Structural investigation of bromide complexation with bipodal, tripodal and tetrapodal cationic molecules

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Supplementary Information

A) Crystallography

Table S1. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **I**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O01W-H01*A*···Br1	0.85	2.58	3.420(3)	170
O01W-H01*B*...Br1^{i}	0.85	2.50	3.347(3)	177
O02W-H02*A*...Br2	0.85	2.62	3.455(4)	168
O02W-H02*B*...Br2^{ii}	0.85	2.62	3.445(3)	165
C10-H10*A*...Br2^{iii}	0.99	2.99	3.860(3)	147
C12-H12*B*...Br1	0.99	3.09	3.858(3)	135
C15-H15*B*...Br2^{iii}	0.99	3.11	3.912(3)	140
C16-H16*B*...Br2^{iii}	0.99	2.83	3.755(3)	156
C40-H40*A*...Br2^{ii}	0.99	2.83	3.724(4)	151
C40-H40*B*...Br1^{iv}	0.99	3.13	3.990(4)	146
C42-H42*A*...Br1	0.99	3.11	3.883(5)	136
C42-H42*B*...O02W	0.99	2.49	3.381(5)	150
C43-H43*A*...Br1	0.99	3.12	3.832(5)	130
C45-H45*A*...Br1^{iv}	0.99	3.08	3.892(3)	140
C45-H45*B*...O01W	0.99	2.54	3.358(5)	140
C46-H46*B*...Br1^{iv}	0.99	3.12	4.033(7)	153
C47'-H47*C*...Br1^{iv}	0.99	2.99	3.804(6)	141

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y, -z+1$; (iii) $x-1, y, z$; (iv) $x, -y+1/2, z+1/2$.

Table S2. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **II**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O01W-H01*A*···Br1	0.85	2.44	3.278(2)	169
O01W-H01*B*···O02W^{i}	0.85	1.95	2.796(3)	172
O02W-H02*A*···Br1	0.85	2.50	3.320(2)	164
O02W-H02*B*···O01W^{ii}	0.85	1.90	2.742(3)	171
C10-H10*A*···Br2^{iii}	0.99	2.82	3.783(2)	165
C10-H10*B*···Br2^{iv}	0.99	3.12	4.007(2)	151
C12-H12*B*···Br1^{i}	0.99	2.92	3.821(3)	152
C16-H16*A*···Br1^{i}	0.99	2.99	3.872(2)	149
C16-H16*B*···O02W^{v}	0.99	2.60	3.509(3)	152
C17-H17*A*···O01W	0.98	2.62	3.416(3)	138
C17-H17*B*···Br1^{i}	0.98	2.93	3.828(2)	153
C40-H40*A*···Br2^{v}	0.99	3.03	3.949(2)	154
C40-H40*B*···Br2	0.99	2.94	3.846(2)	152
C42-H42*A*···Br2	0.99	3.01	3.909(2)	152
C42-H42*B*···Br1	0.99	3.12	3.751(2)	123
C43-H43*A*···Br2^{vi}	0.99	3.00	3.853(2)	145
C43-H43*B*···Br1	0.99	2.89	3.571(2)	127
C45-H45*A*···Br1^{v}	0.99	2.86	3.680(2)	141
C47-H47*A*···Br2^{v}	0.98	2.97	3.900(2)	159
C47-H47*B*···Br2^{vi}	0.98	3.13	4.100(2)	173
C47-H47*C*···Br2	0.98	3.08	3.962(2)	150

Symmetry codes: (i) 1–*x*, 1–*y*, –*z*; (ii) *x*–1, *y*, *z*; (iii) –*x*+1, –*y*+1, –*z*+1; (iv) –*x*+2, –*y*+1, –*z*+1; (v) *x*+1, *y*, *z*; (vi) –*x*+2, –*y*+2, –*z*+1.

Table S3. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **III**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O01W-H01*A*...O06W	0.85	1.80	2.645(8)	180
O01W-H01*B*...O10W	0.85	1.88	2.732(16)	180
O02W-H02*A*...Br1	0.85	2.49	3.341(5)	179
O02W-H02*B*...Br3	0.85	2.55	3.402(4)	179
O03W-H03*A*...Br1	0.85	2.44	3.286(3)	176
O03W-H03*B*...Br3	0.85	2.44	3.288(3)	176
O04W-H04*A*...Br4	0.85	2.51	3.351(5)	173
O04W-H04*B*...Br6^{vii}	0.85	2.65	3.484(6)	166
O04W-H04*B*...Br6'^{vii}	0.85	2.13	2.894(7)	149
O05W-H05*A*...O04W	0.85	1.86	2.710(7)	177
O05W-H05*B*...Br2	0.85	2.44	3.289(5)	177
C110-H11*A*...Br3	0.99	2.76	3.749(7)	173
C110-H11*B*...Br1^{i}	0.99	2.88	3.807(7)	156
C111-H11*C*...O06W	0.99	2.65	3.380(11)	131
C111-H11*D*...Br1^{i}	0.99	2.95	3.911(8)	163
C112-H11*K*...Br2^{ii}	0.98	2.93	3.900(9)	169
C113-H11*F*...O05W^{ii}	0.99	2.62	3.544(10)	156
C114-H11*L*...Br5	0.98	2.86	3.598(9)	132
C115-H11*G*...O01W	0.99	2.57	3.461(9)	149
C115-H11*H*...Br2^{ii}	0.99	3.05	3.981(8)	158
C130-H13*A*...O02W^{i}	0.99	2.48	3.437(9)	162
C132-H13*J*···Br5^{iii}	0.98	3.07	4.012(10)	161
C133-H13*E*...O13W	0.99	2.65	3.561(8)	154
C133-H13*F*...Br3^{i}	0.99	2.83	3.782(8)	161
C134-H13*N*...Br6	0.98	2.93	3.845(9)	156
C135-H13*H*...Br4^{iv}	0.99	2.93	3.764(7)	142
C150-H15*A*...Br5'^{iii}	0.99	2.89	3.795(8)	152
C150-H15*B*...O03W	0.99	2.31	3.229(8)	154
C153-H15*E*...Br6'^{v}	0.99	2.87	3.850(10)	170
C153-H15*F*...Br5'^{iii}	0.99	2.96	3.853(11)	151
C153-H15*F*...O14W^{iii}	0.99	2.58	3.227(18)	123
C155-H15*H*...Br6^{v}	0.99	3.07	3.913(8)	144
C156-H15*Q*···Br5^{iii}	0.98	3.09	4.045(9)	165
C210-H21*A*...Br1^{i}	0.99	2.92	3.908(7)	178
C210-H21*B*...Br3	0.99	2.93	3.908(7)	169
C211-H21*R*...Br2	0.99	3.01	3.970(9)	165
C212-H21*J*...Br3	0.98	2.62	3.477(14)	147
C22'-H22*A*...O07W	0.98	2.53	3.15(2)	121
C214-H21*M*...O08W^{vi}	0.98	2.66	3.622(18)	168
C24'-H24*C*...Br3	0.98	3.14	3.81(3)	127
C215-H21*H*...Br2	0.99	2.87	3.749(10)	149
C216-H21*O*...Br4^{i}	0.98	3.03	3.947(12)	156
C216-H21*Q*...Br1^{i}	0.98	2.96	3.735(15)	136
C230-H23*A*...O03W	0.99	2.48	3.434(8)	161
C230-H23*B*...Br5'^{iii}	0.99	2.92	3.902(8)	171
C231-H23*C*...O04W	0.99	2.59	3.563(8)	167
C232-H23*I*...O11W	0.98	2.45	3.322(16)	148
C232-H23*J*...Br5'^{iii}	0.98	2.86	3.578(12)	131
C233-H23*F*...O14W^{iii}	0.99	2.39	3.272(17)	148
C234-H23*N*...Br6'^{vii}	0.98	3.07	3.989(10)	158
C235-H23*G*...Br4	0.99	3.09	3.925(7)	143
C235-H23*H*...Br2	0.99	2.99	3.860(7)	148
C250-H25*B*...O02W^{i}	0.99	2.42	3.343(10)	155
C251-H25*D*...Br2	0.99	3.05	3.931(9)	149

C253-H25*F*...Br6^{viii}	0.99	2.99	3.964(9)	166
C255-H25*G*...Br6^{viii}	0.99	3.03	3.923(9)	151
C255-H25*H*...Br2	0.99	2.91	3.784(8)	147

Symmetry codes: (i) *x*–1/2, –*y*+1/2, *z*–1/2; (ii) *x*+1/2, –*y*+1/2, *z*–1/2; (iii) –*x*+1/2, *y*–1/2, –*z*+1/2; (iv) *x*, *y*, *z*–1; (v) –*x*+1, –*y*, –*z*; (vi) *x*–1/2, –*y*+1/2, *z*+1/2; (vii) *x*, *y*, *z*+1; (viii) –*x*, –*y*, –*z*.

Table S4. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **IV**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O01W-H01*A*···Br3	0.85	2.45	3.281(4)	167
O01W-H01*B*...Br3^{i}	0.85	2.47	3.317(4)	172
O02W-H02*A*...Br4	0.85	2.47	3.312(4)	174
O02W-H02*B*...Br4^{ii}	0.85	2.47	3.318(4)	178
O03W-H03*A*...Br2	0.85	2.64	3.475(4)	167
O03W-H03*B*...Br1^{iii}	0.85	2.69	3.450(4)	150
C110-H11*A*...Br3^{i}	0.99	3.06	3.988(4)	157
C110-H11*B*...Br6	0.99	2.84	3.707(5)	147
C110-H11*B*...O13W	0.99	2.40	3.321(15)	154
C112-H11*C*...Br3^{i}	0.99	2.87	3.839(6)	166
C112-H11*D*...Br6	0.99	2.54	3.447(7)	152
C112-H11*D*...Br6^{iv}	0.99	3.09	3.923(7)	142
C113-H11*E*...Br7	0.99	3.02	3.975(7)	162
C113-H11*E*...O08W	0.99	2.60	3.503(13)	152
C115-H11*G*...Br2^{v}	0.99	2.86	3.658(6)	139
C115-H11*H*···Br7	0.99	3.11	4.044(6)	158
C116-H11*I*...O01W	0.99	2.54	3.476(7)	158
C116-H11*J*...Br1	0.99	2.93	3.898(5)	165
C117-H11*K*...O13W	0.98	2.63	3.486(15)	146
C117-H11*L*...Br7	0.98	2.72	3.673(6)	164
C130-H13*A*...Br4^{ii}	0.99	2.79	3.754(4)	166
C130-H13*B*...Br3	0.99	2.79	3.765(4)	167
C132-H13*D*...O234^{ii}	0.99	2.54	3.250(6)	129
C133-H13*E*···Br5^{vi}	0.99	3.08	4.037(4)	162
C133-H13*F*···Br1^{vii}	0.99	3.06	4.019(5)	164
C135-H13*H*...O03W^{v}	0.99	2.54	3.335(6)	137
C136-H13*I*...Br1	0.99	2.77	3.705(4)	158
C137-H13*L*...Br1	0.98	3.11	3.919(5)	140
C137-H13*M*...Br1^{vii}	0.98	2.89	3.834(4)	161
C150-H15*A*...Br5	0.99	2.70	3.662(4)	165
C150-H15*B*...Br4	0.99	2.74	3.710(4)	165
C152-H15*C*···Br5	0.99	3.13	4.010(4)	148
C153-H15*E*...O254^{ii}	0.99	2.57	3.201(5)	121
C153-H15*F*...Br7^{viii}	0.99	2.63	3.569(5)	158
C155-H15*G*...Br5^{ix}	0.99	3.04	3.788(4)	133
C155-H15*G*...O05W^{v}	0.99	2.65	3.435(10)	137
C155-H15*G*...O11W	0.99	2.55	3.470(9)	154
C156-H15*I*...Br1	0.99	2.85	3.773(4)	156
C157-H15*M*...Br1	0.98	3.07	3.889(4)	142
C210-H21*A*...Br6	0.99	2.72	3.704(4)	176
C210-H21*B*...Br3^{i}	0.99	2.77	3.751(4)	169
C212-H21*C*...Br6^{iv}	0.99	2.43	3.424(5)	178
C213-H21*E*...O134^{i}	0.99	2.65	3.260(6)	120
C213-H21*F*...Br5^{iv}	0.99	2.91	3.900(5)	175
C215-H21*G*...O10W	0.99	2.33	2.994(9)	124
C216-H21*J*...Br2	0.99	3.07	3.975(5)	153
C216-H21*J*...O09W	0.99	2.48	3.163(14)	126
C217-H21*K*...Br2	0.98	2.98	3.846(5)	148
C230-H23*A*...Br5	0.99	2.92	3.860(4)	159
C230-H23*B*···Br4	0.99	3.14	4.075(4)	158
C232-H23*C*...O154^{viii}	0.99	2.66	3.307(6)	124
C232-H23*D*...Br4	0.99	2.98	3.941(6)	164
C233-H23*E*...O154^{viii}	0.99	2.64	3.233(6)	119
C233-H23*F*...Br5^{viii}	0.99	3.12	3.787(5)	126

C235-H23*G*...Br1^{iii}	0.99	2.92	3.706(5)	137
C236-H23*I*...Br2	0.99	2.93	3.898(4)	166
C236-H23*J*...O02W^{ii}	0.99	2.60	3.535(6)	158
C237-H23*K*···Br7^{iii}	0.98	3.12	4.033(6)	155
C237-H23*L*...O09W	0.98	2.23	2.811(17)	117
C237-H23*M*...O214^{iv}	0.98	2.43	3.135(6)	129
C250-H25*A*...Br3	0.99	2.89	3.845(5)	162
C250-H25*B*...Br4^{ii}	0.99	2.91	3.863(4)	163
C252-H25*D*...Br2	0.99	2.75	3.679(4)	157
C253-H25*F*...O03W	0.99	2.49	3.299(6)	138
C255-H25*H*···Br2^{x}	0.99	3.05	4.005(5)	163
C256-H25*I*...O114^{i}	0.99	2.56	3.268(6)	128
C256-H25*J*...Br4^{ii}	0.99	3.05	3.987(4)	159
C257-H25*K*...Br2	0.98	3.12	3.913(5)	139
C257-H25*L*...Br2^{x}	0.98	2.95	3.890(4)	162

Symmetry codes: (i) –*x*+1, –*y*+1, –*z*+1; (ii) –*x*+1/2, –*y*+1/2, –*z*+1; (iii) *x*, *y*–1, *z*; (iv) –*x*+1, *y*, –*z*+3/2; (v) *x*, *y*+1, *z*; (vi) *x*, –*y*+1, *z*–1/2; (vii) –*x*+1/2, –*y*+3/2, –*z*+1; (viii) –*x*+1/2, *y*–1/2, –*z*+3/2; (ix) –*x*+1/2, *y*+1/2, –*z*+3/2; (x) –*x*+1, –*y*, –*z*+1.

Table S5. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **V**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O01W-H01*A*···Br1	0.85	2.50	3.344(3)	173
O01W-H01*B*...Br2	0.85	2.50	3.335(4)	169
O02W-H02*A*...O01W	0.85	1.99	2.834(4)	176
O02W-H02*B*...Br3	0.85	2.53	3.378(5)	173
O02W-H02*B*...Br4	0.85	2.69	3.352(4)	135
C10-H10*A*...O06W^{i}	0.99	2.38	3.35(2)	166
C10-H10*B*...Br4^{i}	0.99	2.99	3.780(4)	137
C12-H12*A*...Br4^{i}	0.99	2.84	3.741(6)	151
C12-H12*B*...O05W^{i}	0.99	2.46	3.343(7)	149
C13-H13*A*...O06W	0.99	2.30	3.13(2)	141
C14-H14*B*...O05W	0.99	2.46	3.401(8)	158
C15-H15*A*...O04W	0.99	2.34	3.281(7)	159
C15-H15*B*...Br1	0.99	2.82	3.799(5)	171
C32-H32*A*...Br4^{ii}	0.99	3.11	3.877(5)	136
C32-H32*B*...O01W^{ii}	0.99	2.55	3.420(6)	146
C33-H33*A*...Br2	0.99	2.99	3.806(5)	141
C33-H33*B*···Br1^{ii}	0.99	3.12	4.016(4)	151
C35-H35*A*...Br2^{ii}	0.99	2.69	3.675(4)	174
C36-H36*A*···Br2	0.99	3.05	4.034(4)	173
C37-H37*B*...Br4^{iii}	0.99	3.00	3.890(5)	151
C50-H50*A*...Br2^{iv}	0.99	2.96	3.782(4)	142
C50-H50*B*...Br3^{iii}	0.99	3.01	3.939(4)	157
C50-H50*B*...O06W^{iii}	0.99	2.35	3.20(3)	144
C52-H52*A*...Br2^{iv}	0.99	2.91	3.859(5)	160
C52-H52*B*···Br1^{v}	0.99	3.08	4.049(5)	168
C52-H52*A*...Br2^{iv}	0.99	2.91	3.859(5)	160
C53-H53*B*...Br3^{iii}	0.99	2.91	3.482(12)	118
C54-H54*A*...Br3^{iii}	0.99	2.19	3.077(9)	148
C55-H55*D*...Br1	0.99	2.90	3.821(5)	155

Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+1/2, y+1/2, -z+3/2$; (iii) $x-1/2, -y+1/2, z-1/2$; (iv) $x+1/2, -y+1/2, z-1/2$; (v) $-x+1, -y, -z+1$.

Table S6. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **VI**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O01W-H01*A*···Br1	0.85	2.45	3.302(2)	179
O01W-H01*B*...Br3^{i}	0.85	2.55	3.354(2)	157
O02W-H02*A*...O01W	0.85	1.94	2.774(3)	169
O02W-H02*B*...Br2	0.85	2.52	3.352(2)	167
O03W-H03*A*...Br2	0.85	2.47	3.283(2)	160
O03W-H03*B*...Br3	0.85	2.42	3.241(2)	161
O04W-H04*A*...O02W	0.85	1.87	2.720(3)	176
O04W-H04*B*...Br1^{ii}	0.85	2.47	3.316(2)	174
C10-H10*A*...Br3^{iii}	0.99	2.96	3.893(2)	157
C10-H10*B*...Br2^{iv}	0.99	2.83	3.747(2)	155
C15-H15*B*...Br2^{v}	0.99	3.07	3.999(3)	158
C16-H16*A*...Br2^{iv}	0.99	2.89	3.811(3)	156
C17-H17*A*...Br3^{iii}	0.98	2.99	3.904(3)	156
C17-H17*C*...Br3^{i}	0.98	2.84	3.777(2)	161
C32-H32*A*...Br2	0.99	2.72	3.670(3)	161
C32-H32*B*...Br2^{iii}	0.99	2.79	3.773(3)	175
C33-H33*B*...O02W^{iii}	0.99	2.66	3.381(4)	130
C37-H37*A*...O03W^{iii}	0.98	2.33	3.274(4)	161
C37-H37*B*...Br2	0.98	3.11	3.975(3)	148
C37-H37*C*...Br1	0.98	3.04	3.899(3)	147
C50-H50*B*...O04W^{vi}	0.99	2.49	3.412(3)	155
C52-H52*A*...Br3^{iv}	0.99	3.06	3.944(3)	150
C52-H52*B*...Br3^{vii}	0.99	3.06	3.860(3)	139
C55-H55*A*...O04W^{vi}	0.99	2.43	3.400(3)	166
C56-H56*A*...Br1	0.99	2.97	3.782(2)	140
C57-H57*A*...O03W^{iv}	0.98	2.44	3.389(4)	162
C57-H57*C*...O02W^{v}	0.98	2.64	3.469(4)	143

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*+1/2, –*y*+3/2, *z*+1/2; (iii) *x*, –*y*+1, *z*+1/2; (iv) *x*–1/2, *y*+1/2, *z*; (v) *x*–1/2, –*y*+3/2, *z*–1/2; (vi) *x*–1/2, *y*–1/2, *z*; (vii) *x*–1/2, –*y*+1/2, *z*–1/2.

Table S7. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **VII**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
C10-H10*A*···Br2^{ii}	0.99	2.95	3.786(2)	143
C12-H12...Br2^{ii}	0.95	2.73	3.581(2)	149
C14-H14...O01W	0.95	2.36	3.253(3)	157
C15-H15...Br2	0.95	2.76	3.668(2)	160
C16-H16*C*···Br2^{iii}	0.98	3.01	3.776(3)	136
C20-H20*A*···Br1^{iv}	0.99	2.93	3.874(2)	160
C20-H20*B*···Br1^{iii}	0.99	2.68	3.651(2)	166
C22-H22...Br2^{i}	0.95	2.76	3.638(2)	154
C24-H24...Br1^{v}	0.95	3.00	3.878(2)	154
C24-H24...O02W^{vi}	0.95	2.53	3.221(4)	130
C25-H25...O03W^{vi}	0.95	2.62	3.16(13)	117
C26-H26*A*···Br2^{i}	0.98	3.03	3.939(3)	155
C26-H26*B*···Br2^{ii}	0.98	3.11	3.647(3)	116
C26-H26*C*···Br1^{vii}	0.98	3.14	3.945(3)	141

Symmetry codes: (i) –*x*+1, –*y*+1, –*z*+1; (ii) *x*, *y*+1, *z*; (iii) –*x*+1/2, *y*+1/2, –*z*+1/2; (iv) *x*+1/2, *y*+1/2, *z*; (v) –*x*+1/2, *y*+3/2, –*z*+1/2; (vi) *x*, –*y*+1, *z*–1/2; (vii) *x*+1/2, *y*+3/2, *z*.

Table S8. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **VIII**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O1W-H1*A*···Br1	0.85	2.54	3.384(6)	174
O1W-H1*B*...Br5	0.85	2.17	3.014(7)	174
O2W-H2*A*...O1W	0.85	2.11	2.962(9)	178
O2W-H2*B*...O4W	0.85	2.00	2.851(6)	178
O3W-H3*A*...O7W	0.85	1.77	2.59(4)	164
O3W-H3*A*...O7'	0.85	1.94	2.78(3)	174
O3W-H3*B*...O8W	0.85	1.87	2.719(14)	178
O3W-H3*B*...O5'	0.85	1.85	2.67(4)	162
O4W-H4*A*...Br4	0.85	2.43	3.277(4)	173
O4W-H4*B*...O6W	0.85	1.85	2.699(11)	176
O4W-H4*B*...O6'	0.85	2.33	3.156(15)	166
C10-H10*B*...Br2^{i}	0.99	2.89	3.814(7)	156
C10-H10*B*...O8^{i}	0.99	2.58	3.284(10)	128
C11-H11*B*...O3W^{iii}	0.99	2.60	3.522(10)	155
C11-H11*A*...Br1	0.99	3.02	3.887(8)	147
C12-H12*A*...Br5	0.99	2.78	3.742(8)	164
C12-H12*B*...Br2^{iv}	0.99	2.92	3.768(8)	144
C13-H13*B*...Br3	0.99	3.11	3.885(7)	136
C14-H14*A*...Br2^{i}	0.99	3.03	3.902(7)	148
C14-H14*B*...Br3	0.99	3.08	3.839(7)	135
C15-H15*A*...Br1	0.98	3.00	3.888(8)	151
C15-H15*B*...Br2'	0.98	2.54	3.451(11)	155
C15-H15*C*...Br5	0.98	3.12	3.916(8)	140
C20-H20*B*...Br1^{i}	0.99	2.99	3.865(7)	148
C21-H21*B*...Br1^{i}	0.99	2.88	3.743(7)	146
C23-H23*B*...Br3^{v}	0.99	3.13	3.938(8)	139
C24-H24*B*...O6W^{i}	0.99	2.51	3.420(11)	152
C25-H25*A*...O8'	0.98	2.49	3.344(10)	145
C25-H25*B*...Br1^{i}	0.98	2.94	3.819(7)	150
C25-H25*C*...O3W	0.98	2.55	3.488(10)	160
C30-H30*A*...Br5^{ii}	0.99	2.91	3.795(7)	149
C30-H30*B*...Br1^{vi}	0.99	2.96	3.852(7)	151
C31-H31*A*...Br4^{vi}	0.99	3.13	3.753(7)	122
C31-H31*A*...Br5^{ii}	0.99	2.76	3.725(8)	164
C31-H31*B*...Br1^{vi}	0.99	3.00	3.824(8)	141
C32-H32*A*...Br6^{vii}	0.99	2.98	3.938(8)	163
C32-H32*B*...Br2	0.99	3.04	3.878(7)	143
C33-H33*B*...Br4^{viii}	0.99	3.01	3.912(8)	152
C34-H34*B*...Br6^{ii}	0.99	2.70	3.669(8)	166
C35-H35*A*...Br1^{vi}	0.98	3.03	3.894(8)	148
C35-H35*B*...Br2	0.98	2.84	3.800(7)	166
C35-H35*C*...Br2'	0.98	2.67	3.444(10)	136
C40-H40*A*...Br1^{ix}	0.99	3.10	3.957(7)	146
C40-H40*B*...Br2'^{ii}	0.99	2.76	3.493(10)	132
C40-H40*B*...Br3^{ii}	0.99	2.94	3.885(7)	159
C41-H41*A*...Br1^{ix}	0.99	2.88	3.762(7)	148
C42-H42*A*...Br5^{ix}	0.99	2.94	3.909(8)	168
C43-H43*B*...Br4	0.99	3.01	3.915(8)	152
C44-H44*B*...Br6^{ii}	0.99	3.03	3.954(7)	156
C45-H45*B*···Br4	0.98	3.10	4.046(7)	163
C45-H45*C*...Br1^{ix}	0.98	2.91	3.801(7)	152

Symmetry codes: (i) –*x*+1, –*y*+1, –*z*+1; (ii) –*x*+1, –*y*+1, –*z*+2; (iii) *x*–1, *y*, *z*; (iv) *x*–1, *y*+1, *z*; (v) –*x*+1, –*y*+2, –*z*+1; (vi) *x*+1, *y*, *z*; (vii) *x*+1, *y*–1, *z*; (viii) –*x*+1, –*y*, –*z*+2; (ix) –*x*, –*y*+1, –*z*+2.

Table S9. Selected hydrogen-bond parameters and short intermolecular contacts (Å, º) for compound **IX**.

D*—H···*A	**d(*D*—H)**	**d(H···*A*)**	**d(*D*···*A*)**	**∠(*D*—H···*A*)**
O01W-H01*B*···Br1^{ii}	0.848(5)	2.397(6)	3.2421(14)	175(2)
O01W-H01*A*...O02W^{iii}	0.844(5)	1.895(6)	2.732(2)	171(3)
O02W-H02*B*...O01W	0.842(5)	1.976(8)	2.785(2)	161(2)
O02W-H02*A*...Br2	0.845(5)	2.447(6)	3.2874(15)	173(2)
O03W-H03*A*...Br2	0.849(5)	2.513(7)	3.3464(15)	167(2)
O03W-H03*B*...Br2^{iv}	0.851(5)	2.521(10)	3.3377(14)	161(2)
C11-H11*B*...O03W^{i}	0.99	2.55	3.454(2)	151
C12-H12*B*...O02W^{iii}	0.99	2.64	3.528(2)	149
C15-H15*A*...O01W	0.99	2.49	3.366(2)	148
C17-H17*B*...Br1	0.99	2.99	3.7222(17)	132
C32-H32*A*...Br1	0.99	3.01	3.7646(16)	134
C33-H33*A*...Br1^{v}	0.99	2.86	3.7843(18)	156
C35-H35*A*...O01W	0.99	2.58	3.363(2)	136
C35-H35*B*...Br2	0.99	3.01	3.7490(16)	132
C35-H35*B*...O03W	0.99	2.50	3.350(2)	144
C36-H36*A*...O03W	0.99	2.60	3.472(2)	148
C36-H36*B*...Br1^{v}	0.99	2.97	3.9271(16)	162

Symmetry codes: (i) –*x*+1, –*y*+1, –*z*+1; (ii) *x*–1, *y*, *z*; (iii) –*x*, –*y*+1, –*z*+1; (iv) –*x*+1, –*y*+1, –*z*+2; (v) –*x*+1, –*y*, –*z*+1.

B) Hirshfeld surface analysis

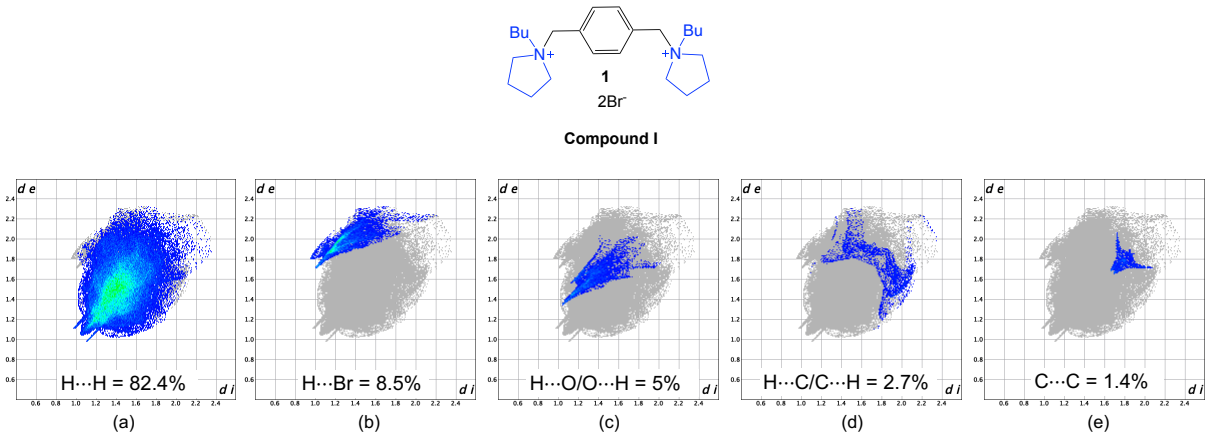

Figure S1. (Top) Chemical diagram for compound **I**. Fingerprint plots delineated into (a) H···H, (b) H···Br, (c) H···O / O···H, (d) H···C / C···H, and (e) C···C contacts.

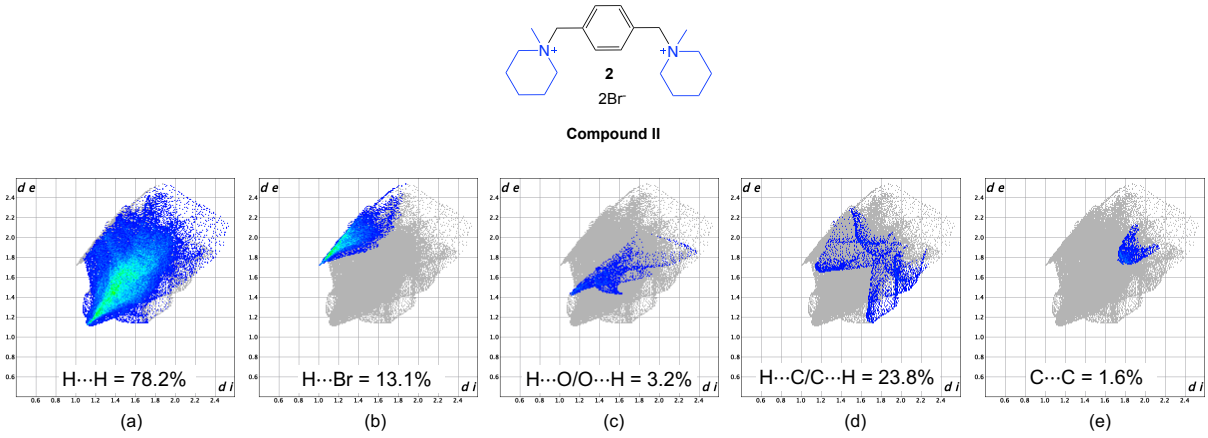

Figure S2. (Top) Chemical diagram for compound **II**. Fingerprint plots delineated into (a) H···H, (b) H···Br, (c) H···O / O···H, (d) H···C / C···H, and (e) C···C contacts.

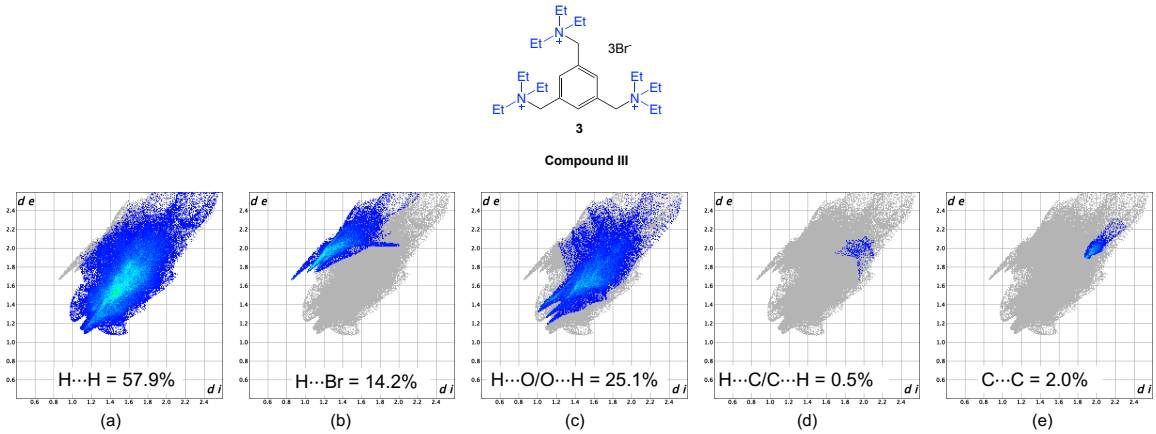

Figure S3. (Top) Chemical diagram for compound **III**. Fingerprint plots delineated into (a) H···H, (b) H···Br, (c) H···O / O···H, (d) H···C / C···H, and (e) C···C contacts.

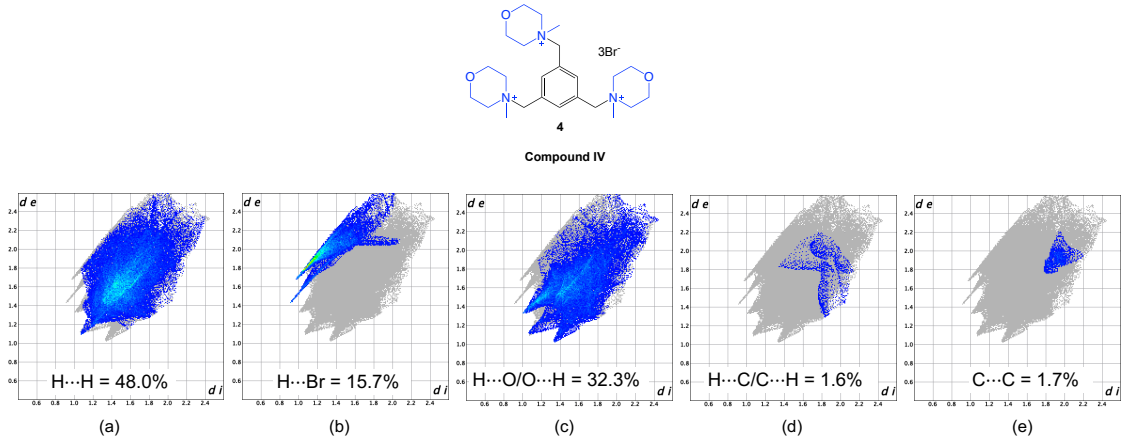

Figure S4. (Top) Chemical diagram for compound **IV**. Fingerprint plots delineated into (a) H···H, (b) H···Br, (c) H···O / O···H, (d) H···C / C···H, and (e) C···C contacts.

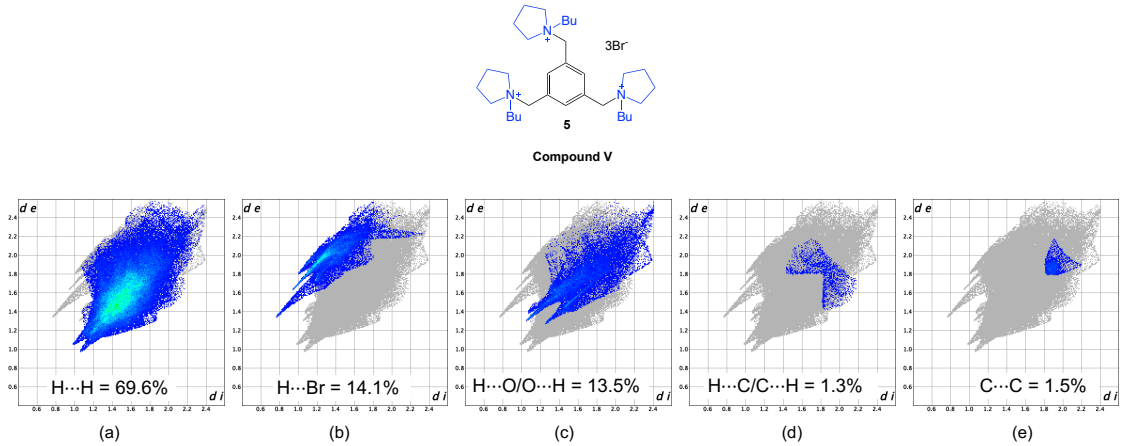

Figure S5. (Top) Chemical diagram for compound **V**. Fingerprint plots delineated into (a) H···H, (b) H···Br, (c) H···O / O···H, (d) H···C / C···H, and (e) C···C contacts.

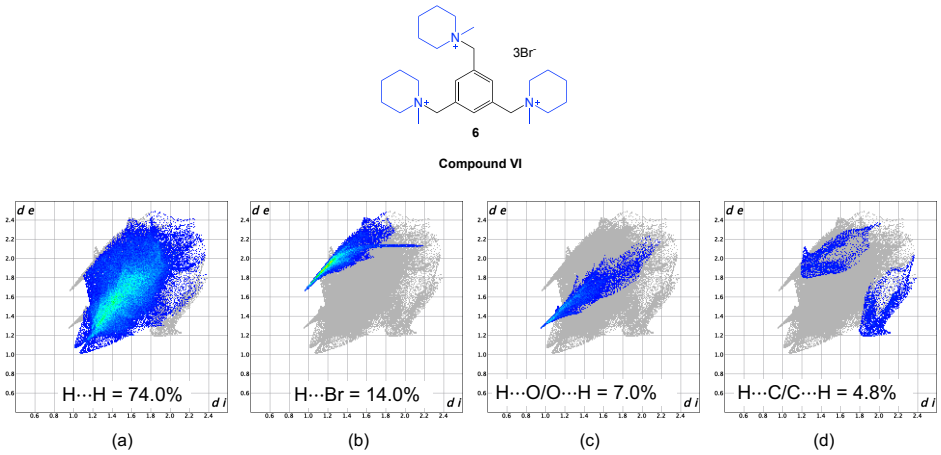

Figure S6. (Top) Chemical diagram for compound **VI**. Fingerprint plots delineated into (a) H···H, (b) H···Br, (c) H···O / O···H, and (d) H···C / C···H contacts.

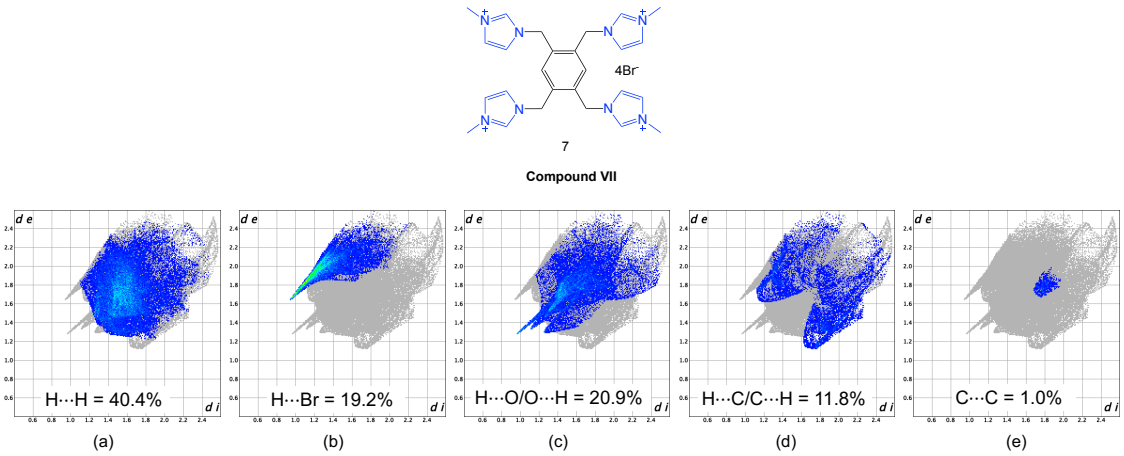

Figure S7. (Top) Chemical diagram for compound **VII**. Fingerprint plots delineated into (a) H···H, (b) H···Br, (c) H···O / O···H, (d) H···C / C···H, and (e) C···C contacts.

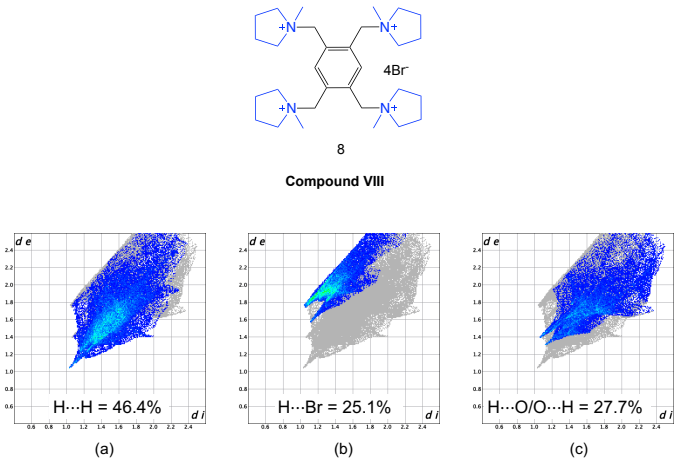

Figure S8. (Top) Chemical diagram for compound **VIII**. Fingerprint plots delineated into (a) H···H, (b) H···Br, and (c) H···O / O···H contacts.

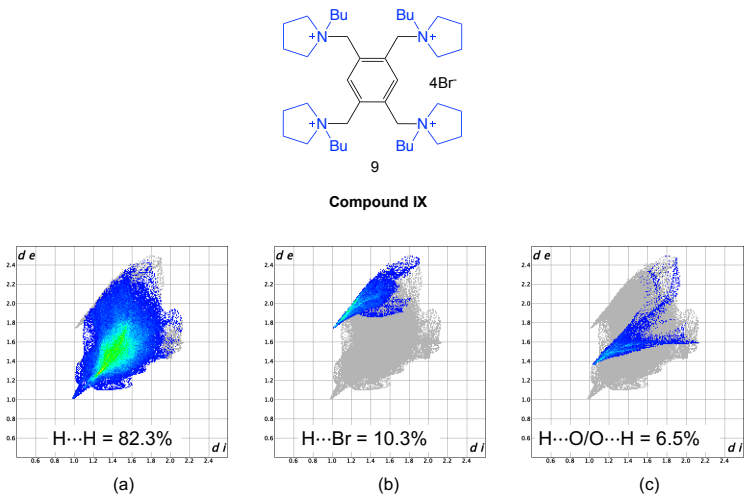

Figure S9. (Top) Chemical diagram for compound **IX**. Fingerprint plots delineated into (a) H···H, (b) H···Br, and (c) H···O / O···H contacts.