-x,-0.5+y,2-z	-1-x,-0.5+y,1-z	0.28	-1.38	0.03	0.25
M1···M15	-x,-0.5+y,1-z	-1-x,-0.5+y,-z	0.61	3.27	0.06	-0.58
M1···M16	-1+x,y,z	x,y,1+z	22.94	0.86	2.25	-0.15
M1···M17	-1+x,y,-1+z	x,y,z	7.43	-14.53	0.73	2.59
M1···M18	-x,0.5+y,2-z	-1-x,0.5+y,1-z	0.28	-1.38	0.03	0.25
M1···M19	-x,0.5+y,1-z	-1-x,0.5+y,-z	0.61	3.27	0.06	-0.58
Total			183.82	-101.01	18.00	18.00

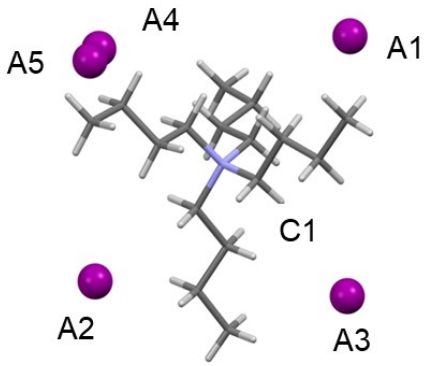


Figure S49. Anions that present contact area with C1 cation of salt **12c**.

Table S49. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **12c**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	-1/2+x,-1/2+y,z	11.29	-615834.14	0.00	5.048
C1···A2	x,y,z	10.95	-615833.85	0.29	5.067
C1···A3	1.5-x,1/2-y,1-z	10.98	-615833.77	0.37	5.079
C1···A4	1-x,1-y,1-z	11.07	-615833.57	0.57	5.090
C1···A5	1-x,y,1/2-z	1.68	-615802.34	31.79	9.124

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

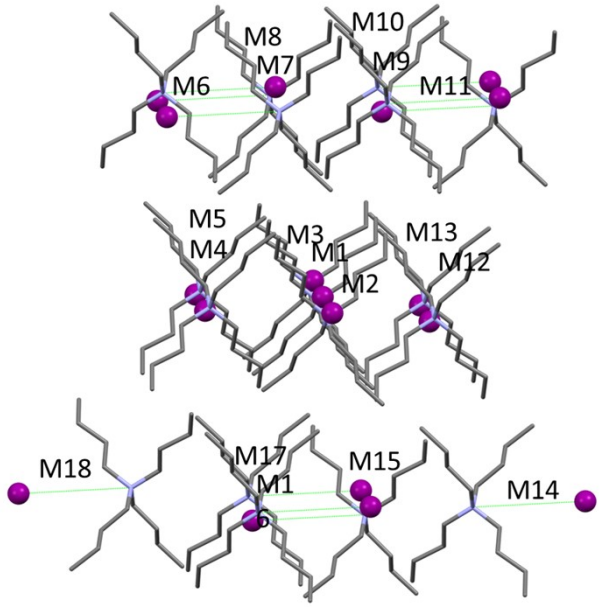


Figure S50. Supramolecular cluster of **12c**. Hydrogens were omitted for clarity.

Table S50. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **12c**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	-0.5+x,-0.5+y,z				
M1···M2	-0.5+x,-0.5+y,z	-1+x,-1+y,z	11.00	-15.98	0.42	1.93
M1···M3	0.5+x,0.5+y,z	x,y,z	11.00	-15.98	0.42	1.93
M1···M4	1-x,-y,1-z	1.5-x,0.5-y,1-z	73.96	-39.77	2.86	4.81
M1···M5	1.5-x,0.5-y,1-z	2-x,1-y,1-z	51.41	-3.05	1.99	0.37
M1···M6	x,-y,-0.5+z	-0.5+x,0.5-y,-0.5+z	7.65	-0.94	0.30	0.11
M1···M7	0.5-x,-0.5+y,0.5-z	1-x,-1+y,0.5-z	13.03	-4.46	0.50	0.54
M1···M8	1-x,y,0.5-z	1.5-x,-0.5+y,0.5-z	22.77	-1.66	0.88	0.20
M1···M9	-0.5+x,0.5-y,-0.5+z	-1+x,1-y,-0.5+z	25.30	-4.06	0.98	0.49
M1···M10	x,1-y,-0.5+z	-0.5+x,1.5-y,-0.5+z	8.70	0.59	0.34	-0.07
M1···M11	0.5-x,0.5+y,0.5-z	1-x,y,0.5-z	13.03	-4.46	0.50	0.54
M1···M12	0.5-x,0.5-y,1-z	1-x,1-y,1-z	73.79	-39.70	2.85	4.80
M1···M13	1-x,1-y,1-z	1.5-x,1.5-y,1-z	52.66	-2.47	2.03	0.30
M1···M14	x,1-y,0.5+z	-0.5+x,1.5-y,0.5+z	8.70	0.59	0.34	-0.07
M1···M15	1-x,y,1.5-z	1.5-x,-0.5+y,1.5-z	30.25	-4.89	1.17	0.59
M1···M16	x,-y,0.5+z	-0.5+x,0.5-y,0.5+z	7.65	-0.94	0.30	0.11
M1···M17	0.5+x,0.5-y,0.5+z	x,1-y,0.5+z	25.3	-4.06	0.98	0.49
M1···M18	2-x,y,1.5-z	2.5-x,-0.5+y,1.5-z	3.96	0.72	0.15	-0.09
Total			440.16	-140.52	17.00	17.00

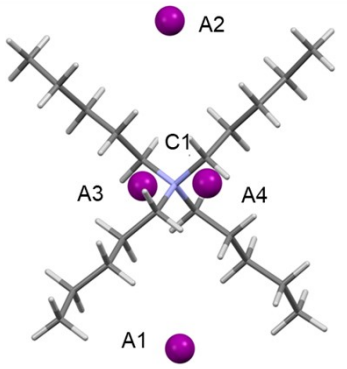


Figure S51. Anions that present contact area with C1 cation of salt **13c**.

Table S51. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **13c**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$ [d]	N···X[e]
C1···A1	-1/2+x,y,-z	7.77	-714707.66824324	2.11	4.750
C1···A2	-1/2+x,y,1-z	7.77	-714707.66825130	2.11	4.750
C1···A3	-1+x,y,z	15.03	-714709.78323328	0.0000109	5.405
C1···A4	x,y,z	15.03	-714709.78324419	0.0000000	5.405
C1···A5	-1/2+x,y,-z	7.77	-714707.66824324	2.11	4.750

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

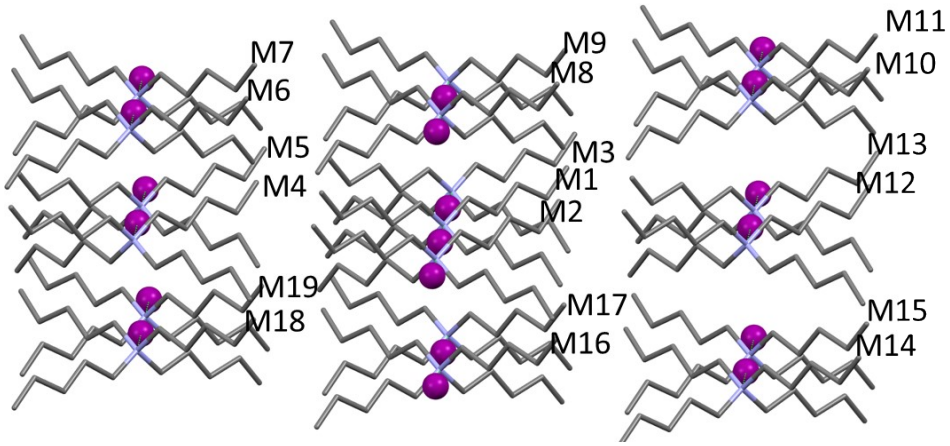


Figure S52. Supramolecular cluster of **13c.** Hydrogens were omitted for clarity.

Table S52. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **13c**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1···M2	1+x,y,z	1+x,y,z	50.70	-21.06	1.66	2.62
M1···M3	-1+x,y,z	-1+x,y,z	50.70	-21.06	1.66	2.62
M1···M4	1/2-x,1-y,z	1/2-x,1-y,z	21.82	-6.45	0.72	0.80
M1···M5	-1/2-x,1-y,z	-1/2-x,1-y,z	21.82	-6.45	0.72	0.80
M1···M6	1-x,1-y,-z	1-x,1-y,-z	12.67	-2.01	0.42	0.25
M1···M7	-x,1-y,-z	-x,1-y,-z	2.64	-2.83	0.09	0.35
M1···M8	1/2+x,y,-z	1/2+x,y,-z	74.62	-14.41	2.45	1.79
M1···M9	-1/2+x,y,-z	-1/2+x,y,-z	74.62	-14.41	2.45	1.79
M1···M10	-x,-y,-z	-x,-y,-z	2.64	-2.83	0.09	0.35
M1···M11	-1-x,-y,-z	-1-x,-y,-z	12.67	-2.01	0.42	0.25
M1···M12	1/2-x,-y,z	1/2-x,-y,z	21.82	-6.45	0.72	0.80
M1···M13	-1/2-x,-y,z	-1/2-x,-y,z	21.82	-6.45	0.72	0.80
M1···M14	1-x,-y,1-z	1-x,-y,1-z	12.67	-2.01	0.42	0.25
M1···M15	-x,-y,1-z	-x,-y,1-z	2.64	-2.83	0.09	0.35
M1···M16	1/2+x,y,1-z	1/2+x,y,1-z	74.62	-14.41	2.45	1.79
M1···M17	-1/2+x,y,1-z	-1/2+x,y,1-z	74.62	-14.41	2.45	1.79
M1···M18	-x,1-y,1-z	-x,1-y,1-z	2.64	-2.83	0.09	0.35
M1···M19	-1-x,1-y,1-z	-1-x,1-y,1-z	12.67	-2.01	0.42	0.25
Total			548.40	-144.89	18.00	18.00

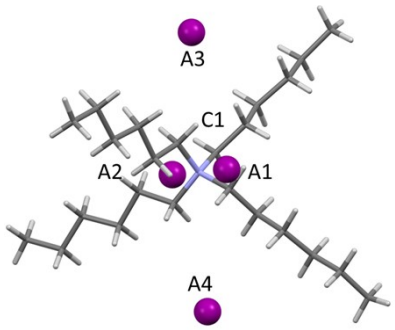


Figure S53. Anions that present contact area with C1 cation of salt **14c**.

Table S53. Symmetry codes, contact area, absolute stabilization energies and N···X distances of each C1···A pair of salt **14c**.

C1···A	Anion symmetry code[a]	$C_{C1\cdots A}$ [b]	$G_{C1\cdots A}$ [c]	$\lvert G_{C1\cdots A1} - G_{C1\cdots A}\rvert$[d]	N···X[e]
C1···A1	x,y,z	12.08	-813042.44972188	0.00000000	5.012
C1···A2	x,1+y,z	12.08	-813042.44972186	0.00000002	5.012
C1···A3	1/2-x,1/2+y,z	11.62	-813042.13406789	0.31565400	5.038
C1···A4	1.5-x,1/2+y,z	11.62	-813042.13406789	0.31565400	5.038

[a]Cation C1 symmetry code: *x,y,z*. [b]Contact area between C1 and each considered anion, in Å^2. [c]Absolute energy of each C1···A pair, in a.u.; [d]Difference of absolute energies between the most stable pair and each considered pair, in kcal mol^{-1}. [e]Distance, in Å.

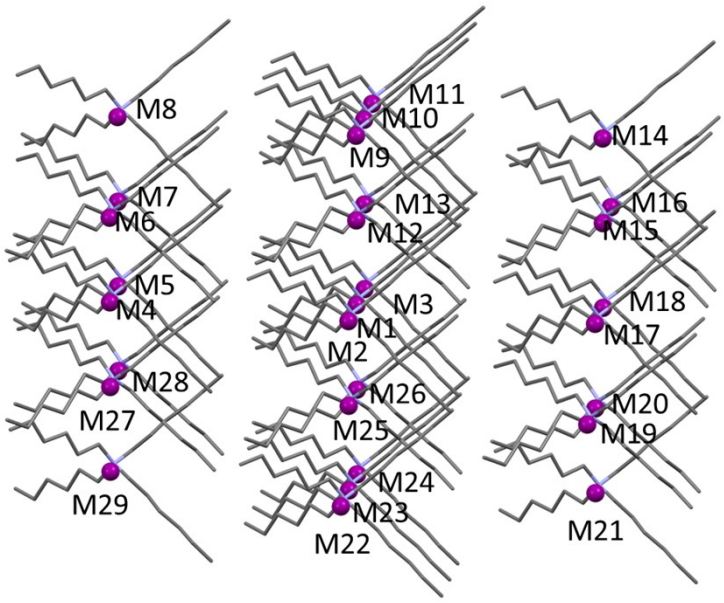


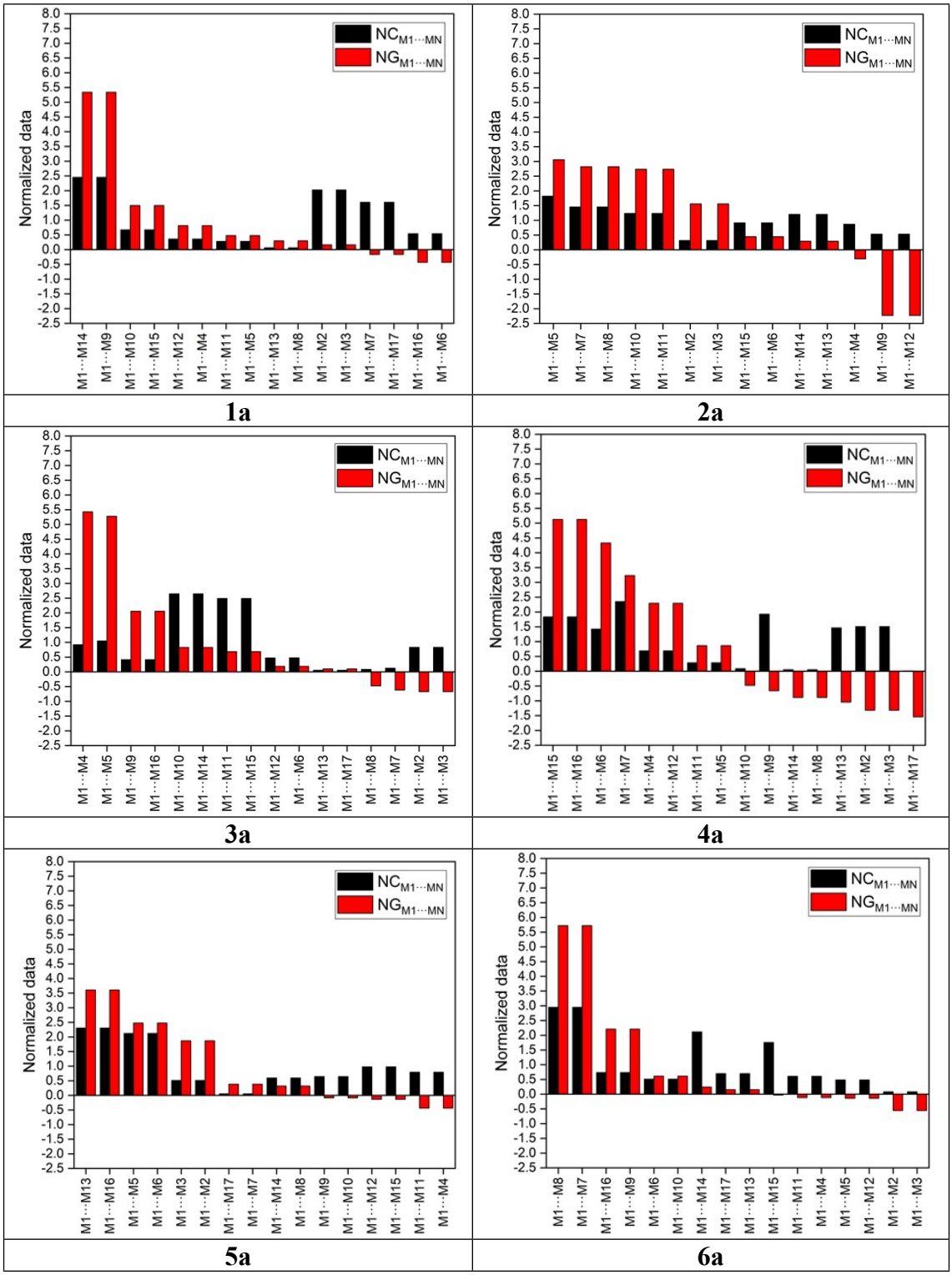
Figure S54. Supramolecular cluster of **14c.** Hydrogens were omitted for clarity.

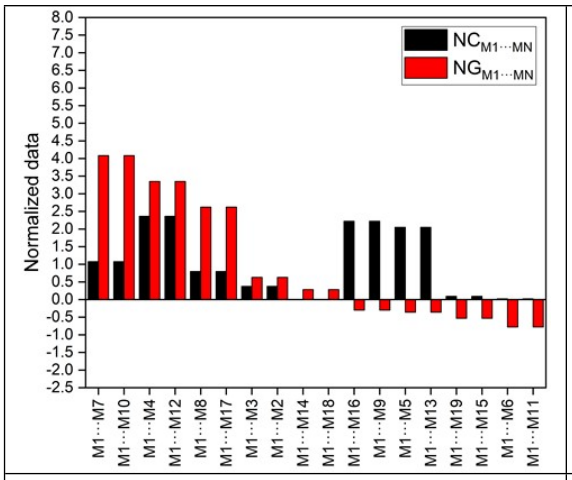
Table S54. Symmetry codes, contact area ($C_{M1\cdots MN}$, in Å^2) and energetic data ($G_{M1\cdots MN}$, in kcal mol^{-1}) for the supramolecular cluster of salt **14c**.

Dimer	Cation symmetry code	Anion symmetry code	$C_{M1\cdots MN}$	$G_{M1\cdots MN}$	$NC_{M1\cdots MN}$	$NG_{M1\cdots MN}$
M1	x,y,z	x,y,z				
M1⋯M2	x,-1+y,z	x,-1+y,z	29.55	-18.77	1.30	3.96
M1⋯M3	x,1+y,z	x,1+y,z	29.55	-18.77	1.30	3.96
M1⋯M4	x,-1/2+y,-1/2+z	x,-1/2+y,-1/2+z	15.17	-0.97	0.67	0.21
M1⋯M5	x,1/2+y,-1/2+z	x,1/2+y,-1/2+z	15.17	-0.97	0.67	0.21
M1⋯M6	1/2-x,-1+y,-1/2+z	1/2-x,-1+y,-1/2+z	8.63	-1.33	0.38	0.28
M1⋯M7	1/2-x,y,-1/2+z	1/2-x,y,-1/2+z	10.17	-1.92	0.45	0.41
M1⋯M8	-1+x,-1/2+y,-1/2+z	-1+x,-1/2+y,-1/2+z	5.28	0.02	0.23	0.00
M1⋯M9	-1+x,-1+y,z	-1+x,-1+y,z	0.16	-1.52	0.01	0.32
M1⋯M10	-1+x,y,z	-1+x,y,z	17.48	1.41	0.77	-0.30
M1⋯M11	-1+x,1+y,z	-1+x,1+y,z	0.32	-1.34	0.01	0.28
M1⋯M12	1/2-x,-1/2+y,z	1/2-x,-1/2+y,z	96.44	-18.82	4.23	3.98
M1⋯M13	1/2-x,1/2+y,z	1/2-x,1/2+y,z	96.44	-18.82	4.23	3.98
M1⋯M14	-1+x,-1/2+y,1/2+z	-1+x,-1/2+y,1/2+z	5.28	0.02	0.23	0.00
M1⋯M15	1/2-x,y,1/2+z	1/2-x,y,1/2+z	10.17	-1.92	0.45	0.41
M1⋯M16	1/2-x,1+y,1/2+z	1/2-x,1+y,1/2+z	8.63	-1.33	0.38	0.28
M1⋯M17	x,-1/2+y,1/2+z	x,-1/2+y,1/2+z	15.17	-0.97	0.67	0.21
M1⋯M18	x,1/2+y,1/2+z	x,1/2+y,1/2+z	15.17	-0.97	0.67	0.21
M1⋯M19	1.5-x,-1+y,1/2+z	1.5-x,-1+y,1/2+z	8.63	-1.33	0.38	0.28
M1⋯M20	1.5-x,y,1/2+z	1.5-x,y,1/2+z	10.17	-1.92	0.45	0.41
M1⋯M21	1+x,1/2+y,1/2+z	1+x,1/2+y,1/2+z	5.28	0.02	0.23	0.00
M1⋯M22	1+x,-1+y,z	1+x,-1+y,z	0.32	-1.34	0.01	0.28
M1⋯M23	1+x,y,z	1+x,y,z	17.48	1.41	0.77	-0.30
M1⋯M24	1+x,1+y,z	1+x,1+y,z	0.16	-1.52	0.01	0.32
M1⋯M25	1.5-x,-1/2+y,z	1.5-x,-1/2+y,z	96.44	-18.82	4.23	3.98
M1⋯M26	1.5-x,1/2+y,z	1.5-x,1/2+y,z	96.44	-18.82	4.23	3.98
M1⋯M27	1.5-x,y,-1/2+z	1.5-x,y,-1/2+z	10.17	-1.92	0.45	0.41
M1⋯M28	1.5-x,1+y,-1/2+z	1.5-x,1+y,-1/2+z	8.63	-1.33	0.38	0.28
M1⋯M29	1+x,1/2+y,-1/2+z	1+x,1/2+y,-1/2+z	5.28	0.02	0.23	0.00
Total			637.78	-132.60	28.00	28.00

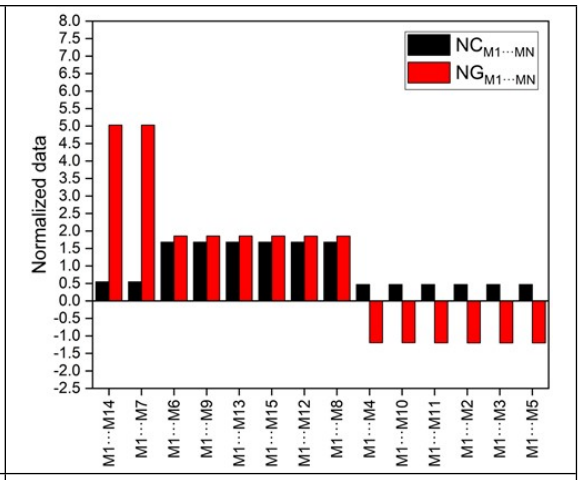
2. Normalized Data

Table S55. Normalized contact area (NC) and stabilization energy (NG) data of all 27 salts.

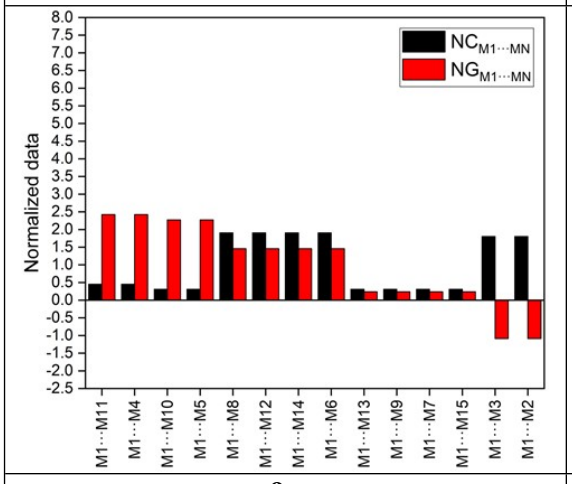




7a



8a



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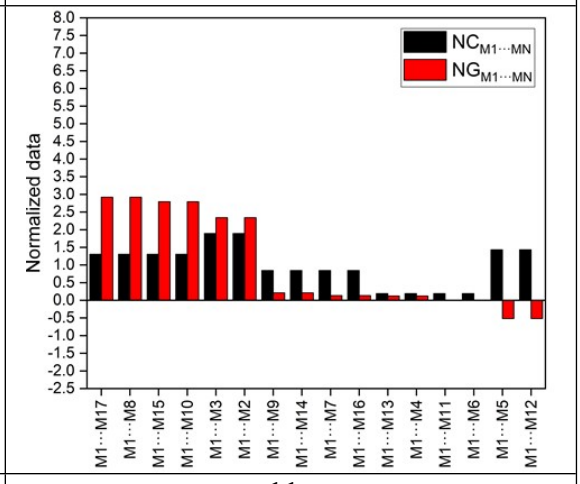

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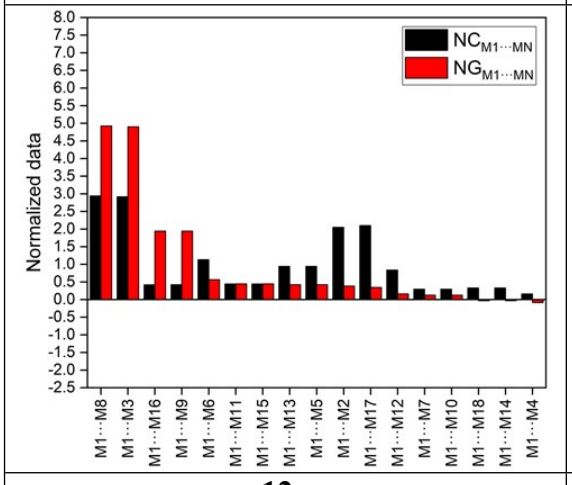
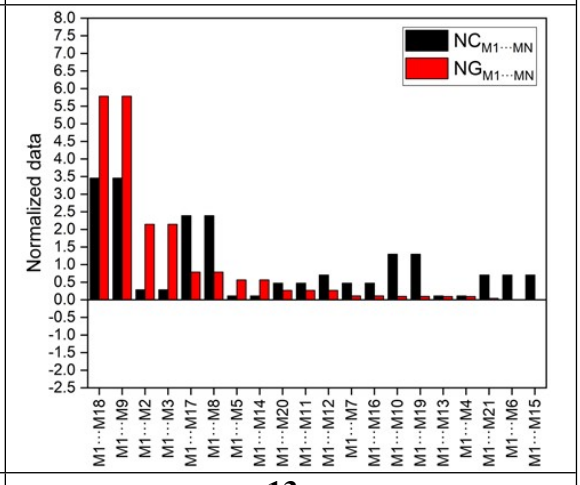
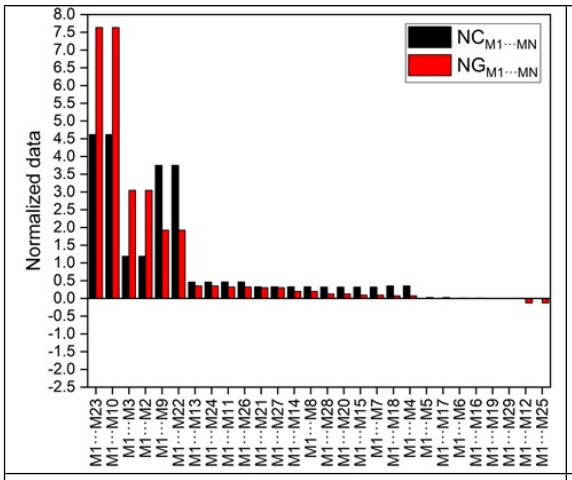


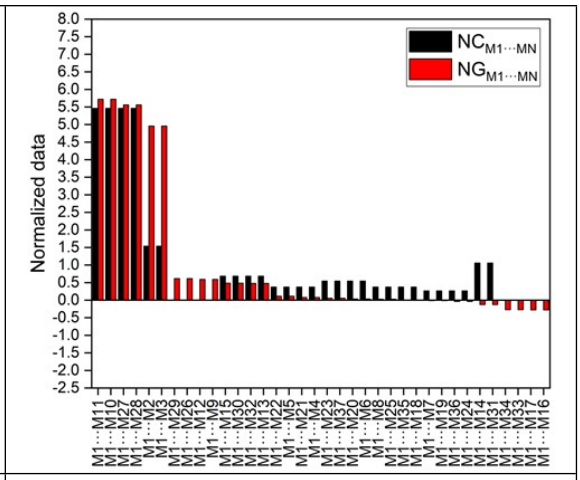
12a



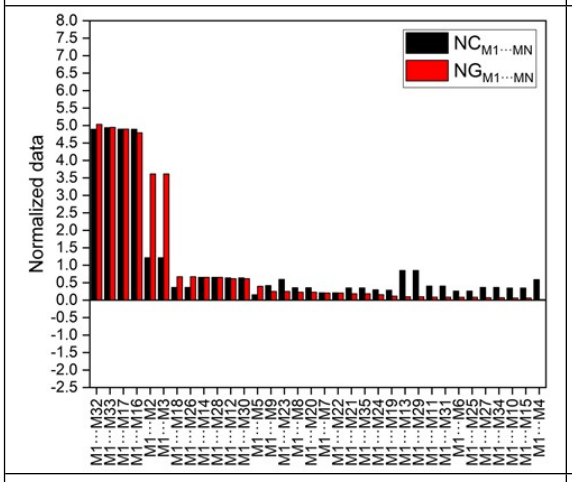
13a



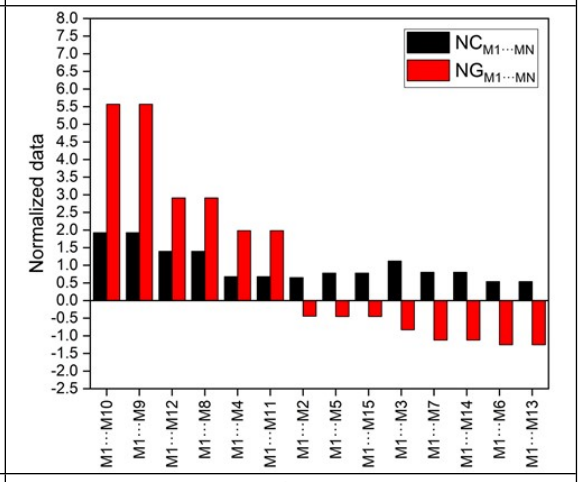
15a



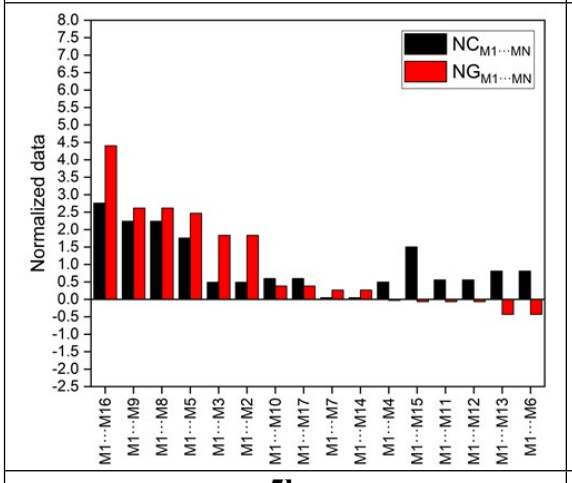
16a



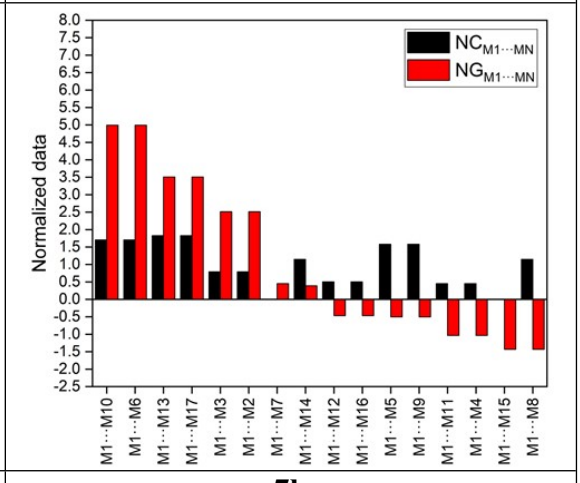
17a



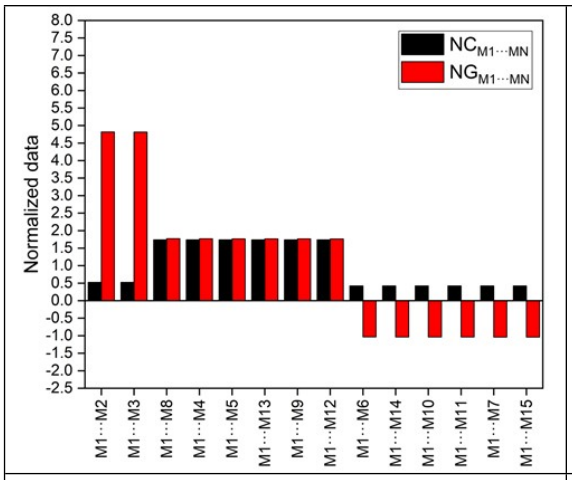
4b



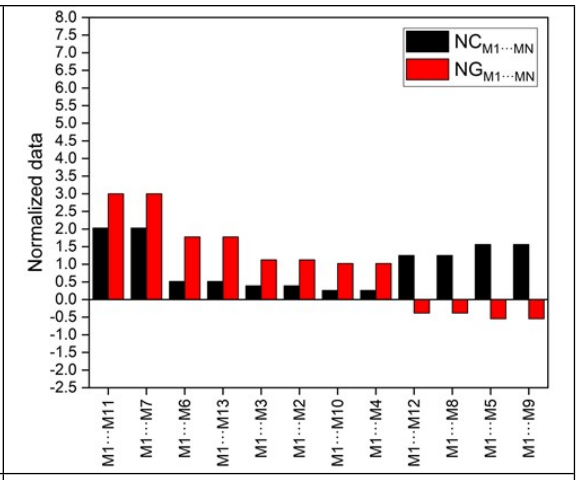
5b



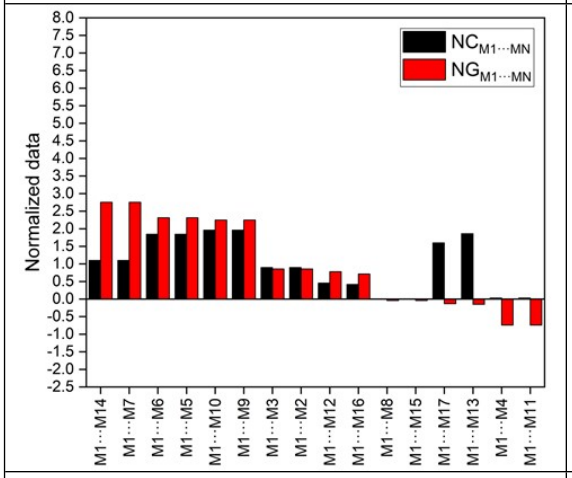
7b



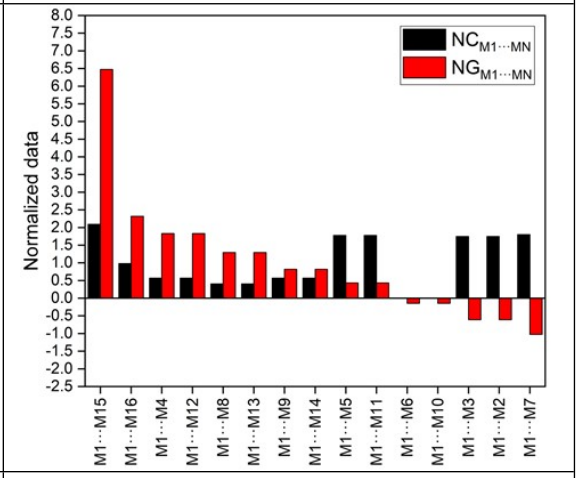
8b



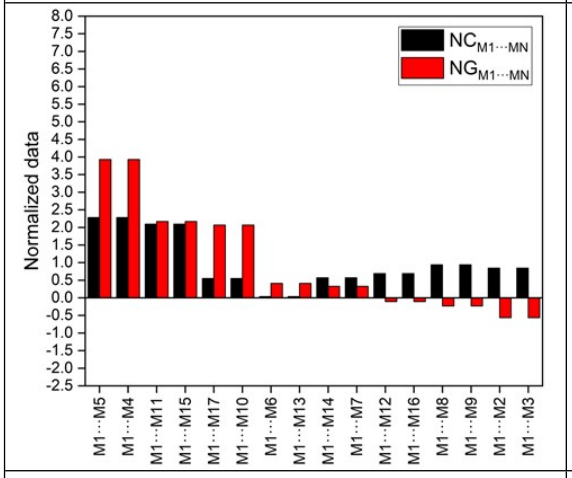
9b



10b



4c



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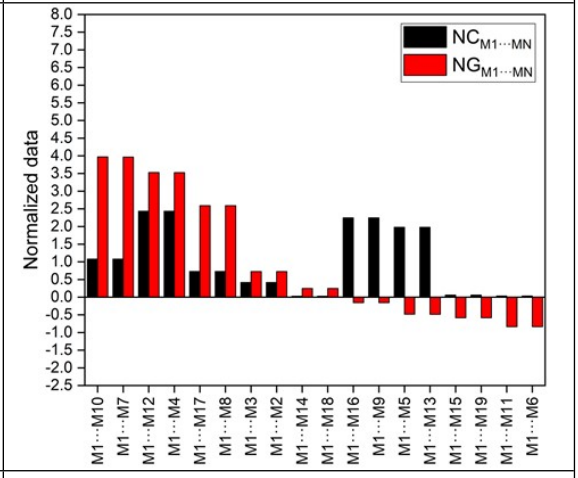

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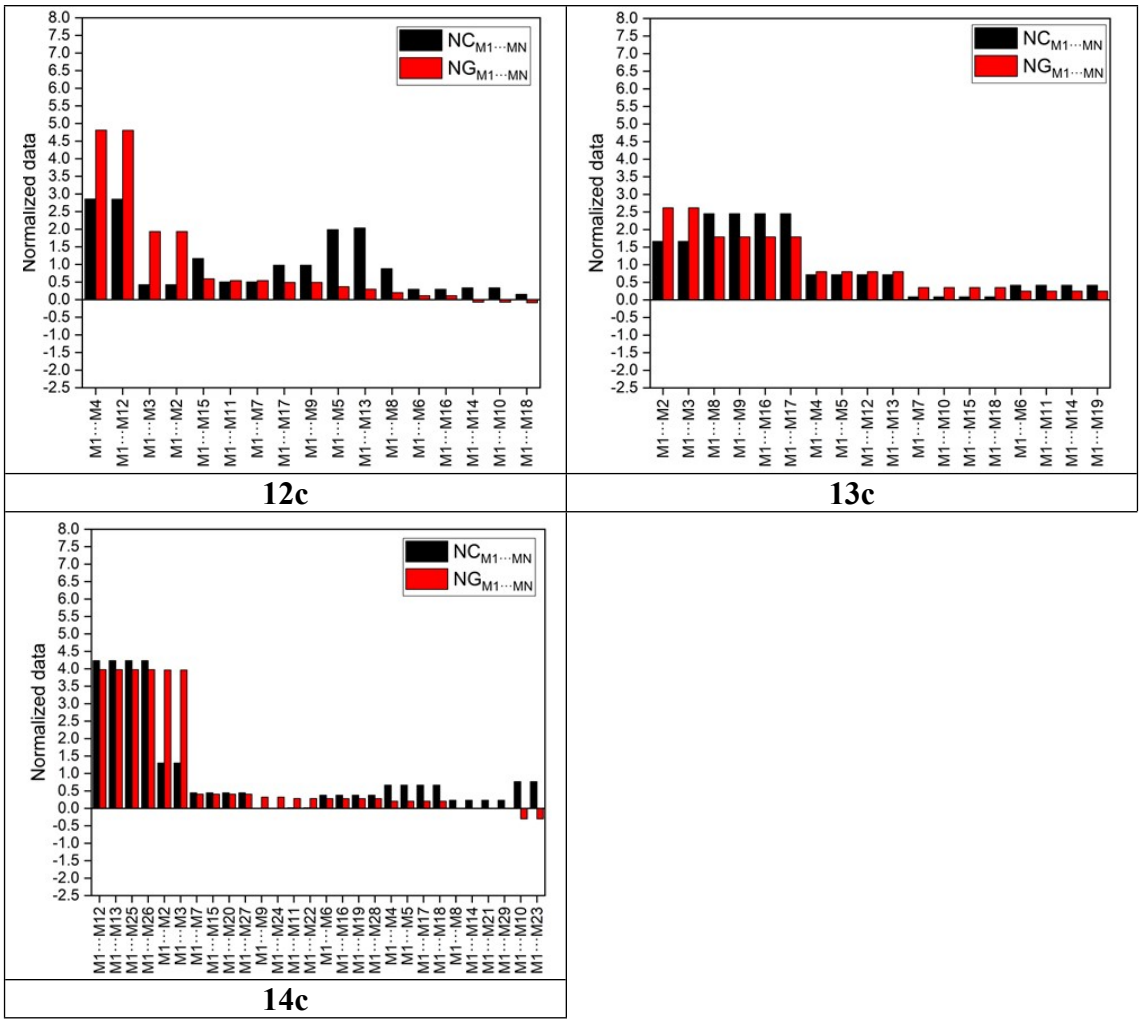

3. Molecular Electrostatic Potential (MEP)

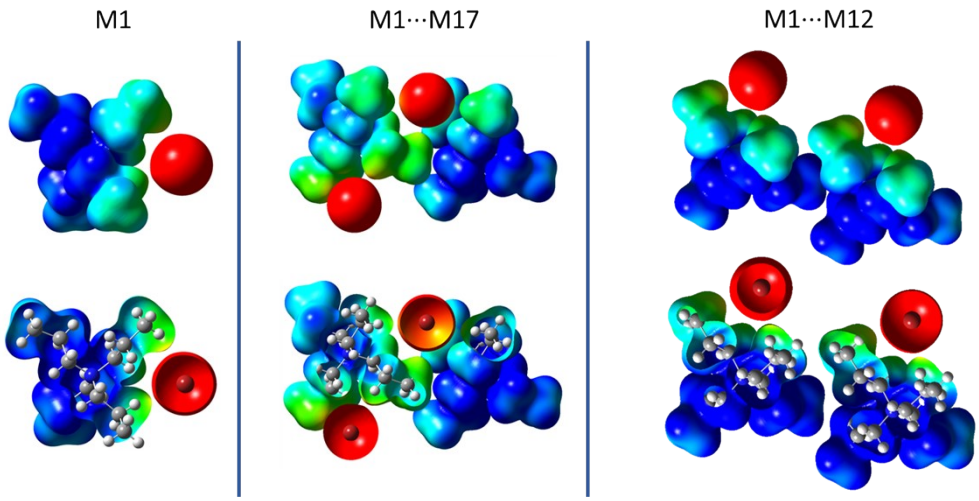

Figure S55. MEPs surfaces of salt **11a.** M1, M1···M17 the most stabilizing dimer and M1···M12 the least stabilizing dimer.

4. Crystallization Mechanisms Proposals

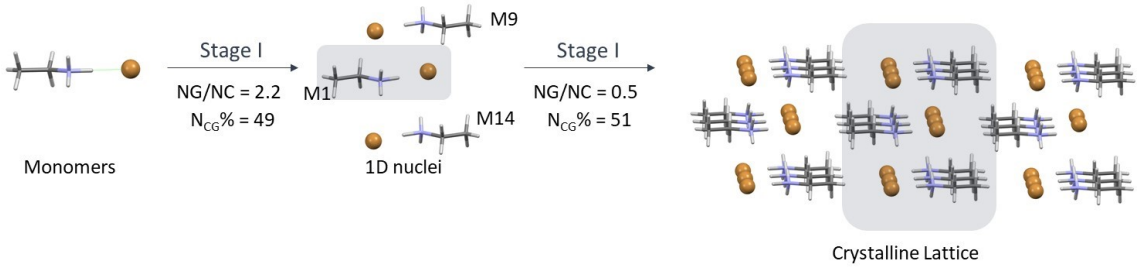

Figure S56. Crystallization mechanism proposal of salt **1a**.

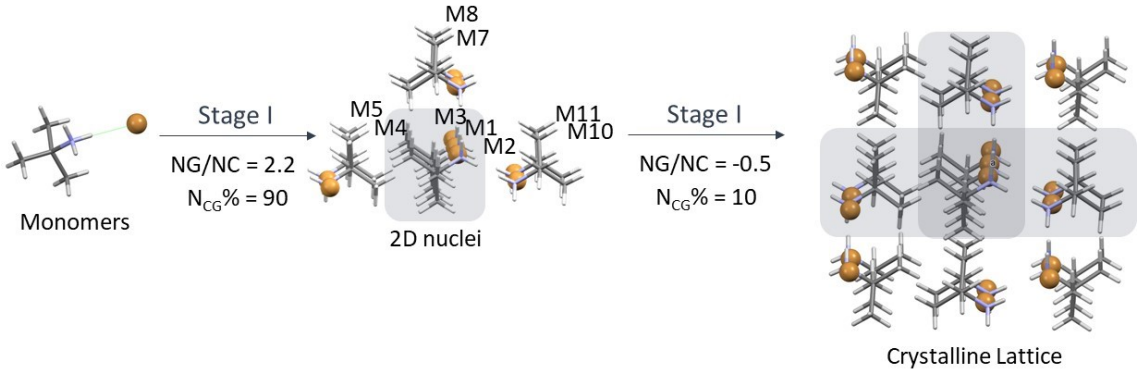

Figure S57. Crystallization mechanism proposal of salt **2a**.

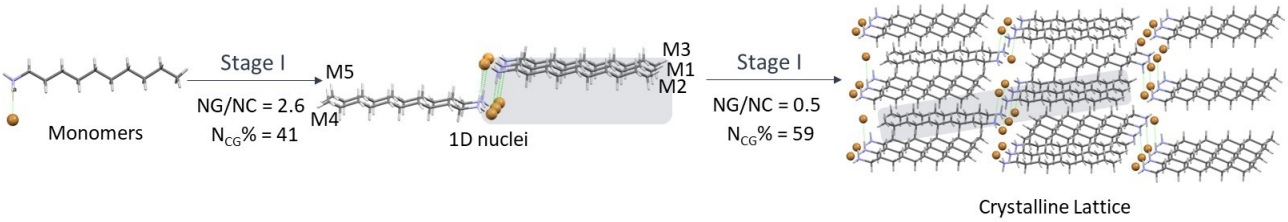

Figure S58. Crystallization mechanism proposal of salt **3a**.

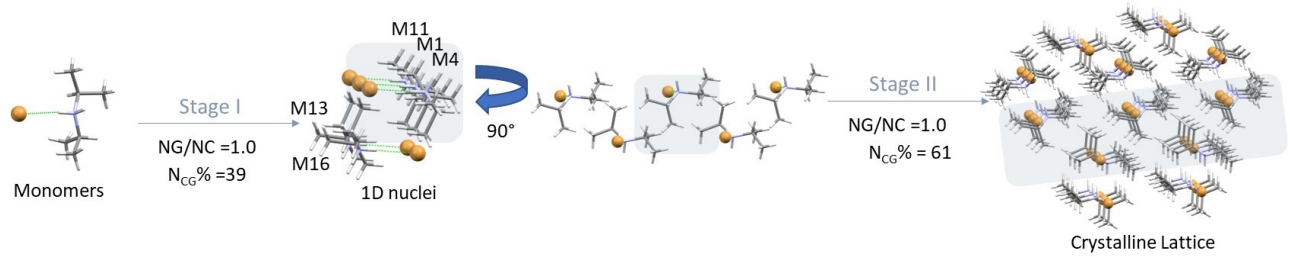

Figure S59. Crystallization mechanism proposal of salt **5a**.

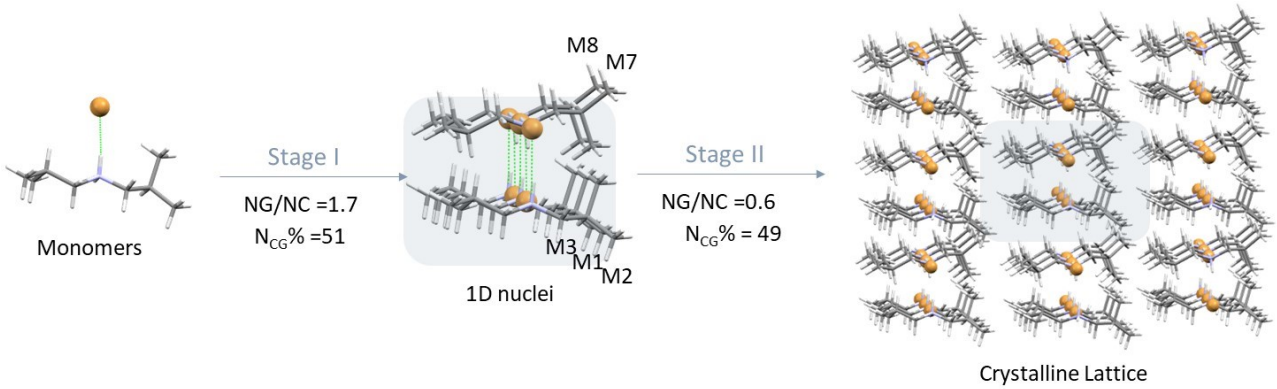

Figure S60. Crystallization mechanism proposal of salt **6a**.

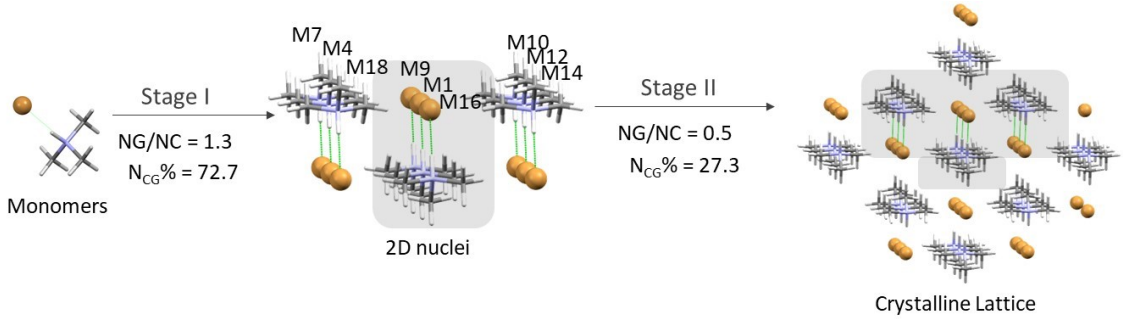

Figure S61. Crystallization mechanism proposal of salt **7a**.

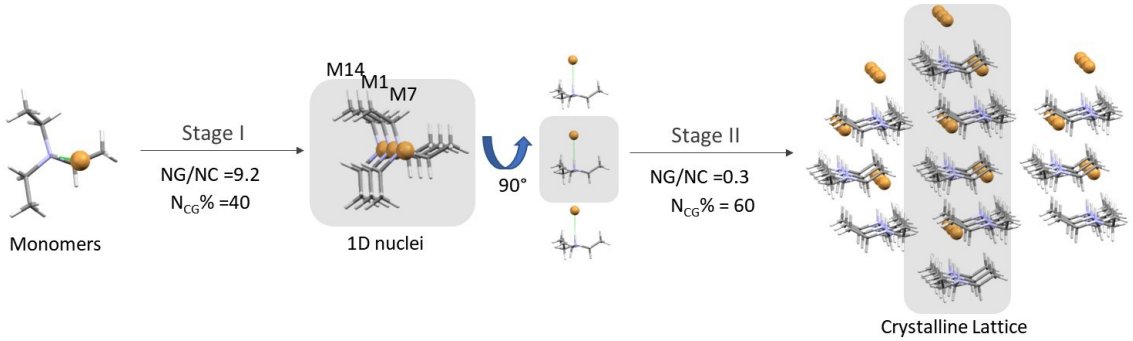

Figure S62 Crystallization mechanism proposal of salt **8a**.

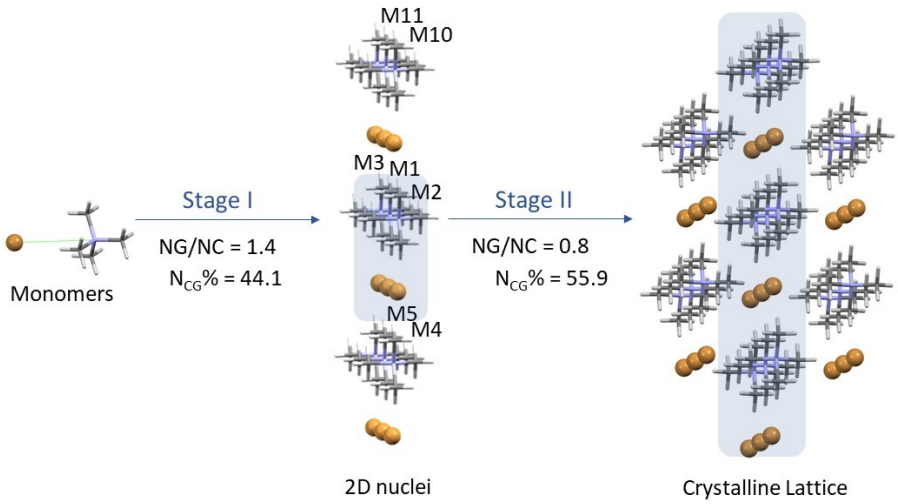

Figure S63. Crystallization mechanism proposal of salt **9a**.

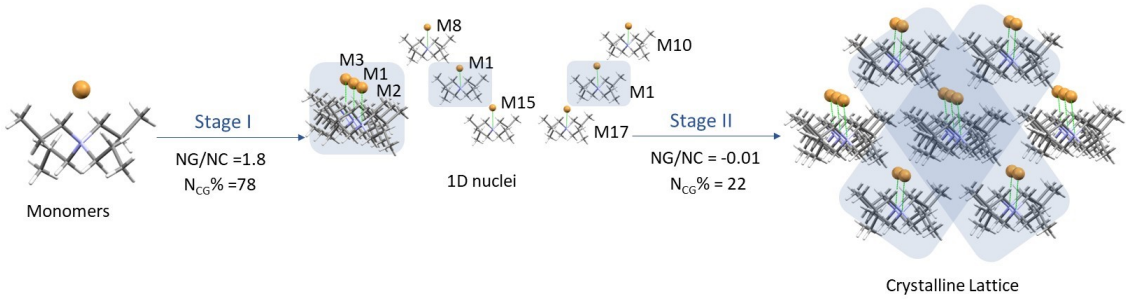

Figure S64. Crystallization mechanism proposal of salt **11a**.

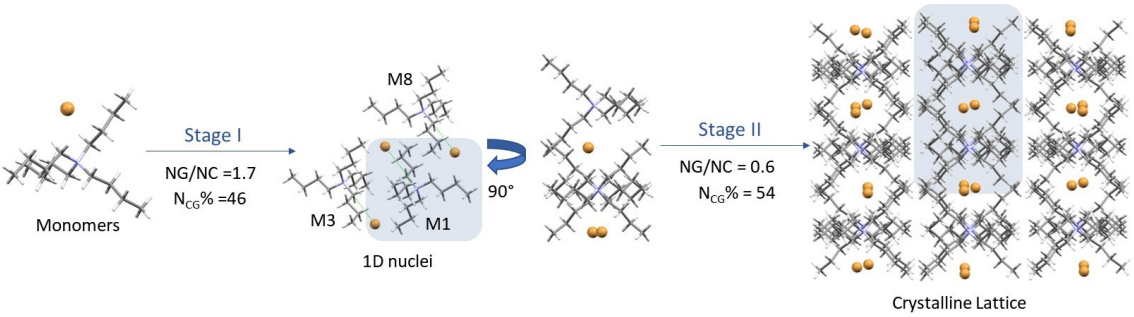

Figure S65. Crystallization mechanism proposal of salt **12a**.

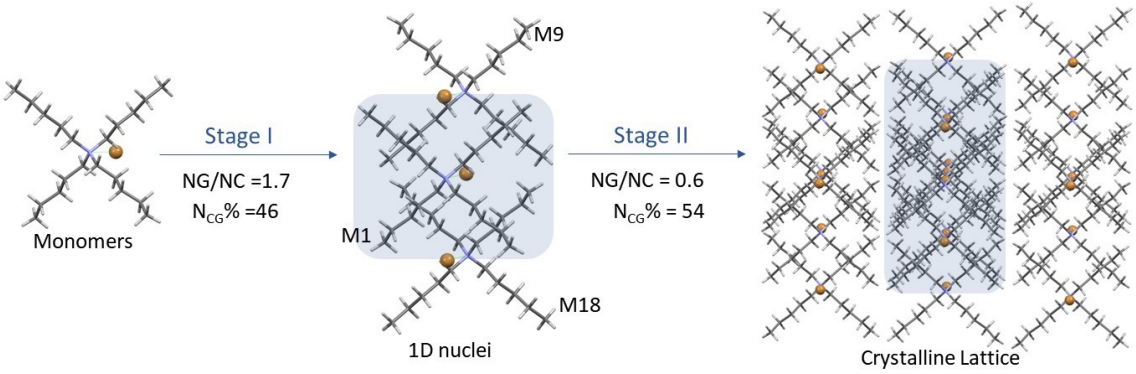

Figure S66. Crystallization mechanism proposal of salt **13a**.

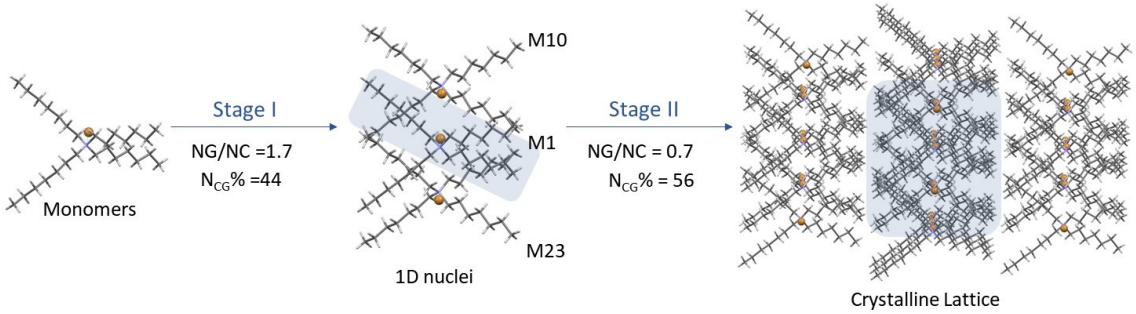

Figure S67. Crystallization mechanism proposal of salt **15a**.

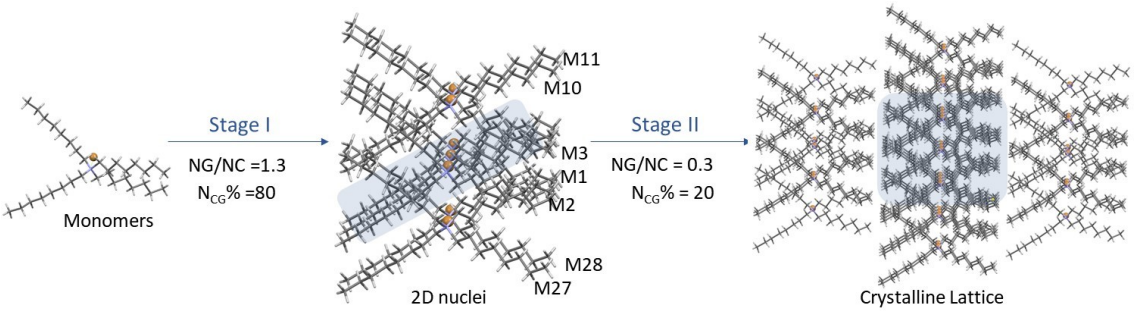

Figure S68. Crystallization mechanism proposal of salt **16a**.

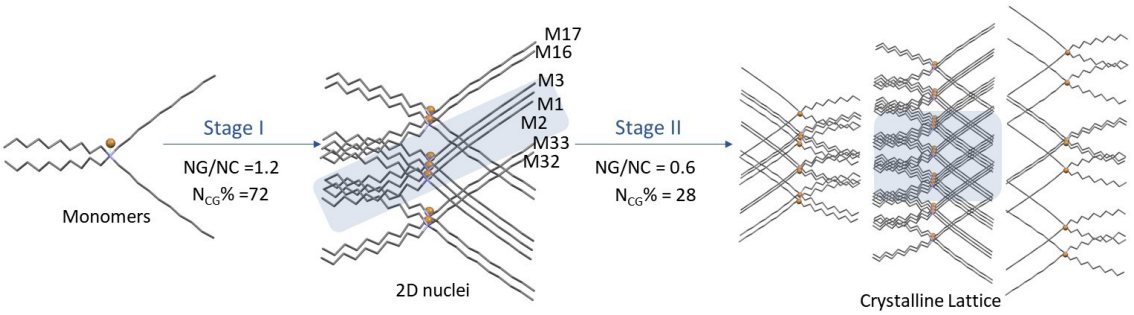

Figure S69. Crystallization mechanism proposal of salt **17a**. Hydrogens were omitted for clarity.

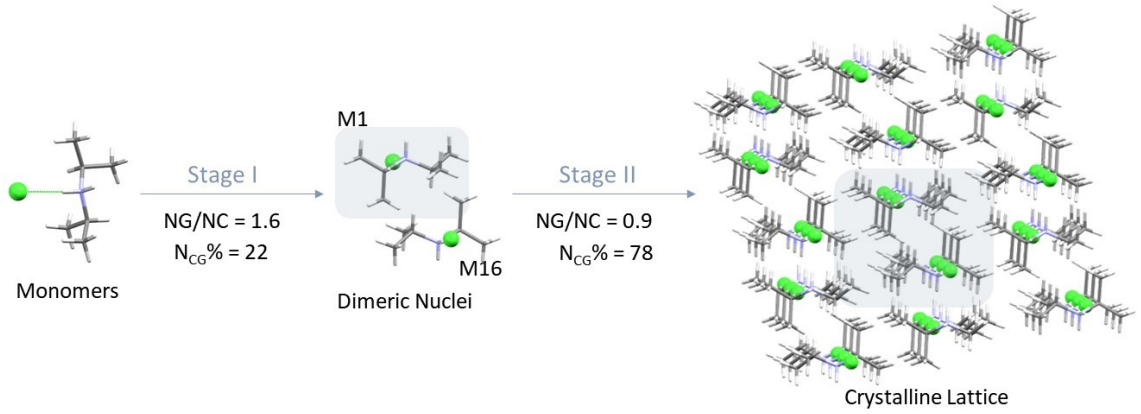

Figure S70. Crystallization mechanism proposal of salt **5b**.

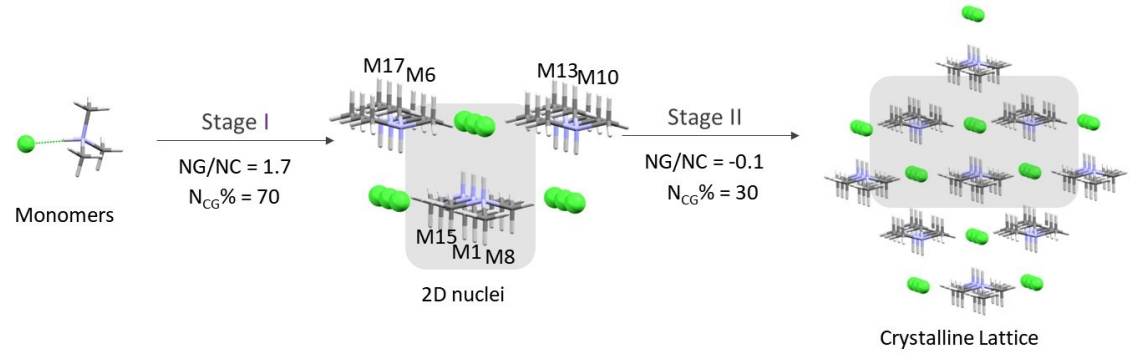

Figure S71. Crystallization mechanism proposal of salt **7b**.

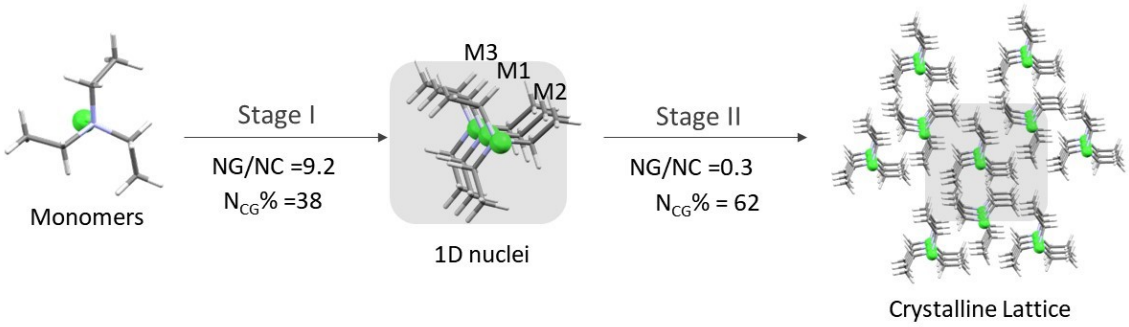

Figure S72. Crystallization mechanism proposal of salt **8b**.

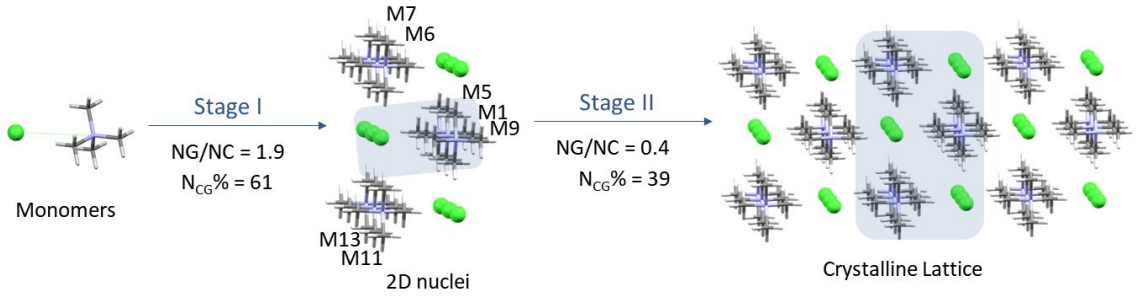

Figure S73. Crystallization mechanism proposal of salt **9b**.

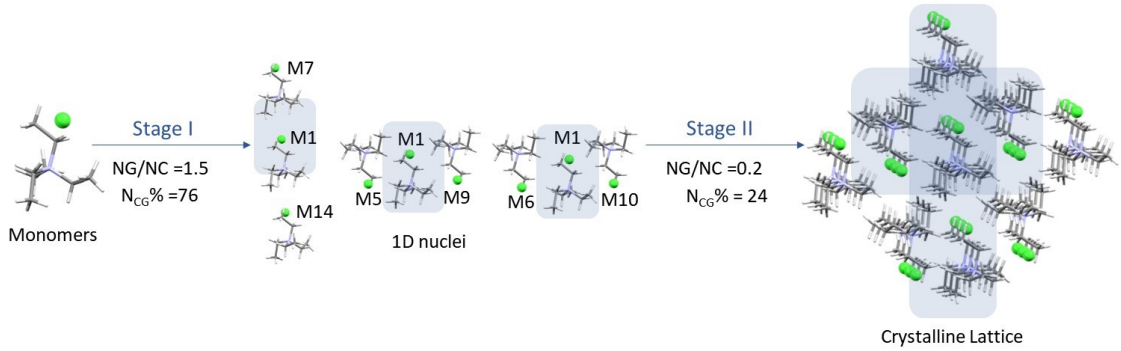

Figure S74. Crystallization mechanism proposal of salt **10b**.

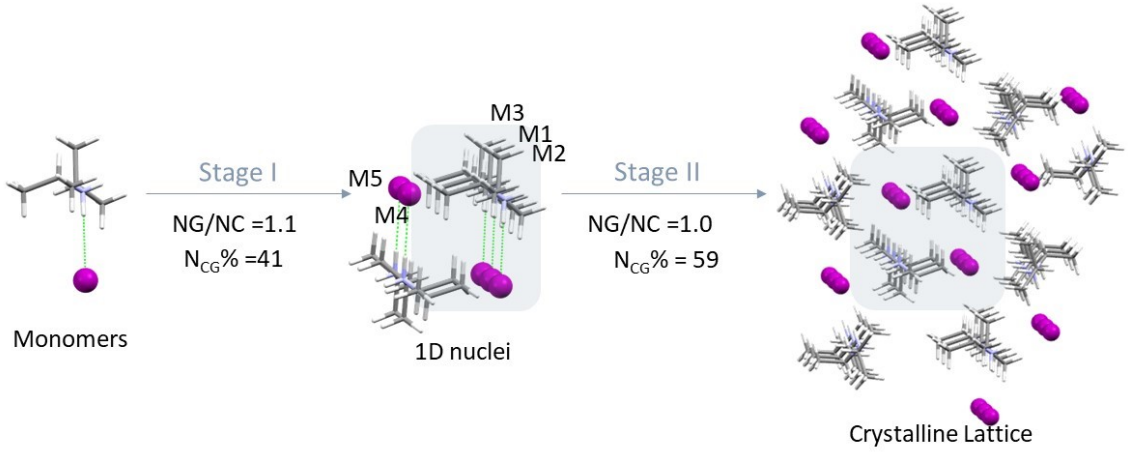

Figure S75. Crystallization mechanism proposal of salt **5c**.

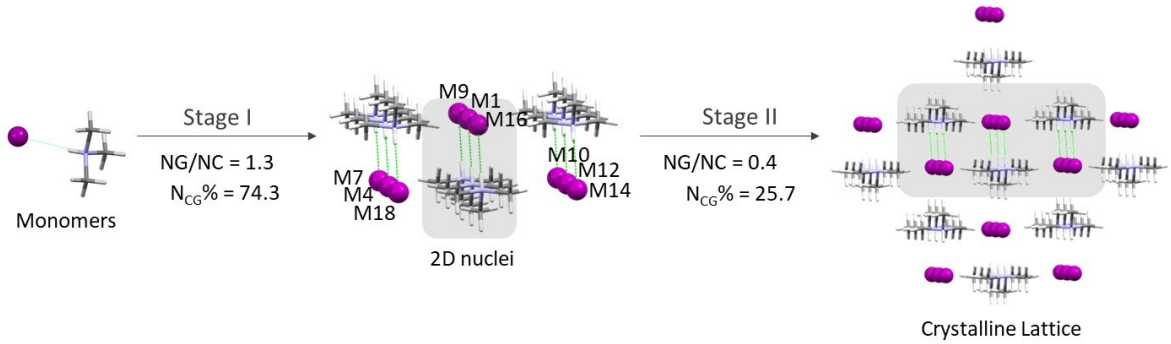

Figure S76. Crystallization mechanism proposal of salt **7c**.

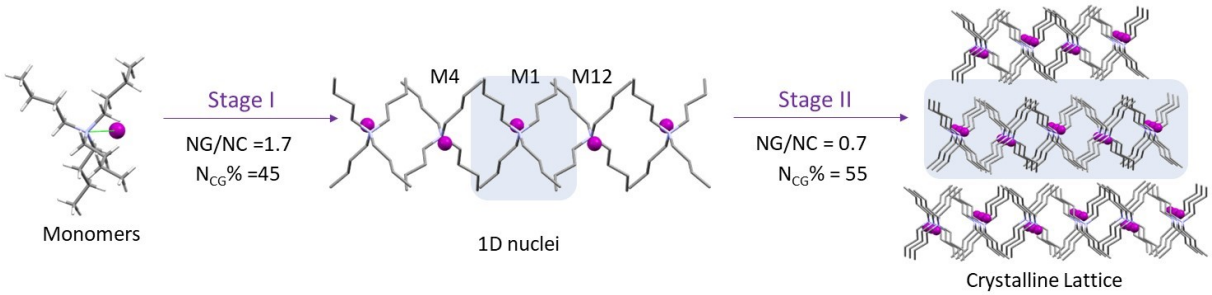

Figure S77. Crystallization mechanism proposal of salt **12c**. Hydrogens were omitted for clarity

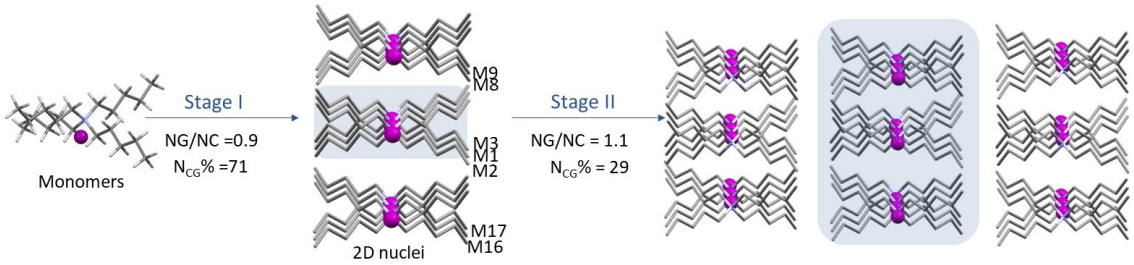

Figure S78. Crystallization mechanism proposal of salt **13c**. Hydrogens were omitted for clarity.

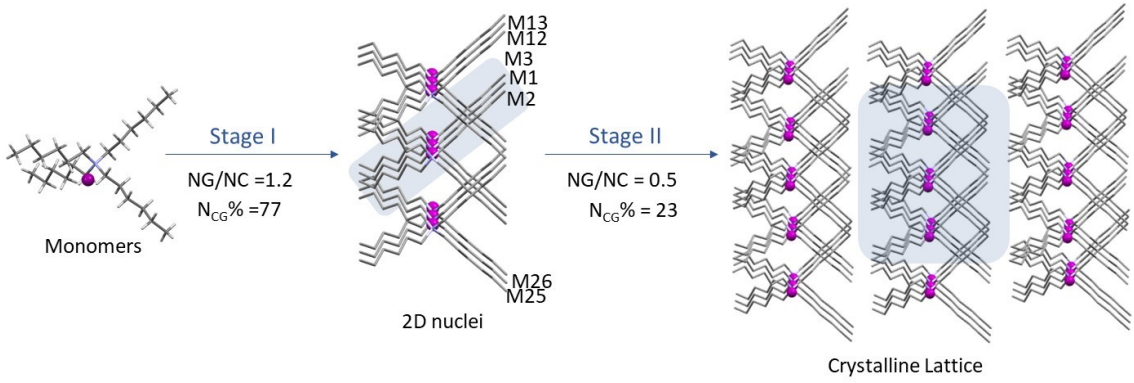

Figure S79. Crystallization mechanism proposal of salt **14c**. Hydrogens were omitted for clarity.

5. Basis Set Comparison

Table S56 Energetic data for **4a**, **4b** and **4c** calculated at ωb97xd/aug-cc-pvdz and ωb97xd/cc-pvdz theory level and basis sets. Pseudopotentials were used for **4c** on both basis sets.

Salt	**4a**		**4b**		**4c**	
Dimer	$G_{M1\cdots MN}$ (kcal mol^{-1})					
Basis set	aug-cc-pvdz	cc-pvdz	aug-cc-pvdz	cc-pvdz	aug-cc-pvdz	cc-pvdz-pp
M1···M2	2.89	3.06	7.44	8.06	3.31	4.19
M1···M3	5.48	5.72	7.44	8.06	3.31	4.19
M1···M4	-14.74	-13.65	-14.84	-14.03	-12.78	-12.58
M1···M5	3.06	3.11	-6.02	-5.29	-3.41	-2.97
M1···M6	8.35	8.64	-27.04	-26.47	0.90	0.99
M1···M7	7.51	7.73	-20.38	-19.76	6.63	7.04
M1···M8	-20.55	-20.07	5.23	5.43	-9.15	-8.88
M1···M9	-37.95	-38.40	3.75	4.03	-7.01	-5.62
M1···M10	-37.95	-38.40	2.86	2.91	0.90	0.99
M1···M11	-14.74	-13.65	-6.01	-5.29	-3.41	-2.97
M1···M12	-20.55	-20.07	-14.84	-14.03	-12.78	-12.58
M1···M13	8.35	8.64	6.01	6.37	-9.15	-8.88
M1···M14	7.51	7.73	5.23	5.43	-7.01	-5.62
M1···M15	3.06	3.11	-30.73	-31.34	-42.92	-44.49
M1···M16	-	-	-30.73	-31.34	-16.35	-15.91
M1···M17	-	-	7.77	9.43	-	-
Total	-100.28	-96.53	-104.88	-97.82	-108.90	-103.09

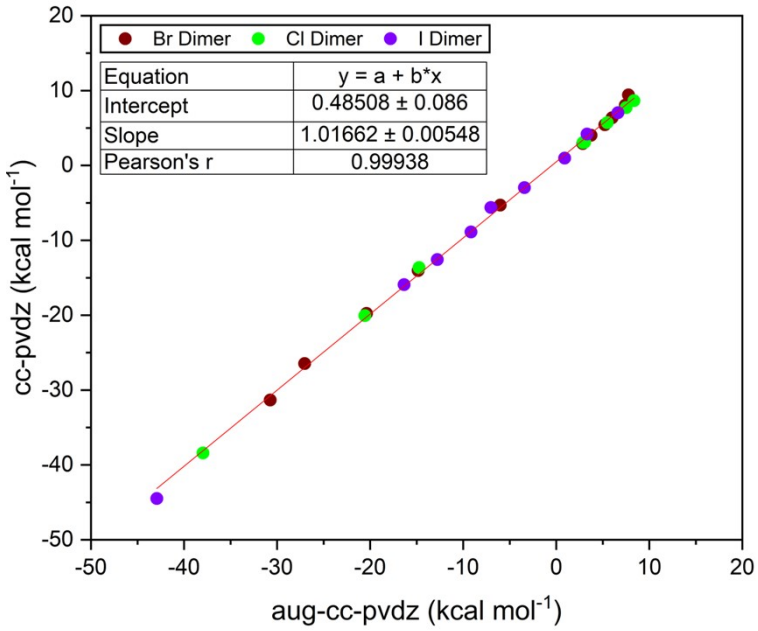

Figure S80. Correlation between raw values of dimer interactions of **4a-c** using both basis sets, aug-cc-pvdz and cc-pvdz. (**4c** energies were calculated using aug-cc-pvdz-pp and cc-pvdz-pp). This correlation considers 45 comparisons of dimer pairs.