Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information for manuscript:

Spodium bonding in five coordinated Zn(II): a new player in crystal engineering?

Rosa M. Gomila,[a] Antonio Bauzá,[b] Tiddo J. Mooibroek*[,c] and Antonio Frontera*[b]

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1. Figure S1

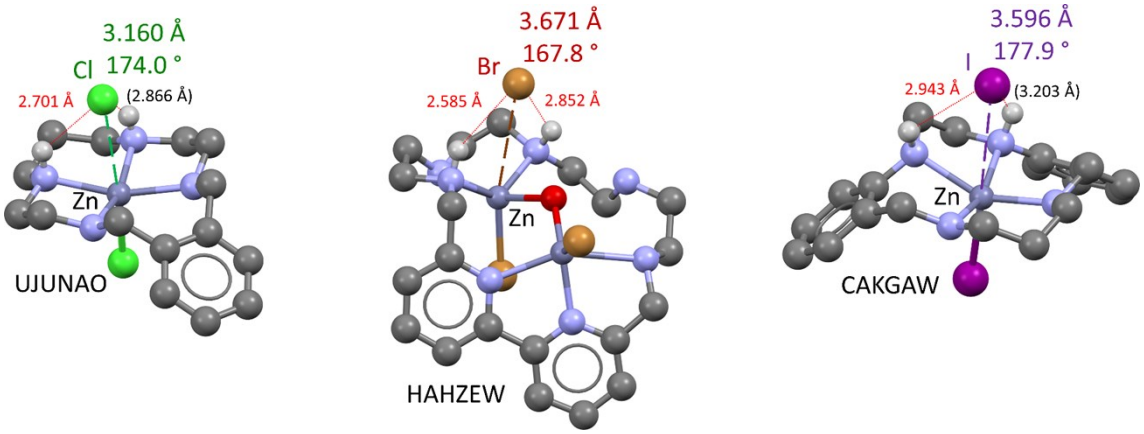

Figure S1. Examples of SpB interactions of azacrown complexes involving a Cl^-, Br^- and I^- anion. The angles are the Hlg–Zn–Hlg angle and the interatomic distances with the shown hydrogen atoms are either hydrogen bonds (red) or longer than the sum of the van der Waals radii of H and the halogen involved (black in brackets). The van der Waals corrected Hlg-Zn distances using the radii of Hu and Robertson are: –0.60 (Cl^-), –0.19 (Br^-) and –0.39 (I^-) Å.

2. Figure S2

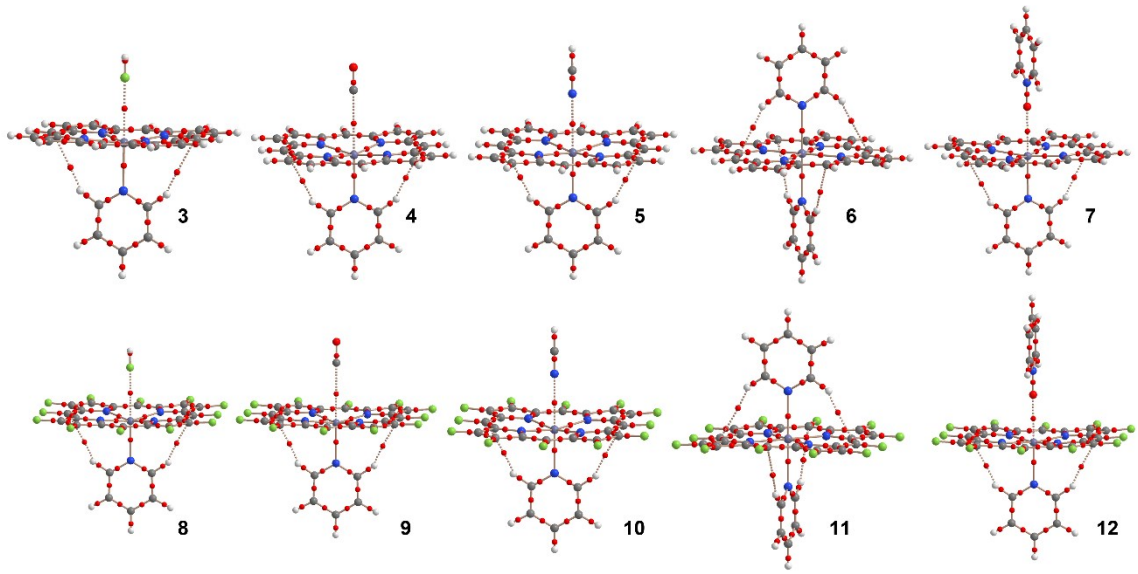

Figure S2. Distribution of bond critical points and bond paths for complexes **3**-**12**.

3. Cartesian Coordinates

1

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6	0.000000	1.146669	-2.431678
7	0.000000	0.000000	-1.757650
30	0.000000	0.000000	0.418097
7	-1.446875	-1.453843	0.696883
6	-1.244817	-2.795468	0.745493
6	0.000000	-3.418808	0.756599
6	1.244817	-2.795468	0.745493
7	1.446875	-1.453843	0.696883
7	-1.446875	1.453843	0.696883
6	-2.788015	1.245545	0.720729
6	-3.408524	0.000000	0.715777
6	-2.788015	-1.245545	0.720729
6	-3.472125	-2.512253	0.777049
6	-2.515077	-3.473764	0.793078
1	-2.646661	-4.545093	0.843089
1	-4.544685	-2.638541	0.811491
6	-3.472125	2.512253	0.777049
1	-4.544685	2.638541	0.811491
6	-2.515077	3.473764	0.793078
1	-2.646661	4.545093	0.843089
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6	1.244817	2.795468	0.745493
7	1.446875	1.453843	0.696883
6	2.788015	1.245545	0.720729
6	3.472125	2.512253	0.777049
6	2.515077	3.473764	0.793078
1	2.646661	4.545093	0.843089
1	4.544685	2.638541	0.811491
6	3.408524	-0.000000	0.715777
6	2.788015	-1.245545	0.720729
6	3.472125	-2.512253	0.777049
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1	0.000000	4.502281	0.797933

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6	0.000000	-3.411875	0.543163
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7	-1.452127	1.458579	0.466645
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6	-3.472811	2.512581	0.535580
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9	4.774554	-2.706012	0.567507
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7	-1.448712	1.455983	0.538152
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6	-3.408273	0.000000	0.561868
6	-2.788450	-1.246349	0.565604
6	-3.473254	-2.513218	0.628044
6	-2.516209	-3.474794	0.645787
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6	-3.473254	2.513218	0.628044
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6	-2.516209	3.474794	0.645787
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7	1.448712	1.455983	0.538152
6	2.788450	1.246349	0.565604
6	3.473254	2.513218	0.628044
6	2.516209	3.474794	0.645787
1	2.648018	4.546011	0.699199
1	4.545834	2.639494	0.664405
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6	1.245665	2.796376	0.496866
7	1.448621	1.455766	0.441731
6	2.788909	1.246420	0.470129
6	3.473243	2.513159	0.533666
6	2.516120	3.474728	0.551090
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1	2.647950	-4.545812	0.605933
6	-0.000000	-1.146287	-2.674808
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  7          1.450898    1.458476    0.446686
  6          2.789804    1.247546    0.471262
  6          3.475043    2.514908    0.530375
  6          2.517980    3.476682    0.549406
  1          2.650480    4.547985    0.600081
  1          4.547722    2.641712    0.562841
  6          3.408722   -0.000000    0.467676
  6          2.789804   -1.247546    0.471262
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  1          0.000000    2.048706   -2.040246
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  1          0.000000    0.000000   -5.813535
  1          0.000000   -4.503133    0.560917
  1          4.492929   -0.000000    0.491020
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  1          0.000000    4.503133    0.560917
  7          0.000000    0.000000    3.153277
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  1          0.000000    0.000000    5.366163

6 (1+ Py)
==> porph_py_py_outTurbo.log.xyz <==
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  7         -1.461906    1.461907   -0.000071
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6	3.482271	2.523113	-0.025800
6	2.523119	3.482262	0.026071
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1	4.554485	2.655822	-0.050304
6	3.416317	0.000000	-0.065506
6	2.799272	-1.251440	-0.039197
6	3.482271	-2.523113	-0.025800
1	4.554485	-2.655822	-0.050304
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7 (1+ Py^{+}O^{-})

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6	0.000000	1.171375	-4.096234
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6	2.798510	1.247186	0.225334
6	3.477616	2.518307	0.158722
6	2.515787	3.475363	0.171337
1	2.642388	4.547704	0.126298

1	4.548646	2.650369	0.100776
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8 (2+HF)

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6	1.250403	-2.803191	0.420722
7	1.454440	-1.461152	0.351904
7	-1.454440	1.461152	0.351904
6	-2.796749	1.251342	0.367002
6	-3.402710	0.000000	0.350458
6	-2.796749	-1.251342	0.367002
6	-3.473924	-2.513435	0.436388
6	-2.516443	-3.474072	0.472121
6	-3.473924	2.513435	0.436388
6	-2.516443	3.474072	0.472121
6	-1.250403	2.803191	0.420722
6	0.000000	3.411212	0.442204
6	1.250403	2.803191	0.420722
7	1.454440	1.461152	0.351904
6	2.796749	1.251342	0.367002
6	3.473924	2.513435	0.436388
6	2.516443	3.474072	0.472121
6	3.402710	-0.000000	0.350458
6	2.796749	-1.251342	0.367002
6	3.473924	-2.513435	0.436388
6	2.516443	-3.474072	0.472121
6	-0.000000	-1.146216	-2.760108
6	-0.000000	-1.193721	-4.142651
1	0.000000	-2.149326	-4.651333
1	0.000000	-2.051286	-2.162514
1	0.000000	2.051286	-2.162514
1	0.000000	2.149326	-4.651333
1	0.000000	0.000000	-5.930518
9	0.000000	0.000000	3.023053
1	0.000000	0.000000	3.943772
9	-4.776286	-2.707636	0.474542
9	-4.737865	0.000000	0.354170
9	-4.776286	2.707636	0.474542
9	-2.715866	4.774294	0.549305
9	0.000000	4.745642	0.501875
9	2.715866	4.774294	0.549305
9	4.776286	2.707636	0.474542

9	4.737865	-0.000000	0.354170
9	4.776286	-2.707636	0.474542
9	2.715866	-4.774294	0.549305
9	-0.000000	-4.745642	0.501875
9	-2.715866	-4.774294	0.549305

9 (2+CO)

6	0.000000	0.000000	-4.917804
6	0.000000	1.193766	-4.213874
6	0.000000	1.146438	-2.831448
7	0.000000	0.000000	-2.154407
30	0.000000	0.000000	0.007367
7	-1.454198	-1.460828	0.290822
6	-1.250490	-2.803690	0.354206
6	0.000000	-3.412235	0.375071
6	1.250490	-2.803690	0.354206
7	1.454198	-1.460828	0.290822
7	-1.454198	1.460828	0.290822
6	-2.797135	1.251426	0.302431
6	-3.403547	0.000000	0.286680
6	-2.797135	-1.251426	0.302431
6	-3.474221	-2.513767	0.365189
6	-2.516583	-3.474666	0.399541
6	-3.474221	2.513767	0.365189
6	-2.516583	3.474666	0.399541
6	-1.250490	2.803690	0.354206
6	0.000000	3.412235	0.375071
6	1.250490	2.803690	0.354206
7	1.454198	1.460828	0.290822
6	2.797135	1.251426	0.302431
6	3.474221	2.513767	0.365189
6	2.516583	3.474666	0.399541
6	3.403547	-0.000000	0.286680
6	2.797135	-1.251426	0.302431
6	3.474221	-2.513767	0.365189
6	2.516583	-3.474666	0.399541
6	-0.000000	-1.146438	-2.831448
6	-0.000000	-1.193766	-4.213874
1	0.000000	-2.149321	-4.722598
1	0.000000	-2.051597	-2.234038
1	0.000000	2.051597	-2.234038
1	0.000000	2.149321	-4.722598
1	0.000000	0.000000	-6.001666
6	0.000000	0.000000	3.245895
8	0.000000	0.000000	4.368603
9	-4.776026	2.707503	0.398407
9	-2.715386	4.774583	0.470308
9	0.000000	4.746004	0.430213
9	2.715386	4.774583	0.470308
9	4.776026	2.707503	0.398407
9	4.737872	-0.000000	0.288161
9	4.776026	-2.707503	0.398407
9	2.715386	-4.774583	0.470308
9	-0.000000	-4.746004	0.430213
9	-2.715386	-4.774583	0.470308
9	-4.776026	-2.707503	0.398407
9	-4.737872	0.000000	0.288161

10 (2+HCN)

6	0.000000	0.000000	-4.878981
6	0.000000	1.193459	-4.174660
6	0.000000	1.145324	-2.791840
7	0.000000	0.000000	-2.114147
30	0.000000	0.000000	0.081849
7	-1.457497	-1.464832	0.291628
6	-1.251925	-2.805796	0.358358
6	0.000000	-3.412743	0.382442
6	1.251925	-2.805796	0.358358
7	1.457497	-1.464832	0.291628
7	-1.457497	1.464832	0.291628
6	-2.798604	1.252983	0.302323
6	-3.403294	0.000000	0.286878
6	-2.798604	-1.252983	0.302323
6	-3.476237	-2.515864	0.366687
6	-2.518887	-3.476747	0.403870
6	-3.476237	2.515864	0.366687
6	-2.518887	3.476747	0.403870

6	-1.251925	2.805796	0.358358
6	0.000000	3.412743	0.382442
6	1.251925	2.805796	0.358358
7	1.457497	1.464832	0.291628
6	2.798604	1.252983	0.302323
6	3.476237	2.515864	0.366687
6	2.518887	3.476747	0.403870
6	3.403294	-0.000000	0.286878
6	2.798604	-1.252983	0.302323
6	3.476237	-2.515864	0.366687
6	2.518887	-3.476747	0.403870
6	-0.000000	-1.145324	-2.791840
6	-0.000000	-1.193459	-4.174660
1	0.000000	-2.149202	-4.683209
1	0.000000	-2.050780	-2.194871
1	0.000000	2.050780	-2.194871
1	0.000000	2.149202	-4.683209
1	0.000000	0.000000	-5.962902
7	0.000000	0.000000	2.901353
6	0.000000	0.000000	4.045505
1	0.000000	0.000000	5.114694
9	4.778935	2.710444	0.398433
9	4.738724	-0.000000	0.289780
9	4.778935	-2.710444	0.398433
9	2.718990	-4.777370	0.476235
9	0.000000	-4.747332	0.443669
9	-2.718990	-4.777370	0.476235
9	-4.778935	-2.710444	0.398433
9	-4.738724	0.000000	0.289780
9	-4.778935	2.710444	0.398433
9	-2.718990	4.777370	0.476235
9	0.000000	4.747332	0.443669
9	2.718990	4.777370	0.476235

11 (2+Py)

6	0.000000	0.000000	5.098978
6	0.000000	1.192653	4.393493
6	0.000000	1.142164	3.009732
7	0.000000	0.000000	2.329045
30	0.000000	0.000000	0.000021
7	1.469217	-1.469218	0.000009
6	1.257195	-2.807471	-0.064987
6	0.000000	-3.408807	-0.110538
6	-1.257195	-2.807471	-0.064987
7	-1.469217	-1.469218	0.000009
7	1.469217	1.469218	0.000009
6	2.807472	1.257195	0.064990
6	3.408808	-0.000000	0.110540
6	2.807472	-1.257195	0.064990
6	3.482454	-2.524263	0.043112
6	2.524263	-3.482453	-0.043126
6	3.482454	2.524263	0.043112
6	2.524263	3.482453	-0.043126
6	1.257195	2.807471	-0.064987
6	0.000000	3.408807	-0.110538
6	-1.257195	2.807471	-0.064987
7	-1.469217	1.469218	0.000009
6	-2.807472	1.257195	0.064990
6	-3.482454	2.524263	0.043112
6	-2.524263	3.482453	-0.043126
6	-3.408808	0.000000	0.110540
6	-2.807472	-1.257195	0.064990
6	-3.482454	-2.524263	0.043112
6	-2.524263	-3.482453	-0.043126
6	-0.000000	-1.142164	3.009732
6	-0.000000	-1.192653	4.393493
1	0.000000	-2.148883	4.901589
1	0.000000	-2.049637	2.415597
1	0.000000	2.049637	2.415597
1	0.000000	2.148883	4.901589
1	0.000000	0.000000	6.182977
6	0.000000	0.000000	-5.098965
6	-1.192653	0.000000	-4.393480
6	-1.142164	0.000000	-3.009718
7	0.000000	0.000000	-2.329031
6	1.142164	-0.000000	-3.009718
6	1.192653	-0.000000	-4.393480

1	2.148883	-0.000000	-4.901576
1	2.049637	-0.000000	-2.415585
1	-2.049637	0.000000	-2.415585
1	-2.148883	0.000000	-4.901576
1	0.000000	0.000000	-6.182964
9	-4.784098	2.725061	0.089972
9	-2.725062	4.784096	-0.090002
9	0.000000	4.743234	-0.177950
9	2.725062	4.784096	-0.090002
9	4.784098	2.725061	0.089972
9	4.743235	-0.000000	0.177945
9	4.784098	-2.725061	0.089972
9	2.725062	-4.784096	-0.090002
9	-0.000000	-4.743234	-0.177950
9	-2.725062	-4.784096	-0.090002
9	-4.784098	-2.725061	0.089972
9	-4.743235	0.000000	0.177945

12 (2+Py^{+}O^{-})

6	0.000000	0.000000	-6.154136
6	0.000000	1.187439	-5.438283
6	0.000000	1.170199	-4.063043
7	0.000000	0.000000	-3.374210
30	0.000000	0.000000	0.410511
7	-1.467928	-1.459351	0.245354
6	-1.254072	-2.798837	0.217906
6	0.000000	-3.402260	0.226635
6	1.254072	-2.798837	0.217906
7	1.467928	-1.459351	0.245354
7	-1.467928	1.459351	0.245354
6	-2.807233	1.252539	0.172192
6	-3.413456	0.000000	0.149406
6	-2.807233	-1.252539	0.172192
6	-3.478006	-2.519804	0.108921
6	-2.517032	-3.476812	0.138906
6	-3.478006	2.519804	0.108921
6	-2.517032	3.476812	0.138906
6	-1.254072	2.798837	0.217906
6	0.000000	3.402260	0.226635
6	1.254072	2.798837	0.217906
7	1.467928	1.459351	0.245354
6	2.807233	1.252539	0.172192
6	3.478006	2.519804	0.108921
6	2.517032	3.476812	0.138906
6	3.413456	-0.000000	0.149406
6	2.807233	-1.252539	0.172192
6	3.478006	-2.519804	0.108921
6	2.517032	-3.476812	0.138906
6	-0.000000	-1.170199	-4.063043
6	-0.000000	-1.187439	-5.438283
1	0.000000	-2.146911	-5.940090
1	0.000000	-2.047844	-3.432897
1	0.000000	2.047844	-3.432897
1	0.000000	2.146911	-5.940090
1	0.000000	0.000000	-7.236029
6	0.000000	0.000000	5.394655
6	1.193277	-0.000000	4.690095
6	1.144644	-0.000000	3.307019
7	0.000000	0.000000	2.628953
6	-1.144644	0.000000	3.307019
6	-1.193277	0.000000	4.690095
1	-2.149127	0.000000	5.198565
1	-2.050270	0.000000	2.710289
1	2.050270	-0.000000	2.710289
1	2.149127	-0.000000	5.198565
1	0.000000	0.000000	6.478620
8	0.000000	0.000000	-2.108880
9	-2.710875	-4.779942	0.089359
9	0.000000	-4.738771	0.205554
9	2.710875	-4.779942	0.089359
9	4.778571	-2.719901	0.027116
9	4.748230	-0.000000	0.082221
9	4.778571	2.719901	0.027116
9	2.710875	4.779942	0.089359
9	0.000000	4.738771	0.205554
9	-2.710875	4.779942	0.089359
9	-4.778571	2.719901	0.027116

9	-4.748230	0.000000	0.082221
9	-4.778571	-2.719901	0.027116