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Theoretical Study of Chloride Complexes with Hybrid Macrocycles

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Supplementary Material

Table S1. Optimized Cartesian coordinates of the complexes investigated.

Complex Atom	1...2Cl ⁻ (B3LYP/SVP)		
	X	Y	Z
C	-3.252563	-0.892531	-0.164959
C	-4.144528	-1.927686	0.191820
C	-3.457385	-3.161489	-0.019633
C	-2.168807	-2.832835	-0.483993
C	-0.949744	-3.618933	-0.720498
C	-0.919126	-4.991172	-1.063320
C	0.327801	-5.603557	-1.205800
H	0.384397	-6.661724	-1.483874
C	1.503231	-4.875552	-1.009766
H	2.479162	-5.347230	-1.133580
C	1.388135	-3.507030	-0.669794
C	2.515871	-2.608480	-0.386577
C	3.807423	-2.813437	0.136162
C	4.367328	-1.520010	0.366404
C	3.400357	-0.573784	-0.039101
C	-5.505366	-1.769757	0.818238
H	-5.620809	-0.724520	1.147355
H	-5.561387	-2.375963	1.742885
C	-6.700038	-2.151670	-0.074134
H	-6.726464	-1.540944	-0.989633
H	-7.660033	-2.010020	0.455324
H	-6.645829	-3.205951	-0.391366
C	-3.972318	-4.524632	0.374715
H	-3.805372	-5.259947	-0.433090
H	-5.067395	-4.476520	0.493334
C	-3.364356	-5.072414	1.677797
H	-2.272907	-5.184067	1.588149
H	-3.552702	-4.382957	2.516345
C	4.427630	-4.121031	0.565307
H	4.365943	-4.872085	-0.242874

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ARTICLE

Journal Name

C	3.813237	-4.716543	1.844093
H	4.315793	-5.657768	2.134834
H	2.742405	-4.930340	1.704978
H	3.896565	-4.007763	2.683504
C	5.676543	-1.236529	1.054800
H	5.745165	-1.836706	1.982437
H	5.677295	-0.186084	1.386900
C	6.942817	-1.502900	0.221257
H	7.003367	-2.557258	-0.094628
H	7.859115	-1.271804	0.794870
H	6.954878	-0.891611	-0.694209
N	-2.086523	-1.471698	-0.565062
H	-1.275948	-0.967013	-1.019857
N	0.186016	-2.936049	-0.547358
N	2.311784	-1.261448	-0.483478
H	1.477349	-0.835166	-0.973479
C	3.325886	0.891569	0.033315
C	4.205503	1.928621	-0.347470
C	3.514480	3.160438	-0.137089
C	2.234952	2.829069	0.349425
C	1.017888	3.613168	0.601879
C	0.993703	4.987417	0.939565
H	1.917287	5.549792	1.083378
C	-0.249314	5.598761	1.108530
H	-0.300962	6.657355	1.385888
C	-1.428916	4.868395	0.944095
H	-2.399265	5.339857	1.099987
C	-1.321053	3.499752	0.602052
C	-2.451349	2.600175	0.333370
C	-3.741431	2.810986	-0.191186
C	-4.292354	1.519549	-0.460903
C	-3.323089	0.570941	-0.068144
C	5.555723	1.775581	-0.997167
H	5.669563	0.730973	-1.328087
H	5.592309	2.380863	-1.923288
C	6.764803	2.163474	-0.127172
H	7.715581	2.027408	-0.674488
H	6.710421	3.217306	0.191592
C	4.017015	4.522559	-0.550435
H	3.864192	5.262646	0.255853
H	5.109695	4.476934	-0.690231
C	3.381840	5.060449	-1.844616
H	2.291962	5.168949	-1.734349
H	3.556056	4.366562	-2.682563
C	-4.381567	4.133333	-0.521828
H	-3.608188	4.844558	-0.861060
H	-5.063405	4.003662	-1.381964
C	-5.171596	4.782759	0.629841
H	-4.524103	4.968106	1.501871
H	-5.615194	5.748442	0.324190
H	-5.987664	4.127631	0.974162
C	-5.557547	1.234138	-1.226172
H	-5.559440	1.826923	-2.162171
H	-5.533863	0.181403	-1.549330
C	-6.882760	1.506252	-0.494252
H	-6.988887	2.571192	-0.233531
H	-7.750399	1.230053	-1.120744
H	-6.948142	0.932904	0.443765
N	2.162031	1.468337	0.444675
H	1.358646	0.962261	0.910423
N	-0.120406	2.929650	0.453292
N	-2.241245	1.252009	0.401790

H	–1.404122	0.820302	0.882578
H	6.811486	1.552427	0.787280
H	3.798359	6.047067	–2.120517
H	–3.789469	–6.059190	1.939597
Cl	0.003207	0.105755	2.246385
Cl	0.087032	–0.123822	–2.355514
H	–1.839542	–5.552882	–1.228781
H	5.507096	–3.971033	0.732439
Complex	2a ···2Cl [–] (B3LYP/SVP)		
Atom	X	Y	Z
C	–3.444230	–0.887790	–0.119934
C	–4.231662	–1.944181	0.356696
C	–3.476518	–3.159871	0.177602
C	–2.263719	–2.783274	–0.399988
N	–1.075610	–3.497292	–0.719313
B	–1.022087	–4.564954	–1.663598
N	0.269048	–5.075845	–2.026070
H	0.307816	–5.822542	–2.708437
B	1.505617	–4.466131	–1.627866
H	2.555211	–4.856832	–2.088437
N	1.448354	–3.397901	–0.684661
C	2.565604	–2.589524	–0.335162
C	3.784582	–2.861675	0.286060
C	4.430017	–1.586484	0.482642
C	3.574895	–0.601402	–0.028920
C	–5.581936	–1.822563	1.009053
H	–5.726361	–0.775125	1.324574
H	–5.610495	–2.423317	1.937946
C	–6.768767	–2.246382	0.125484
H	–6.820157	–1.630286	–0.786061
H	–7.730975	–2.143794	0.660570
H	–6.673738	–3.296510	–0.197010
C	–3.837366	–4.534724	0.675909
H	–3.345646	–5.296509	0.047601
H	–4.922294	–4.710271	0.557698
C	–3.450632	–4.786386	2.144629
H	–2.364579	–4.668130	2.284552
H	–3.942868	–4.064500	2.816472
C	4.240505	–4.199859	0.805862
H	3.840482	–5.002116	0.162872
C	3.818423	–4.480226	2.259553
H	4.171729	–5.469989	2.604441
H	2.721548	–4.454590	2.355748
H	4.220226	–3.717339	2.946079
C	5.739477	–1.350797	1.185159
H	5.783480	–1.948759	2.115218
H	5.781529	–0.295644	1.505096
C	6.992161	–1.669256	0.349563
H	6.999049	–2.722289	0.022564
H	7.920098	–1.488097	0.922989
H	7.027824	–1.047211	–0.558781
N	–2.271219	–1.436461	–0.582701
H	–1.516943	–0.948427	–1.115339
B	0.158437	–2.906922	–0.226848
N	2.468974	–1.247736	–0.528485
H	1.693036	–0.824700	–1.085444
C	3.510166	0.868402	0.022260
C	4.287192	1.923200	–0.474158
C	3.529379	3.137677	–0.296584
C	2.325175	2.761885	0.299356
N	1.137807	3.473754	0.625594
B	1.094846	4.559516	1.549052

ARTICLE

Journal Name

H	2.102090	5.039705	2.019276
N	-0.192259	5.076728	1.915186
H	-0.224884	5.836765	2.582917
B	-1.433156	4.462754	1.537538
H	-2.474952	4.866359	2.001939
N	-1.388796	3.375442	0.615956
C	-2.509662	2.570323	0.272104
C	-3.713297	2.842119	-0.381414
C	-4.353817	1.564344	-0.593138
C	-3.510395	0.581790	-0.057700
C	5.627332	1.800817	-1.147011
H	5.767409	0.752929	-1.462875
H	5.640263	2.399462	-2.077543
C	6.828849	2.227022	-0.284705
H	7.781559	2.126175	-0.836867
H	6.737492	3.276988	0.039460
C	3.879141	4.508471	-0.813686
H	3.396636	5.275616	-0.184803
H	4.965577	4.686814	-0.714929
C	3.467817	4.745215	-2.278223
H	2.379912	4.623200	-2.399156
H	3.950518	4.017896	-2.951111
C	-4.164346	4.188254	-0.878617
H	-3.271293	4.808225	-1.075403
H	-4.668765	4.070476	-1.856236
C	-5.098028	4.974762	0.059638
H	-4.606186	5.168692	1.025238
H	-5.385668	5.947955	-0.380087
H	-6.023384	4.414567	0.269821
C	-5.604293	1.306420	-1.389115
H	-5.595160	1.926826	-2.306187
H	-5.581769	0.258852	-1.735495
C	-6.934663	1.553823	-0.656613
H	-7.028505	2.602678	-0.332511
H	-7.800373	1.325056	-1.305120
H	-7.012220	0.925554	0.244732
N	2.341196	1.417063	0.495360
H	1.592108	0.929982	1.035208
B	-0.101265	2.872495	0.157718
N	-2.419549	1.228957	0.472204
H	-1.645317	0.805325	1.030710
H	6.897754	1.611138	0.625938
H	3.741139	5.760815	-2.620692
H	-3.731667	-5.804567	2.472838
H	-2.024295	-5.035475	-2.153950
H	5.340265	-4.282762	0.731367
H	-0.064799	2.036268	-0.697504
H	0.114021	-2.080752	0.638199
Cl	0.094186	-0.672206	-2.453597
Cl	-0.024619	0.661305	2.375764
Complex			
2b⁺·2Cl⁻ (B3LYP/SVP)			
Atom	X	Y	Z
C	-3.583117	-0.849333	-0.180754
C	-4.460475	-1.898191	0.160650
C	-3.739522	-3.117145	-0.039242
C	-2.443687	-2.786059	-0.477413
B	-1.109820	-3.576428	-0.653028
N	-1.019403	-4.971051	-1.058182
B	0.232871	-5.627556	-1.240921
H	0.278072	-6.790052	-1.605575
N	1.431190	-4.891928	-1.006221
H	2.322401	-5.334233	-1.191088

Journal Name	ARTICLE		
B	1.414292	-3.494732	-0.600115
C	2.687028	-2.621603	-0.372656
C	3.984412	-2.872300	0.111226
C	4.622179	-1.611562	0.333682
C	3.695309	-0.618016	-0.041307
C	-5.841330	-1.766026	0.746880
H	-5.975357	-0.733353	1.108116
H	-5.925586	-2.405792	1.646295
C	-7.001409	-2.121909	-0.199916
H	-7.002137	-1.474286	-1.090547
H	-7.980829	-2.011047	0.300735
H	-6.923090	-3.161807	-0.557346
C	-4.233606	-4.501003	0.311025
H	-4.008002	-5.212362	-0.506309
H	-5.334437	-4.492213	0.383974
C	-3.657666	-5.064738	1.621322
H	-2.563071	-5.159005	1.554505
H	-3.878139	-4.394216	2.467652
C	4.549937	-4.223532	0.480270
H	4.392263	-4.948063	-0.341341
C	3.969107	-4.819132	1.774103
H	4.437485	-5.789743	2.022565
H	2.884763	-4.979319	1.673840
H	4.122332	-4.135061	2.624418
C	5.970457	-1.398879	0.969736
H	6.059937	-2.035869	1.870552
H	6.028863	-0.361921	1.338038
C	7.184190	-1.680566	0.066205
H	7.182851	-2.722233	-0.294676
H	8.135949	-1.511858	0.602814
H	7.178341	-1.031442	-0.823298
N	-2.401811	-1.416218	-0.564855
H	-1.595337	-0.878512	-0.956829
N	0.127328	-2.921339	-0.383991
N	2.564979	-1.256829	-0.464421
H	1.740659	-0.768941	-0.880891
C	3.647341	0.846327	0.052040
C	4.517283	1.896014	-0.305699
C	3.794341	3.113997	-0.106642
C	2.504189	2.782008	0.346431
B	1.171349	3.571705	0.531807
N	1.084598	4.967663	0.933521
H	1.938710	5.467920	1.144414
B	-0.165641	5.623940	1.128539
H	-0.207425	6.788161	1.487977
N	-1.366645	4.885930	0.913865
H	-2.254838	5.330678	1.106666
B	-1.353341	3.488084	0.509841
C	-2.626673	2.612077	0.295642
C	-3.921386	2.867991	-0.192032
C	-4.556835	1.608433	-0.437300
C	-3.629578	0.613124	-0.068586
C	5.891639	1.768354	-0.907700
H	6.025356	0.736798	-1.271494
H	5.962580	2.408518	-1.807917
C	7.061861	2.128510	0.024839
H	8.035511	2.022310	-0.487992
H	6.983246	3.167818	0.383932
C	4.280670	4.496980	-0.470846
H	4.060225	5.213162	0.343638
H	5.380830	4.491414	-0.553721
C	3.690973	5.050179	-1.779545

ARTICLE

Journal Name

H	2.596683	5.140995	-1.703504
H	3.906129	4.375002	-2.623545
C	-4.498473	4.232286	-0.472524
H	-3.697992	4.901387	-0.834324
H	-5.230523	4.168712	-1.298500
C	-5.181659	4.901904	0.734666
H	-4.473168	5.028759	1.570062
H	-5.586301	5.898111	0.476503
H	-6.011321	4.285824	1.116942
C	-5.870800	1.391189	-1.139493
H	-5.905787	2.020540	-2.050404
H	-5.905203	0.351031	-1.501437
C	-7.140638	1.677894	-0.319882
H	-7.185635	2.731688	-0.001167
H	-8.053635	1.468424	-0.906752
H	-7.176477	1.060204	0.591514
N	2.467887	1.412661	0.443912
H	1.665282	0.875197	0.842866
N	-0.068433	2.915724	0.278281
N	-2.503498	1.246761	0.372952
H	-1.678014	0.755569	0.783664
H	7.076484	1.480397	0.915007
H	4.101641	6.048080	-2.021896
H	-4.073951	-6.062705	1.853558
H	-1.871362	-5.470159	-1.280210
H	5.645662	-4.149204	0.585623
H	-0.033516	1.977295	-0.138179
H	0.089088	-1.983837	0.034525
Cl	0.054140	0.170265	-1.939299
Cl	0.013715	-0.178799	1.831113
Complex			
3---2Cl ⁻ (B3LYP/SVP)			
Atom	X	Y	Z
C	-3.313732	-0.837762	-0.223626
C	-4.221888	-1.890393	0.059626
C	-3.526691	-3.109131	-0.169290
C	-2.221443	-2.760443	-0.573140
C	-1.001818	-3.535601	-0.721140
N	-1.013117	-4.896746	-0.712258
C	0.200392	-5.444097	-0.714950
H	0.234492	-6.544554	-0.745011
N	1.377067	-4.823883	-0.662142
C	1.283433	-3.465804	-0.673802
C	2.446763	-2.618399	-0.477523
C	3.750208	-2.887944	-0.013154
C	4.361758	-1.629902	0.239284
C	3.408137	-0.632563	-0.091765
C	-5.610884	-1.763222	0.629115
H	-5.742793	-0.741526	1.018904
H	-5.709199	-2.427211	1.508162
C	-6.760985	-2.087107	-0.340851
H	-6.746217	-1.422080	-1.218170
H	-7.744149	-1.976056	0.151371
H	-6.689645	-3.120086	-0.717588
C	-4.034530	-4.501443	0.108274
H	-3.577531	-5.201122	-0.607379
H	-5.126049	-4.538247	-0.052307
C	-3.721609	-4.999702	1.529606
H	-2.633441	-5.047878	1.684601
H	-4.139707	-4.326481	2.296002
C	4.327706	-4.245526	0.298377
H	3.952712	-4.974948	-0.435018
C	3.973866	-4.757530	1.705084

Journal Name			ARTICLE
H	4.439446	−5.740665	1.902313
H	2.884223	−4.871972	1.804898
H	4.310120	−4.057250	2.487306
C	5.712973	−1.426801	0.873185
H	5.809688	−2.094728	1.749228
H	5.765682	−0.404463	1.278856
C	6.924009	−1.670856	−0.044611
H	6.931928	−2.702098	−0.432853
H	7.875076	−1.507352	0.493950
H	6.910150	−0.998185	−0.915995
N	−2.138658	−1.394669	−0.612410
H	−1.307820	−0.859237	−0.991031
N	0.121688	−2.822225	−0.772964
N	2.286330	−1.259915	−0.529330
H	1.441869	−0.776198	−0.945599
C	3.358117	0.827252	0.069289
C	4.257088	1.885295	−0.223944
C	3.559750	3.100451	0.017439
C	2.261388	2.745307	0.435817
C	1.041268	3.515294	0.605880
N	1.049033	4.876919	0.628787
C	−0.164772	5.420743	0.671522
H	−0.200682	6.520038	0.728445
N	−1.342183	4.798937	0.635609
C	−1.244610	3.441820	0.597037
C	−2.407998	2.597356	0.394951
C	−3.703582	2.875747	−0.087810
C	−4.308656	1.621693	−0.376580
C	−3.359237	0.619844	−0.048248
C	5.637738	1.771006	−0.815371
H	5.768589	0.754978	−1.219223
H	5.718373	2.445033	−1.688500
C	6.801385	2.091017	0.139482
H	7.777155	1.992316	−0.369842
H	6.729131	3.119149	0.529158
C	4.057668	4.495839	−0.262617
H	3.611117	5.190261	0.464692
H	5.151703	4.536037	−0.121244
C	3.717505	5.000093	−1.675591
H	2.626578	5.044139	−1.811532
H	4.124872	4.332886	−2.452962
C	−4.292714	4.239546	−0.333395
H	−3.535264	4.880236	−0.813267
H	−5.134059	4.151245	−1.043259
C	−4.771335	4.957220	0.939112
H	−3.914360	5.137234	1.605268
H	−5.228794	5.934863	0.699917
H	−5.516296	4.356605	1.487685
C	−5.630883	1.423001	−1.068498
H	−5.671199	2.068999	−1.966411
H	−5.678641	0.391779	−1.450605
C	−6.880912	1.711088	−0.220178
H	−6.894871	2.755791	0.129774
H	−7.806946	1.538254	−0.797936
H	−6.916338	1.068741	0.673990
N	2.184887	1.379166	0.472213
H	1.358986	0.841019	0.855954
N	−0.079542	2.798432	0.648851
N	−2.245921	1.238474	0.420199
H	−1.402891	0.748873	0.833667
H	6.805291	1.416004	1.009217
H	4.123465	6.013941	−1.847428

ARTICLE

Journal Name

H	–4.135166	–6.010787	1.699596
H	5.426223	–4.214029	0.194036
Cl	–0.003941	–0.289597	2.012944
Cl	0.054580	0.266361	–2.142455
Complex			
4···2Cl [–] (B97D3/Def2–TZVP)			
Atom	X	Y	Z
C	3.399712	–0.844610	0.207032
C	4.270834	–1.912831	–0.099365
C	3.544694	–3.115062	0.090188
C	2.238561	–2.750903	0.497619
C	1.035898	–3.508975	0.675648
C	0.976942	–4.847296	1.083587
C	–0.261470	–5.463158	1.238110
H	–0.306217	–6.496920	1.570937
C	–1.444121	–4.760649	1.027233
H	–2.406911	–5.217878	1.210491
C	–1.388296	–3.422108	0.619563
C	–2.524073	–2.579803	0.389294
C	–3.832423	–2.849065	–0.079402
C	–4.462165	–1.597844	–0.295119
C	–3.533119	–0.594636	0.057392
C	5.661377	–1.794906	–0.649051
H	5.809764	–0.771025	–1.006174
H	5.756668	–2.438397	–1.534138
C	6.772797	–2.159294	0.349320
H	6.727131	–1.524888	1.239736
H	7.762100	–2.036717	–0.106521
H	6.678515	–3.197592	0.684231
C	4.027303	–4.485590	–0.291117
H	3.865828	–5.198681	0.527115
H	5.111477	–4.449245	–0.435599
C	3.370946	–5.015564	–1.577978
H	2.286312	–5.103886	–1.462232
H	3.558866	–4.330295	–2.411130
C	–4.392487	–4.181167	–0.489757
H	–4.319952	–4.905436	0.331354
C	–3.715652	–4.753849	–1.747366
H	–4.169545	–5.708836	–2.036448
H	–2.646654	–4.919287	–1.581349
H	–3.815009	–4.055199	–2.584657
C	–5.814332	–1.382165	–0.906798
H	–5.915158	–2.018794	–1.796190
H	–5.872782	–0.351314	–1.269235
C	–6.992815	–1.664458	0.039774
H	–6.988735	–2.706669	0.375870
H	–7.949335	–1.471051	–0.459464
H	–6.941304	–1.034563	0.933098
N	2.195085	–1.379567	0.563659
H	1.425954	–0.814878	0.972900
N	–0.149539	–2.869490	0.418022
H	–0.105322	–1.977160	–0.130037
N	–2.386922	–1.215225	0.465382
H	–1.598389	–0.707922	0.910331
C	–3.476659	0.845703	–0.060394
C	–4.339636	1.915090	0.264130
C	–3.610246	3.115713	0.078798
C	–2.309288	2.750151	–0.344220
C	–1.107840	3.507721	–0.531043
C	–1.056288	4.850373	–0.926809
H	–1.978171	5.376015	–1.134771
C	0.178497	5.468319	–1.093080
H	0.218048	6.505803	–1.414872

Journal Name			ARTICLE
C	1.365502	4.763760	−0.911296
H	2.321325	5.224405	−1.115060
C	1.318443	3.420370	−0.516908
C	2.456591	2.575341	−0.309107
C	3.768419	2.847298	0.149607
C	4.389219	1.596845	0.401849
C	3.453763	0.593449	0.069326
C	−5.725600	1.799868	0.825160
H	−5.873406	0.776037	1.182001
H	−5.811710	2.441879	1.712191
C	−6.844229	2.168879	−0.163289
H	−7.830223	2.046929	0.299876
H	−6.750436	3.207948	−0.496077
C	−4.085539	4.484224	0.476146
H	−3.931405	5.203620	−0.337945
H	−5.168273	4.448883	0.631384
C	−3.415033	5.002508	1.760429
H	−2.331443	5.089451	1.634609
H	−3.596034	4.310928	2.589880
C	4.365747	4.194911	0.419439
H	3.589402	4.875327	0.791397
H	5.101752	4.103920	1.227582
C	5.052232	4.825177	−0.806459
H	4.351349	4.946723	−1.639518
H	5.466761	5.809603	−0.560048
H	5.866371	4.189864	−1.167486
C	5.710726	1.370059	1.074419
H	5.767006	1.999923	1.973431
H	5.735735	0.336831	1.433902
C	6.951271	1.641386	0.209076
H	7.030782	2.701414	−0.048712
H	7.864932	1.356395	0.743349
H	6.913761	1.075531	−0.727150
N	−2.272994	1.379250	−0.423940
H	−1.508186	0.814944	−0.839780
N	0.081507	2.866755	−0.297288
H	0.043438	1.972170	0.246247
N	2.311263	1.209800	−0.354454
H	1.520621	0.697841	−0.790055
H	−6.806589	1.536904	−1.055845
H	−3.808186	5.987464	2.037696
H	3.768825	−6.001882	−1.843410
Cl	−0.022436	−0.487186	−1.713917
Cl	−0.056676	0.478623	1.836629
H	1.895100	−5.371951	1.310026
H	−5.463548	−4.068104	−0.683928
Complex			4···2Cl [−] (B3LYP/SVP)
Atom	X	Y	Z
C	3.424479	−0.859140	0.169731
C	4.289638	−1.929083	−0.148096
C	3.553648	−3.129707	0.041135
C	2.255249	−2.751758	0.456901
C	1.040649	−3.504508	0.668862
C	0.984100	−4.827782	1.132749
C	−0.256738	−5.435421	1.321091
H	−0.301828	−6.459927	1.698899
C	−1.441025	−4.737987	1.085918
H	−2.409034	−5.188022	1.294558
C	−1.381284	−3.414324	0.623328
C	−2.528978	−2.574151	0.369441
C	−3.832665	−2.855965	−0.101483
C	−4.474123	−1.605081	−0.308077

ARTICLE	Journal Name		
C	-3.549786	-0.600975	0.055008
C	5.692619	-1.825582	-0.686422
H	5.856251	-0.800246	-1.052146
H	5.788316	-2.471996	-1.576464
C	6.802983	-2.194979	0.310920
H	6.777018	-1.548329	1.201396
H	7.797950	-2.093157	-0.152492
H	6.702638	-3.233726	0.663188
C	4.037411	-4.512056	-0.321008
H	3.843148	-5.221178	0.501650
H	5.132873	-4.486806	-0.419157
C	3.437557	-5.064871	-1.624716
H	2.342575	-5.160636	-1.559162
H	3.657726	-4.397411	-2.472450
C	-4.396237	-4.198062	-0.497907
H	-4.277457	-4.928451	0.320293
C	-3.790489	-4.774032	-1.788710
H	-4.260110	-5.736657	-2.049171
H	-2.707171	-4.943232	-1.687469
H	-3.936390	-4.082892	-2.633497
C	-5.843525	-1.401475	-0.901385
H	-5.947837	-2.035931	-1.798962
H	-5.920589	-0.366192	-1.266752
C	-7.016443	-1.696375	0.047986
H	-7.005335	-2.742031	0.393836
H	-7.982339	-1.519718	-0.452991
H	-6.979373	-1.059680	0.945286
N	2.222944	-1.384565	0.533902
H	1.449444	-0.813912	0.939475
N	-0.143846	-2.873242	0.395185
H	-0.100150	-1.986733	-0.183858
N	-2.403820	-1.213310	0.462362
H	-1.605811	-0.702968	0.899376
C	-3.493604	0.856187	-0.044413
C	-4.348796	1.927471	0.295786
C	-3.609840	3.126236	0.107940
C	-2.318967	2.746749	-0.329571
C	-1.105858	3.498352	-0.552810
C	-1.056417	4.827153	-1.003152
H	-1.982940	5.350888	-1.227702
C	0.180690	5.435801	-1.205493
H	0.220519	6.464618	-1.571993
C	1.369033	4.734173	-1.001000
H	2.331183	5.185237	-1.229824
C	1.317111	3.405625	-0.551369
C	2.467707	2.564213	-0.316142
C	3.766575	2.852064	0.165188
C	4.400164	1.602161	0.411526
C	3.477894	0.596166	0.050535
C	-5.745234	1.828275	0.851415
H	-5.910589	0.802118	1.213212
H	-5.825655	2.469447	1.746701
C	-6.865816	2.210905	-0.129367
H	-7.855590	2.111767	0.345648
H	-6.763526	3.251428	-0.475767
C	-4.083272	4.507052	0.489162
H	-3.902728	5.221807	-0.331767
H	-5.176794	4.483727	0.607094
C	-3.458466	5.048986	1.785699
H	-2.364629	5.142629	1.701104
H	-3.664875	4.375881	2.632420
C	4.339069	4.210371	0.472783

H	3.534238	4.878120	0.824075
H	5.036929	4.118188	1.321751
C	5.077381	4.885551	-0.696800
H	4.417750	5.037953	-1.566146
H	5.472883	5.869541	-0.396216
H	5.922079	4.273157	-1.045655
C	5.725244	1.388482	1.095441
H	5.765993	2.024804	1.997905
H	5.757840	0.353628	1.469059
C	6.979868	1.660775	0.251240
H	7.044743	2.716369	-0.052573
H	7.892626	1.424520	0.822127
H	6.990274	1.054363	-0.667806
N	-2.294842	1.380162	-0.421090
H	-1.526925	0.810423	-0.836770
N	0.082272	2.863831	-0.305673
H	0.045331	1.974294	0.268398
N	2.339574	1.202260	-0.386295
H	1.543205	0.686858	-0.820490
H	-6.854756	1.570586	-1.024822
H	-3.864430	6.043609	2.032544
H	3.850195	-6.060250	-1.857040
Cl	-0.031757	-0.491476	-1.698487
Cl	-0.039715	0.482581	1.790351
H	1.906885	-5.348726	1.378531
H	-5.483715	-4.098470	-0.631021
Complex	5...2Cl ⁻ (B3LYP/SVP)		
Atom	X	Y	Z
C	-3.395143	-0.978552	-0.139745
C	-4.224969	-2.063011	0.221751
C	-3.448558	-3.244196	0.083834
C	-2.162137	-2.839579	-0.345336
C	-0.922869	-3.558394	-0.517627
C	-0.828853	-4.901679	-0.905653
C	0.437412	-5.458870	-1.050024
C	1.606400	-4.729556	-0.859342
H	2.574108	-5.185683	-1.051852
C	1.495717	-3.387367	-0.472098
C	2.614047	-2.501145	-0.256942
C	3.926128	-2.720333	0.225122
C	4.523730	-1.441734	0.383964
C	3.565836	-0.484599	-0.018521
C	-5.631644	-1.983464	0.754760
H	-5.829821	-0.948992	1.074683
H	-5.706371	-2.592743	1.672444
C	-6.727809	-2.433037	-0.225205
H	-6.720108	-1.827783	-1.144569
H	-7.726093	-2.340434	0.232727
H	-6.595350	-3.483426	-0.528754
C	-3.885752	-4.626314	0.501321
H	-3.653231	-5.363132	-0.286110
H	-4.982705	-4.638630	0.583251
C	-3.284444	-5.096593	1.836371
H	-2.185622	-5.150327	1.790165
H	-3.544410	-4.402256	2.650511
C	4.534602	-4.026736	0.670950
H	4.436711	-4.791600	-0.117923
C	3.953134	-4.570954	1.986544
H	4.452869	-5.508459	2.279877
H	2.874922	-4.776575	1.899248
H	4.082771	-3.844327	2.803686
C	5.883719	-1.168062	0.970765

ARTICLE				Journal Name
H	6.005698	−1.761357	1.893813	
H	5.924502	−0.116628	1.293292	
C	7.069145	−1.461804	0.036676	
H	7.095805	−2.520755	−0.264838	
H	8.026315	−1.230708	0.531955	
H	7.013267	−0.864891	−0.886538	
N	−2.175614	−1.476231	−0.480653	
H	−1.421258	−0.896651	−0.910394	
N	0.239923	−2.872497	−0.278088	
H	0.166218	−1.964249	0.264042	
N	2.442376	−1.149702	−0.402832	
H	1.630143	−0.683088	−0.862135	
C	3.459922	0.972549	0.021830	
C	4.279982	2.056641	−0.362817	
C	3.500735	3.235998	−0.227675	
C	2.221721	2.831549	0.223373	
C	0.983898	3.550065	0.405644	
C	0.896370	4.898579	0.778675	
H	1.785948	5.488181	0.984684	
C	−0.366698	5.457072	0.936760	
C	−1.539134	4.724515	0.777736	
H	−2.500597	5.182192	0.992819	
C	−1.435684	3.377804	0.404214	
C	−2.556910	2.490971	0.208532	
C	−3.864115	2.715563	−0.285252	
C	−4.454070	1.436598	−0.481425	
C	−3.498454	0.477668	−0.079813	
C	5.680076	1.979686	−0.912844	
H	5.879254	0.944515	−1.228903	
H	5.740567	2.583303	−1.835239	
C	6.785965	2.440753	0.050700	
H	7.779301	2.347963	−0.417871	
H	6.653149	3.493045	0.347440	
C	3.927700	4.614626	−0.666813	
H	3.704824	5.359679	0.115601	
H	5.023297	4.628986	−0.764794	
C	3.305846	5.068130	−1.998247	
H	2.207664	5.119352	−1.936988	
H	3.556075	4.365230	−2.808067	
C	−4.481146	4.040242	−0.647850	
H	−3.701307	4.714592	−1.040450	
H	−5.184979	3.886984	−1.482624	
C	−5.226407	4.746938	0.498472	
H	−4.562926	4.958994	1.352235	
H	−5.653039	5.704188	0.157499	
H	−6.049327	4.127601	0.885181	
C	−5.772185	1.150635	−1.152194	
H	−5.833987	1.743460	−2.082515	
H	−5.773023	0.099201	−1.477572	
C	−7.032525	1.422883	−0.316578	
H	−7.128201	2.488692	−0.060339	
H	−7.938924	1.134015	−0.873042	
H	−7.022377	0.858445	0.628759	
N	2.243080	1.469831	0.374473	
H	1.494056	0.892068	0.814198	
N	−0.182165	2.861612	0.193093	
H	−0.114777	1.950104	−0.343589	
N	−2.382439	1.137802	0.333532	
H	−1.571637	0.666275	0.790596	
H	6.790793	1.843054	0.975079	
H	3.674825	6.066205	−2.285270	
H	−3.660140	−6.096808	2.106750	

Cl	0.038426	-0.422311	1.718574
Cl	0.028036	0.411393	-1.803967
H	-1.714836	-5.489017	-1.132845
H	5.618724	-3.886435	0.794038
F	0.534500	-6.728443	-1.437923
F	-0.458747	6.731511	1.309889
Complex			
6---2Cl- (B3LYP/SVP)			
Atom	X	Y	Z
C	-0.361150	3.523910	-0.099507
C	-1.261572	4.538275	0.302819
C	-2.565790	3.985395	0.237121
C	-2.419870	2.641677	-0.191619
C	-3.354663	1.552145	-0.300151
C	-4.721168	1.701898	-0.587580
C	-5.497366	0.554058	-0.684276
C	-4.984327	-0.728597	-0.539441
H	-5.625107	-1.593174	-0.681551
C	-3.616098	-0.863448	-0.253193
C	-2.935064	-2.122748	-0.101355
C	-3.362210	-3.386610	0.378417
C	-2.206771	-4.204229	0.464455
C	-1.112568	-3.423234	0.023032
C	-0.906966	5.912221	0.808550
H	0.161300	5.927281	1.072573
H	-1.444364	6.098121	1.754678
C	-1.209471	7.063735	-0.164442
H	-0.667632	6.943108	-1.114926
H	-0.916085	8.032149	0.271994
H	-2.281813	7.118367	-0.408813
C	-3.824091	4.665384	0.715579
H	-4.631465	4.557585	-0.027846
H	-3.637904	5.747761	0.773976
C	-4.318774	4.173936	2.086440
H	-4.566711	3.101217	2.069366
H	-3.547333	4.319547	2.858571
C	-4.733377	-3.761966	0.882050
H	-5.504087	-3.514132	0.133166
C	-5.102388	-3.121246	2.230657
H	-6.099674	-3.452299	2.561835
H	-5.116499	-2.021930	2.169084
H	-4.374178	-3.396362	3.009456
C	-2.155022	-5.603197	1.020344
H	-2.714953	-5.634353	1.971097
H	-1.114476	-5.840057	1.287939
C	-2.704973	-6.695626	0.088449
H	-3.765797	-6.526847	-0.153978
H	-2.623182	-7.688948	0.558590
H	-2.157253	-6.726776	-0.865871
N	-1.084512	2.410552	-0.395275
H	-0.673716	1.566456	-0.851636
N	-2.875652	0.281686	-0.103191
H	-1.933631	0.188288	0.377676
N	-1.583217	-2.191997	-0.314765
H	-1.004986	-1.471984	-0.800388
C	0.338808	-3.578943	-0.012736
C	1.240200	-4.583543	-0.437472
C	2.542678	-4.027164	-0.373385
C	2.395886	-2.690640	0.077346
C	3.330356	-1.602245	0.197066
C	4.699537	-1.759266	0.470032
H	5.141042	-2.738368	0.626863
C	5.477633	-0.615124	0.581286

ARTICLE

Journal Name

C	4.964350	0.671436	0.469305
H	5.607170	1.530116	0.632483
C	3.594210	0.814263	0.195683
C	2.914245	2.076126	0.062480
C	3.344964	3.334269	-0.429747
C	2.185431	4.143651	-0.556621
C	1.089818	3.365286	-0.115932
C	0.889617	-5.952059	-0.959920
H	-0.178882	-5.968505	-1.221600
H	1.425162	-6.123585	-1.909729
C	1.199905	-7.114289	-0.002224
H	0.907432	-8.078386	-0.448757
H	2.273531	-7.168408	0.236594
C	3.798892	-4.696497	-0.871993
H	4.611055	-4.600946	-0.132146
H	3.613817	-5.777937	-0.948144
C	4.283721	-4.180539	-2.237364
H	4.530515	-3.107977	-2.203521
H	3.507175	-4.313691	-3.006605
C	4.740615	3.717315	-0.844262
H	5.247025	2.844840	-1.290290
H	4.677282	4.464083	-1.652650
C	5.617717	4.287004	0.285107
H	5.744890	3.569431	1.111147
H	6.620258	4.545147	-0.091565
H	5.172929	5.194571	0.719556
C	2.109754	5.503846	-1.199467
H	2.655698	5.472688	-2.159307
H	1.061419	5.701650	-1.468765
C	2.651034	6.677535	-0.368640
H	3.728536	6.573767	-0.172080
H	2.502227	7.631056	-0.900494
H	2.145890	6.752450	0.606845
N	1.061342	-2.467909	0.295671
H	0.651531	-1.629520	0.761932
N	2.851716	-0.328223	0.027187
H	1.908381	-0.227849	-0.448780
N	1.558631	2.142510	0.252966
H	0.975546	1.425005	0.736587
H	0.662379	-7.006533	0.952332
H	5.185517	-4.723057	-2.563377
H	-5.222091	4.723004	2.396927
Cl	-0.324523	0.031042	1.735261
Cl	0.299359	-0.087459	-1.812877
H	-5.162733	2.677311	-0.766104
H	-4.782519	-4.855837	0.984978
N	6.926348	-0.773386	0.888669
O	7.587677	0.243741	0.995010
O	7.350536	-1.908996	1.005465
N	-6.943421	0.704216	-1.007736
O	-7.368467	1.836950	-1.147020
O	-7.601704	-0.315882	-1.103691
Complex			
7...2Cl ⁻ (B3LYP/SVP)			
Atom	X	Y	Z
C	3.467140	-0.722980	0.019730
C	4.395130	-1.734320	-0.276280
C	3.716210	-2.961580	-0.194110
C	2.376440	-2.694800	0.141890
C	1.208750	-3.533910	0.210210
C	1.217310	-4.919700	0.422630
C	0.000000	-5.599890	0.501180
H	-0.000010	-6.680120	0.664930

C	-1.217310	-4.919690	0.422640
C	-1.208760	-3.533900	0.210220
C	-2.376440	-2.694800	0.141910
C	-3.716220	-2.961570	-0.194070
C	-4.395140	-1.734310	-0.276240
C	-3.467150	-0.722970	0.019730
N	2.278350	-1.334960	0.284430
H	1.480780	-0.834430	0.746670
N	0.000000	-2.914070	0.047860
N	-2.278350	-1.334960	0.284430
H	-1.480780	-0.834420	0.746650
C	-3.467140	0.722980	-0.019740
C	-4.395130	1.734320	0.276260
C	-3.716210	2.961580	0.194060
C	-2.376440	2.694800	-0.141920
C	-1.208750	3.533900	-0.210240
C	-1.217300	4.919690	-0.422660
C	0.000010	5.599880	-0.501200
H	0.000010	6.680120	-0.664960
C	1.217320	4.919690	-0.422650
C	1.208760	3.533900	-0.210230
C	2.376440	2.694800	-0.141900
C	3.716220	2.961570	0.194110
C	4.395130	1.734310	0.276290
C	3.467140	0.722970	-0.019720
N	-2.278350	1.334960	-0.284450
H	-1.480780	0.834430	-0.746680
N	0.000010	2.914070	-0.047880
N	2.278350	1.334950	-0.284410
H	1.480770	0.834430	-0.746650
H	0.000000	1.957030	0.396040
H	0.000000	-1.957040	-0.396060
Cl	0.000010	-0.260480	-1.760080
Cl	0.000000	0.260500	1.760080
H	2.170290	5.434520	-0.537840
H	-2.170270	5.434520	-0.537860
H	-2.170280	-5.434530	0.537830
H	2.170270	-5.434530	0.537810
F	-4.226260	4.160390	0.458760
F	-5.661440	1.561350	0.630450
F	-5.661460	-1.561330	-0.630390
F	-4.226270	-4.160380	-0.458770
F	4.226260	-4.160390	-0.458820
F	5.661450	-1.561340	-0.630430
F	5.661440	1.561330	0.630470
F	4.226260	4.160380	0.458830
Complex	8...2Cl⁻ (B3LYP/SVP)		
Atom	X	Y	Z
C	-3.435385	-0.727450	-0.031296
C	-4.320545	-1.739698	0.343723
C	-3.668026	-2.975539	0.119700
C	-2.385045	-2.689820	-0.372000
C	-1.202386	-3.499673	-0.650195
C	-1.214168	-4.771936	-1.229634
C	0.000012	-5.406954	-1.494256
H	0.000029	-6.398437	-1.952635
C	1.214167	-4.771900	-1.229635
C	1.202324	-3.499626	-0.650223
C	2.384970	-2.689768	-0.372061
C	3.667988	-2.975557	0.119452
C	4.320559	-1.739761	0.343541
C	3.435384	-0.727457	-0.031330

ARTICLE		Journal Name	
N	-5.665031	-1.532821	0.841810
O	-5.882134	-0.466900	1.398368
O	-6.467328	-2.426540	0.658591
N	-4.152311	-4.285394	0.530120
O	-4.677503	-4.364054	1.619975
O	-3.971434	-5.215310	-0.246389
N	4.152269	-4.285494	0.529613
O	4.677740	-4.364308	1.619324
N	5.665063	-1.532997	0.841629
O	6.467256	-2.426800	0.658419
O	5.882268	-0.467081	1.398144
N	-2.294796	-1.327744	-0.460366
H	-1.499395	-0.790788	-0.892681
N	-0.000037	-2.930870	-0.345920
N	2.294745	-1.327687	-0.460347
H	1.499350	-0.790705	-0.892636
C	3.435396	0.727256	0.031156
C	4.320785	1.739602	-0.343231
C	3.668150	2.975373	-0.119293
C	2.384980	2.689590	0.371770
C	1.202345	3.499531	0.649558
C	1.214166	4.772085	1.228373
C	-0.000003	5.407295	1.492579
H	-0.000001	6.399024	1.950425
C	-1.214180	4.772130	1.228285
C	-1.202361	3.499572	0.649484
C	-2.384990	2.689631	0.371643
C	-3.668124	2.975376	-0.119544
C	-4.320714	1.739587	-0.343479
C	-3.435378	0.727272	0.031100
N	5.665337	1.533078	-0.841058
O	5.883269	0.466624	-1.396266
O	6.466933	2.427698	-0.659046
N	4.152525	4.285453	-0.529104
O	4.676414	4.364890	-1.619512
O	3.972966	5.214639	0.248557
N	-4.152494	4.285413	-0.529469
O	-4.676527	4.364732	-1.619823
O	-3.972752	5.214715	0.248017
N	-5.665255	1.532976	-0.841335
O	-6.466928	2.427528	-0.659312
O	-5.883129	0.466480	-1.396500
N	2.294668	1.327467	0.459848
H	1.499210	0.790463	0.892058
N	-0.000009	2.930663	0.345419
N	-2.294682	1.327519	0.459839
H	-1.499234	0.790538	0.892093
O	3.971106	-5.215283	-0.246979
H	-0.000017	2.060134	-0.261916
H	-0.000047	-2.060434	0.261516
Cl	-0.000038	-0.454222	1.686484
Cl	-0.000029	0.454192	-1.686947
H	-2.171359	5.229422	1.469066
H	2.171345	5.229344	1.469228
H	2.171353	-5.229069	-1.470528
H	-2.171330	-5.229142	-1.470529
Complex		9---2Cl ⁻ (B3LYP/SVP)	
Atom	X	Y	Z
C	-3.477531	-0.818119	-0.211280
C	-4.366203	-1.899365	0.030484
C	-3.626190	-3.093328	-0.149709
C	-2.301671	-2.708447	-0.478248

Journal Name	ARTICLE		
C	-1.084095	-3.452096	-0.571226
N	-1.048614	-4.766852	-0.830220
C	0.162335	-5.321157	-0.878624
H	0.192882	-6.406020	-1.038278
N	1.340553	-4.707031	-0.779164
C	1.300154	-3.392088	-0.520339
C	2.475817	-2.591395	-0.377348
C	3.803319	-2.916580	0.000103
C	4.481352	-1.691078	0.207706
C	3.554559	-0.649519	-0.066063
C	-5.801989	-1.818019	0.479479
H	-5.994707	-0.814180	0.886490
H	-5.953761	-2.511029	1.324543
C	-6.839171	-2.137999	-0.609987
H	-6.746794	-1.457458	-1.470329
H	-7.863383	-2.046763	-0.213694
H	-6.719077	-3.162455	-0.994793
C	-4.105026	-4.495331	0.116931
H	-3.621631	-5.180524	-0.593983
H	-5.188128	-4.549013	-0.072676
C	-3.818503	-4.978037	1.549310
H	-2.736592	-4.995429	1.751817
H	-4.287453	-4.321892	2.299702
C	4.336511	-4.295482	0.283723
H	3.915912	-5.000269	-0.447601
C	4.013966	-4.796277	1.702133
H	4.441344	-5.798379	1.867589
H	2.926587	-4.864706	1.859476
H	4.420389	-4.121686	2.472395
C	5.897198	-1.551916	0.702286
H	6.053639	-2.248807	1.543162
H	6.033813	-0.546622	1.126770
C	6.978420	-1.813003	-0.359809
H	6.913139	-2.836724	-0.759547
H	7.986143	-1.682875	0.066798
H	6.880684	-1.126452	-1.214785
N	-2.261619	-1.337415	-0.524871
H	-1.480929	-0.775103	-0.930467
N	0.087551	-2.775678	-0.342814
N	2.376001	-1.223463	-0.425329
H	1.586797	-0.697244	-0.861297
C	3.517149	0.807564	0.072967
C	4.401332	1.892379	-0.172340
C	3.658778	3.083897	0.010805
C	2.336800	2.695572	0.345054
C	1.118998	3.437615	0.443535
N	1.084573	4.753642	0.699105
C	-0.125521	5.307690	0.753582
H	-0.155856	6.393722	0.904950
N	-1.304596	4.691231	0.671570
C	-1.265256	3.375636	0.415684
C	-2.441621	2.575735	0.285242
C	-3.764089	2.904729	-0.109734
C	-4.436284	1.679614	-0.343988
C	-3.512463	0.637638	-0.064276
C	5.836892	1.820565	-0.622758
H	6.033606	0.822526	-1.040644
H	5.985953	2.523202	-1.460207
C	6.872571	2.132944	0.470364
H	7.897350	2.049206	0.073811
H	6.748558	3.153087	0.865339
C	4.133890	4.486959	-0.256825

ARTICLE

Journal Name

H	3.652774	5.170683	0.456975
H	5.217789	4.542239	-0.072259
C	3.839754	4.970530	-1.687366
H	2.756878	4.986359	-1.884697
H	4.306225	4.315871	-2.440601
C	-4.312327	4.288966	-0.317983
H	-3.549588	4.908680	-0.815908
H	-5.172522	4.234652	-1.004527
C	-4.732580	4.995763	0.981742
H	-3.862877	5.131341	1.640831
H	-5.152602	5.990652	0.761974
H	-5.493996	4.419084	1.530189
C	-5.826236	1.531152	-0.903662
H	-5.930014	2.196900	-1.778351
H	-5.944230	0.511810	-1.298688
C	-6.965263	1.836241	0.081818
H	-6.928166	2.879614	0.430005
H	-7.946610	1.677365	-0.393646
H	-6.912741	1.192975	0.974227
N	2.301204	1.324304	0.392732
H	1.523304	0.761311	0.801862
N	-0.053684	2.760935	0.223703
N	-2.340622	1.207547	0.319581
H	-1.552515	0.677926	0.753698
H	6.781870	1.443606	1.323878
H	4.224155	5.991957	-1.839517
H	-4.205283	-5.998684	1.700669
H	5.427882	-4.297033	0.139348
H	-0.021988	1.850468	-0.322204
H	0.052645	-1.865144	0.203058
Cl	-0.002396	-0.429636	1.701121
Cl	0.042940	0.414166	-1.820487
Complex			
10 ⁻² Cl ⁻ (B3LYP/SVP)			
Atom	X	Y	Z
C	-3.464256	0.722815	0.029338
C	-4.398349	1.743704	-0.229235
C	-3.722295	2.970369	-0.134375
C	-2.371836	2.690267	0.172138
C	-1.188457	3.493387	0.195747
N	-1.195618	4.814473	0.379868
C	-0.000002	5.407649	0.400548
H	-0.000002	6.501710	0.471668
N	1.195615	4.814474	0.379866
C	1.188455	3.493389	0.195743
C	2.371835	2.690269	0.172133
C	3.722293	2.970372	-0.134380
C	4.398346	1.743706	-0.229246
C	3.464255	0.722817	0.029334
F	-5.667019	1.575182	-0.566816
F	-4.241111	4.155614	-0.382757
F	4.241109	4.155616	-0.382763
F	5.667015	1.575185	-0.566833
N	-2.271857	1.323906	0.281862
H	-1.478907	0.822949	0.754672
N	-0.000001	2.837718	-0.002654
N	2.271854	1.323907	0.281850
H	1.478902	0.822950	0.754655
C	3.464256	-0.722815	-0.029338
C	4.398348	-1.743702	0.229241
C	3.722294	-2.970369	0.134380
C	2.371836	-2.690267	-0.172135
C	1.188457	-3.493388	-0.195743

N	1.195618	-4.814474	-0.379857
C	0.000002	-5.407650	-0.400538
H	0.000002	-6.501712	-0.471645
N	-1.195615	-4.814474	-0.379860
C	-1.188455	-3.493387	-0.195749
C	-2.371835	-2.690268	-0.172142
C	-3.722292	-2.970370	0.134379
C	-4.398349	-1.743705	0.229229
C	-3.464256	-0.722816	-0.029342
F	5.667017	-1.575180	0.566827
F	4.241110	-4.155612	0.382768
F	-4.241106	-4.155614	0.382768
F	-5.667020	-1.575185	0.566807
N	2.271853	-1.323906	-0.281845
H	1.478898	-0.822948	-0.754643
N	0.000001	-2.837716	0.002648
N	-2.271856	-1.323907	-0.281862
H	-1.478907	-0.822949	-0.754671
H	0.000000	-1.888501	0.475445
H	-0.000003	1.888508	-0.475460
Cl	0.000004	0.228370	-1.779958
Cl	0.000004	-0.228377	1.779955
Complex	11...2Cl ⁻ (B3LYP/SVP)		
Atom	X	Y	Z
C	3.479970	0.725436	-0.070040
C	4.361044	1.782293	0.236489
C	3.673916	2.988178	-0.004192
C	2.379427	2.653619	-0.420923
C	1.180137	3.440187	-0.569699
N	1.191968	4.722993	-0.908842
C	-0.000221	5.319598	-1.003038
H	-0.000230	6.396781	-1.202916
N	-1.192412	4.722964	-0.908921
C	-1.180549	3.440158	-0.569811
C	-2.379792	2.653504	-0.421129
C	-3.674273	2.987901	-0.004261
C	-4.361254	1.781938	0.236445
C	-3.480063	0.725187	-0.070093
N	5.642570	1.652694	0.897888
O	5.956662	0.538201	1.280998
O	6.285134	2.676269	1.047149
N	4.151864	4.358882	0.208500
O	3.686923	4.943207	1.167702
O	4.936861	4.785763	-0.607827
N	-4.152361	4.358543	0.208559
O	-3.687403	4.942869	1.167750
N	-5.642764	1.652245	0.897863
O	-6.285784	2.675627	1.046363
O	-5.956456	0.537856	1.281602
N	2.315047	1.283958	-0.471366
H	1.525931	0.732533	-0.896505
N	-0.000205	2.801775	-0.312642
N	-2.315255	1.283840	-0.471567
H	-1.526180	0.732514	-0.896854
C	-3.479983	-0.725414	0.070160
C	-4.361064	-1.782242	-0.236418
C	-3.673932	-2.988141	0.004189
C	-2.379485	-2.653604	0.421066
C	-1.180185	-3.440182	0.569804
N	-1.192023	-4.723006	0.908878
C	0.000178	-5.319605	1.003001
H	0.000194	-6.396773	1.202960

ARTICLE

Journal Name

N	1.192361	-4.722965	0.908862
C	1.180492	-3.440144	0.569771
C	2.379743	-2.653499	0.421026
C	3.674275	-2.987912	0.004331
C	4.361212	-1.781942	-0.236535
C	3.480069	-0.725185	0.070121
N	-5.642599	-1.652636	-0.897811
O	-5.956471	-0.538218	-1.281339
O	-6.285496	-2.676069	-1.046444
N	-4.151866	-4.358825	-0.208688
O	-3.686853	-4.943061	-1.167915
O	-4.936868	-4.785826	0.607555
N	4.152429	-4.358530	-0.208530
O	3.687068	-4.943066	-1.167384
O	4.937957	-4.785188	0.607403
N	5.642709	-1.652243	-0.898018
O	6.285558	-2.675681	-1.046855
O	5.956613	-0.537819	-1.281424
N	-2.315101	-1.283950	0.471594
H	-1.526035	-0.732535	0.896875
N	0.000133	-2.801754	0.312718
N	2.315222	-1.283845	0.471486
H	1.526103	-0.732538	0.896770
O	-4.937363	4.785430	-0.607739
H	0.000101	-1.903725	-0.267678
H	-0.000272	1.903808	0.267760
Cl	0.000096	0.438601	1.700313
Cl	0.000123	-0.438847	-1.700225
Complex			
Atom			
12--2Cl⁻ (B3LYP/SVP)			
	X	Y	Z
C	0.725828	3.297236	0.138597
N	1.762426	4.100868	-0.283425
N	2.888452	3.486386	-0.102017
N	2.603398	2.262472	0.455967
C	3.478455	1.148805	0.395534
C	4.819440	1.220790	-0.008224
C	5.482063	-0.000664	-0.183076
H	6.527353	-0.000865	-0.507149
C	4.818992	-1.221868	-0.008121
H	5.285186	-2.184071	-0.218353
C	3.478027	-1.149398	0.395615
N	2.602571	-2.262794	0.456040
N	2.887519	-3.486996	-0.101319
N	1.761404	-4.101308	-0.282808
C	0.724854	-3.297303	0.138615
C	1.264527	2.126769	0.631520
H	0.760097	1.254960	1.067225
N	2.878581	-0.000176	0.648948
C	1.263647	-2.126674	0.631054
H	0.759274	-1.254572	1.066231
C	-0.725871	-3.297285	-0.138808
N	-1.762505	-4.100718	0.283535
N	-2.888578	-3.486673	0.100987
N	-2.603350	-2.262477	-0.456266
C	-3.478393	-1.148797	-0.395501
C	-4.819291	-1.220854	0.008509
H	-5.285750	-2.182906	0.218833
C	-5.481903	0.000575	0.183637
H	-6.527129	0.000721	0.507914
C	-4.818881	1.221804	0.008667
H	-5.285015	2.183997	0.219079
C	-3.478016	1.149380	-0.395395

N	-2.602621	2.262830	-0.456005
N	-2.887531	3.486986	0.101465
N	-1.761407	4.101321	0.282779
C	-0.724916	3.297297	-0.138726
C	-1.264474	-2.126818	-0.631813
H	-0.759941	-1.255020	-1.067458
N	-2.878589	0.000207	-0.648977
C	-1.263743	2.126776	-0.631390
H	-0.759369	1.254742	-1.066739
Cl	0.987450	-0.000306	-2.107803
Cl	-0.987517	0.000428	2.107947
H	5.285979	2.182811	-0.218518
Complex			
13---2Cl⁻ (B3LYP/SVP)			
Atom	X	Y	Z
C	0.725370	-3.298901	-0.140545
N	1.755007	-4.116883	0.249493
N	2.883524	-3.502837	0.053286
N	2.602480	-2.268091	-0.477042
C	3.497235	-1.151551	-0.459694
C	4.868636	-1.235624	-0.164748
C	5.545463	0.000184	-0.022427
C	4.868393	1.235878	-0.164696
C	3.497005	1.151546	-0.459604
N	2.602003	2.267849	-0.476785
N	2.883200	3.503150	0.052131
N	1.754679	4.117202	0.248442
C	0.724964	3.298775	-0.140382
C	1.266510	-2.121468	-0.625485
H	0.762477	-1.244191	-1.053336
N	2.882230	-0.000066	-0.627167
C	1.265988	2.120872	-0.624313
H	0.761984	1.243149	-1.051134
C	-0.725407	3.298904	0.140510
N	-1.755059	4.116833	-0.249560
N	-2.883594	3.502910	-0.053064
N	-2.602507	2.268083	0.477084
C	-3.497283	1.151558	0.459710
C	-4.868677	1.235645	0.164765
C	-5.545516	-0.000161	0.022454
C	-4.868448	-1.235853	0.164679
C	-3.497061	-1.151538	0.459614
N	-2.602062	-2.267860	0.476811
N	-2.883238	-3.503144	-0.052202
N	-1.754709	-4.117163	-0.248553
C	-0.725007	-3.298772	0.140348
C	-1.266517	2.121432	0.625377
H	-0.762534	1.244093	1.053118
N	-2.882287	0.000066	0.627211
C	-1.266046	-2.120936	0.624424
H	-0.762088	-1.243238	1.051317
Cl	0.910839	0.000597	2.159794
Cl	-0.910473	-0.000632	-2.159735
N	5.567404	2.436201	0.117101
H	4.896555	3.207102	0.210938
H	6.236022	2.661310	-0.621972
N	6.900281	0.000320	0.311811
H	7.132108	0.849464	0.829830
H	7.132371	-0.849077	0.829302
N	5.567893	-2.435848	0.117035
H	6.236032	-2.661188	-0.622405
H	4.897081	-3.206720	0.211397
N	-5.567490	-2.436164	-0.117212

ARTICLE

Journal Name

H	–6.235923	–2.661403	0.622001
H	–4.896599	–3.207033	–0.211161
N	–6.900347	–0.000287	–0.311770
H	–7.132366	0.848995	–0.829497
H	–7.132213	–0.849542	–0.829613
N	–5.567934	2.435856	–0.117111
H	–4.897121	3.206706	–0.211704
H	–6.235931	2.661341	0.622422
Complex	14[–]2Cl[–] (B3LYP/SVP)		
Atom	X	Y	Z
C	–0.716986	3.328189	–0.173569
N	–1.755842	4.162665	0.170742
N	–2.885310	3.574379	–0.071059
N	–2.601041	2.334994	–0.591861
C	–3.488449	1.219793	–0.594164
C	–4.836938	1.230775	–0.178121
C	–5.440629	–0.027356	0.013066
C	–4.737479	–1.226277	–0.157516
C	–3.424428	–1.094076	–0.623189
N	–2.537998	–2.205928	–0.647966
N	–2.876993	–3.403242	–0.070633
N	–1.777971	–4.042892	0.203709
C	–0.715716	–3.274535	–0.186167
C	–1.254565	2.166321	–0.684723
H	–0.753829	1.273221	–1.065163
N	–2.880263	0.076667	–0.858720
C	–1.199621	–2.100145	–0.745410
H	–0.642456	–1.249067	–1.170875
C	0.715699	–3.274536	0.185700
N	1.777964	–4.042997	–0.203953
N	2.876986	–3.403361	0.070415
N	2.537988	–2.205966	0.647588
C	3.424474	–1.094179	0.622975
C	4.737656	–1.226403	0.157667
C	5.440876	–0.027483	–0.012687
C	4.837165	1.230656	0.178408
C	3.488564	1.219704	0.594077
N	2.601189	2.334917	0.591725
N	2.885504	3.574402	0.071120
N	1.756052	4.162691	–0.170708
C	0.717156	3.328176	0.173395
C	1.199608	–2.100127	0.744887
H	0.642532	–1.248989	1.170238
N	2.880280	0.076572	0.858380
C	1.254709	2.166257	0.684439
H	0.754074	1.273058	1.064654
Cl	–1.168575	–0.125090	2.015427
Cl	1.167423	–0.124172	–2.015429
O	5.336825	–2.396603	–0.179529
H	4.604199	–3.077328	–0.218601
O	6.730720	–0.050399	–0.475978
H	6.906216	–0.970613	–0.731761
O	5.550814	2.355385	–0.077199
H	6.383789	2.064427	–0.478613
O	–5.550504	2.355492	0.077764
H	–6.383315	2.064502	0.479498
O	–5.336571	–2.396466	0.179860
H	–4.603910	–3.077169	0.218803
O	–6.730334	–0.050277	0.476749
H	–6.905696	–0.970479	0.732677
Complex	15[–]2Cl[–] (B3LYP/SVP)		
Atom	X	Y	Z

C	0.726550	3.277275	0.126017
N	1.747559	4.092025	−0.311062
N	2.883824	3.502448	−0.138880
N	2.620505	2.271991	0.434169
C	3.501670	1.170066	0.397484
C	4.878256	1.224412	0.129758
C	5.547550	−0.000173	0.009830
F	6.860878	−0.000286	−0.240558
C	4.878003	−1.224656	0.129473
F	5.574061	−2.353125	−0.015359
C	3.501440	−1.170114	0.397300
N	2.620010	−2.271813	0.433748
N	2.883432	−3.502789	−0.138085
N	1.747165	−4.092466	−0.310092
C	0.726086	−3.277173	0.125747
C	1.282791	2.116539	0.617371
H	0.788711	1.243775	1.062143
N	2.913164	0.000030	0.555702
C	1.282245	−2.116009	0.616197
H	0.788139	−1.242856	1.060101
C	−0.726578	−3.277249	−0.126113
N	−1.747566	−4.092248	0.310542
N	−2.883785	−3.502286	0.139336
N	−2.620594	−2.271989	−0.434107
C	−3.501767	−1.170078	−0.397519
C	−4.878325	−1.224392	−0.129631
F	−5.574597	−2.352759	0.015011
C	−5.547586	0.000212	−0.009708
F	−6.860883	0.000356	0.240836
C	−4.878039	1.224683	−0.129474
F	−5.574068	2.353165	0.015412
C	−3.501499	1.170112	−0.397406
N	−2.620046	2.271790	−0.433872
N	−2.883436	3.502745	0.138007
N	−1.747195	4.092618	0.309560
C	−0.726101	3.277147	−0.125901
C	−1.282877	−2.116455	−0.617247
H	−0.788862	−1.243605	−1.061873
N	−2.913259	−0.000052	−0.555828
C	−1.282262	2.115905	−0.616153
H	−0.788178	1.242660	−1.059858
Cl	0.977254	−0.000261	−2.080697
Cl	−0.976956	0.000161	2.080659
F	5.574535	2.352802	−0.014675
Complex	16[−]2Cl[−] (B3LYP/SVP)		
Atom	X	Y	Z
C	−0.768953	−3.268285	−0.032394
N	−1.796759	−3.987940	−0.610879
N	−2.922064	−3.420514	−0.369259
N	−2.659846	−2.296708	0.403078
C	−3.519568	−1.189317	0.444102
C	−4.908766	−1.219110	0.218687
C	−5.551620	0.017829	0.055848
C	−4.836284	1.221000	0.098117
C	−3.468670	1.143909	0.433355
N	−2.570967	2.211182	0.535239
N	−2.840202	3.526585	0.194268
N	−1.707352	4.123279	0.062907
C	−0.677792	3.237316	0.305891
C	−1.319397	−2.193543	0.625862
H	−0.823577	−1.388512	1.177189
N	−2.898788	−0.036422	0.607834

ARTICLE	Journal Name		
C	-1.225499	2.017059	0.623393
H	-0.731503	1.086207	0.904672
C	0.768961	3.268269	0.032409
N	1.796780	3.987947	0.610847
N	2.922079	3.420514	0.369219
N	2.659841	2.296692	-0.403096
C	3.519563	1.189303	-0.444122
C	4.908761	1.219104	-0.218716
C	5.551628	-0.017829	-0.055898
C	4.836303	-1.221005	-0.098168
C	3.468683	-1.143924	-0.433386
N	2.570977	-2.211197	-0.535240
N	2.840214	-3.526596	-0.194248
N	1.707363	-4.123297	-0.062906
C	0.677804	-3.237330	-0.305862
C	1.319389	2.193525	-0.625855
H	0.823545	1.388490	-1.177153
N	2.898791	0.036405	-0.607852
C	1.225508	-2.017071	-0.623365
H	0.731495	-1.086232	-0.904659
Cl	-1.149866	0.089047	-1.899765
Cl	1.149818	-0.089058	1.899898
N	5.670814	2.477164	-0.161052
O	6.383283	2.647271	0.812317
O	5.541152	3.236063	-1.100751
N	7.019605	-0.062501	0.100607
O	7.464175	-0.768761	0.986203
O	7.672799	0.595852	-0.689055
N	5.546332	-2.505314	0.117173
O	6.210898	-2.908286	-0.822994
O	5.425440	-3.029154	1.198891
N	-5.670828	-2.477166	0.161035
O	-5.541330	-3.235967	1.100834
O	-6.383188	-2.647345	-0.812402
N	-7.019601	0.062520	-0.100625
O	-7.672795	-0.595649	0.689192
O	-7.464173	0.768684	-0.986299
N	-5.546294	2.505318	-0.117220
O	-5.425399	3.029154	-1.198941
O	-6.210876	2.908282	0.822942

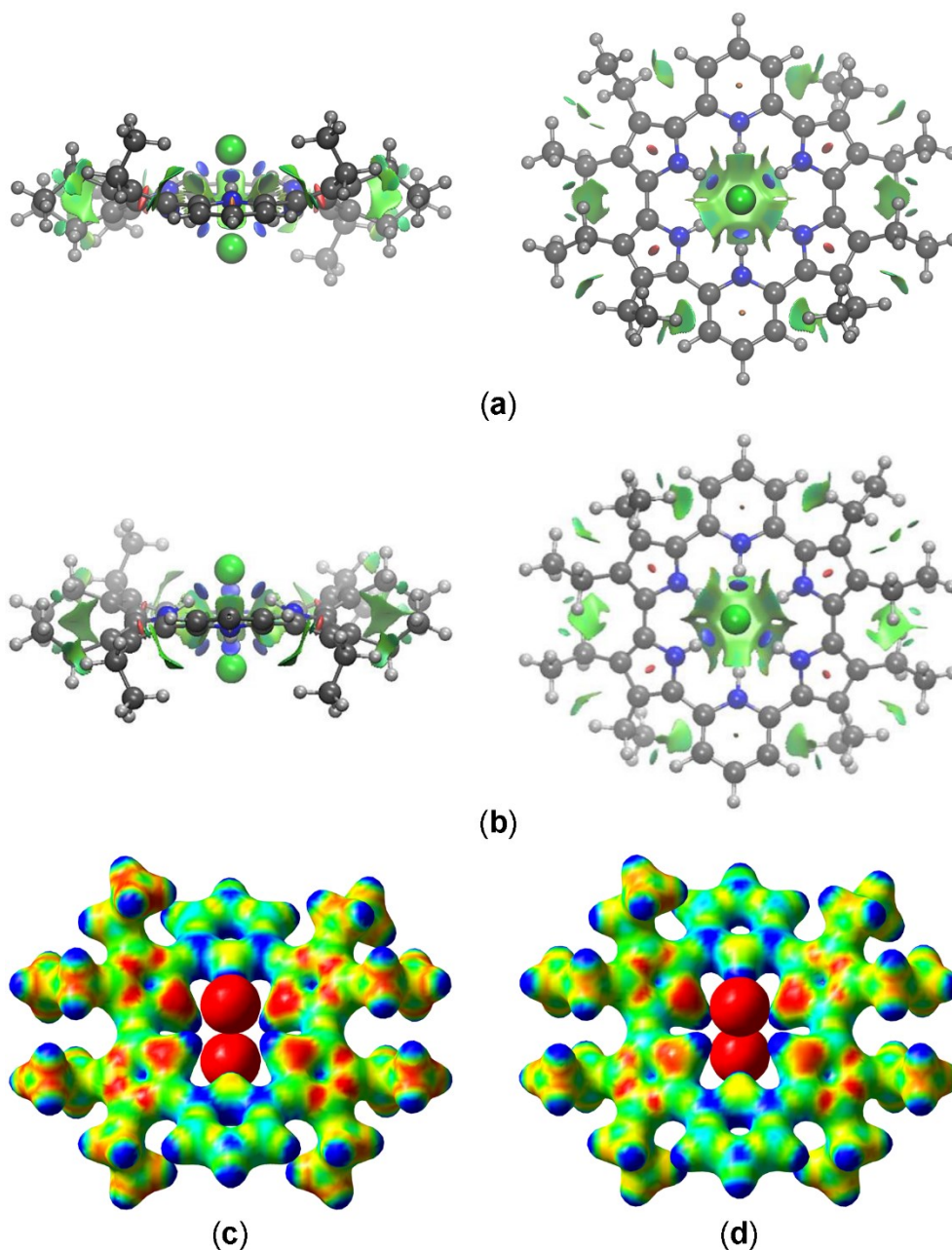


Figure S1. Front (left) and top (right) views of the NCI topology for the system: $4 \cdots 2\text{Cl}^-$ from the: (a) B97D3/Def2-TZVP; and (b) B3LYP/SVP, computational approach. Atoms color: H = silver; C = black; N = blue; and Cl = green. MEP surfaces for the complex $4 \cdots 2\text{Cl}^-$ obtained from the: (c) B97D3/Def2-TZVP; and (d) B3LYP/SVP, computational approach. The isovalue used to represent the MEP surfaces is equal to 0.050 a.u., while that the values of the scale (red – blue a.u.) are: 0.100 – 0.250 a.u.

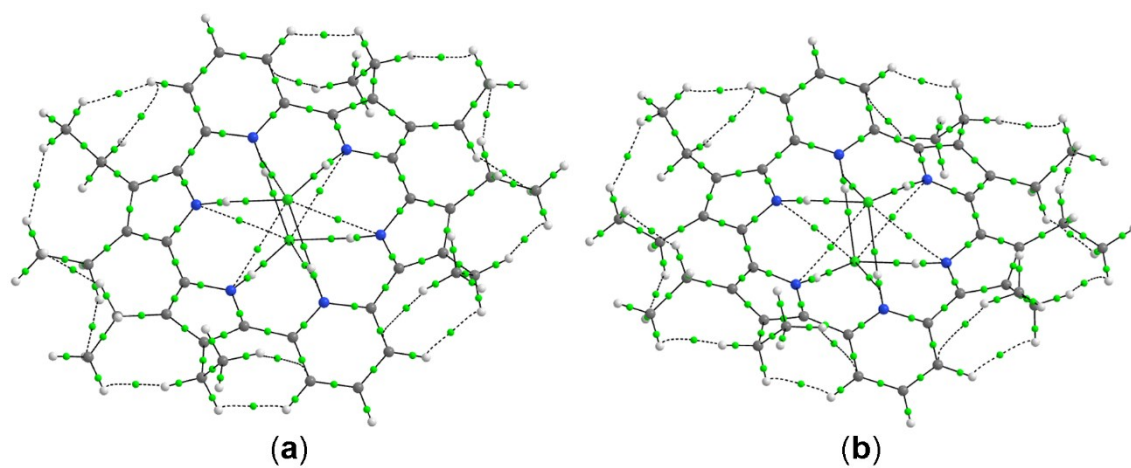


Figure S2. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (light green points) for the structure $4 \cdots 2\text{Cl}^-$ using the: (a) B97D3/Def2-TZVP; and (b) B3LYP/SVP, computational model. Atoms color: H = white; C = gray; N = blue; and Cl = light green.

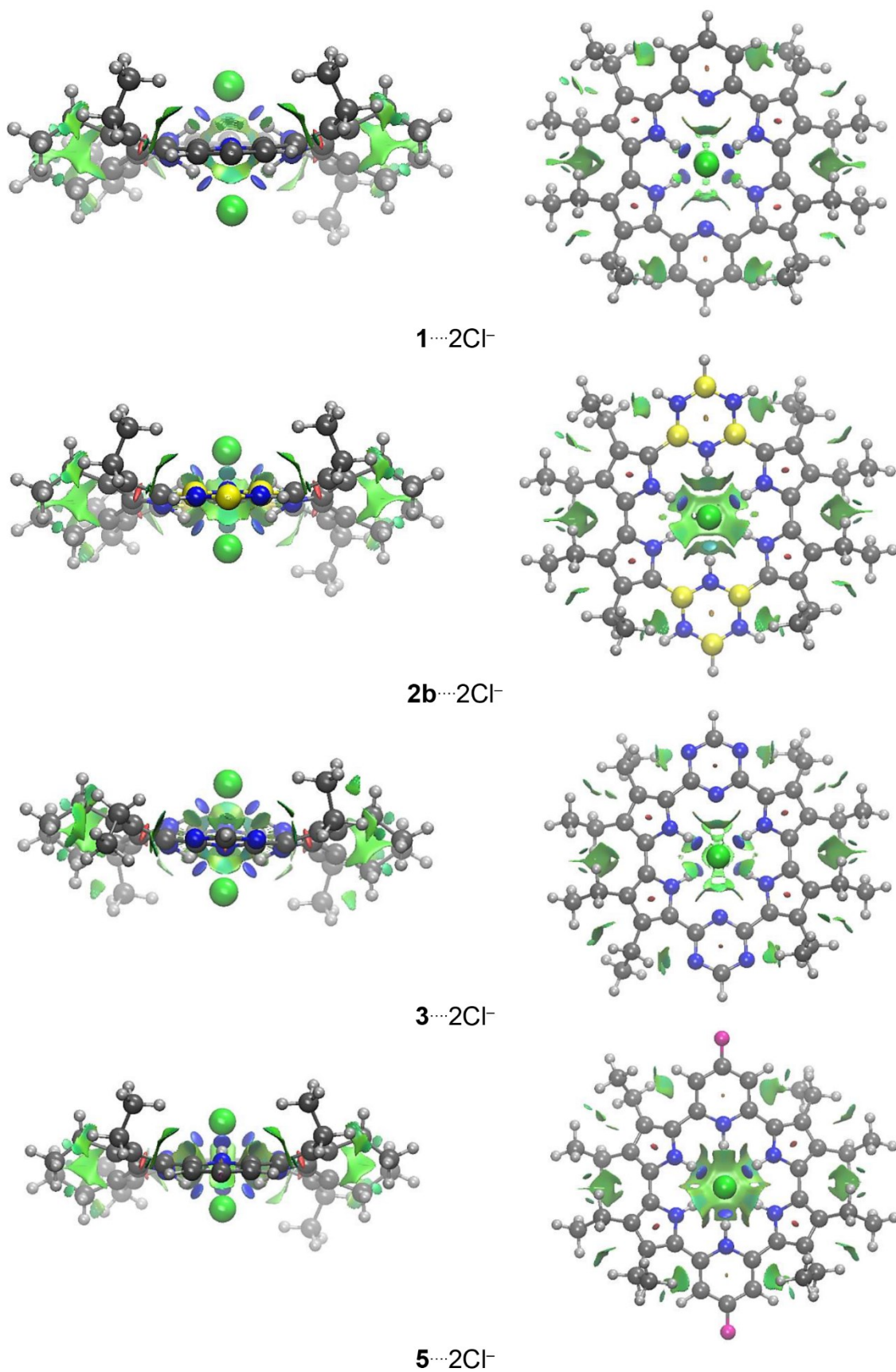


Figure S3. Front (left) and top (right) views of the NCI topology for the systems: (**1**, **2b**, **3** and **5**)... 2Cl^- . Atoms color: H = silver; B = yellow; C = black; N = blue; F = pink; and Cl = green.

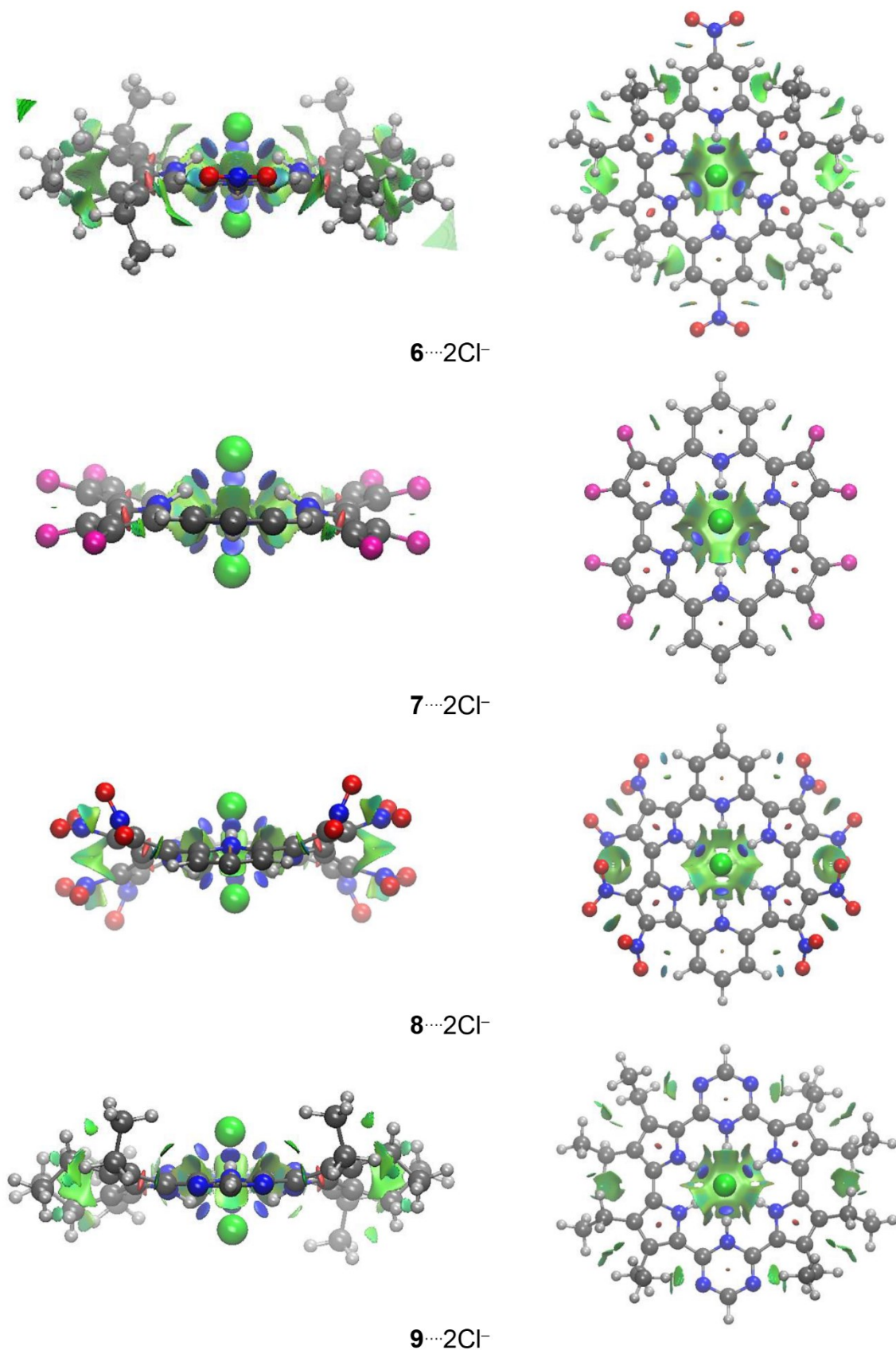


Figure S4. Front (left) and top (right) views of the NCI topology for the systems: (6, 7, 8 and 9) $\cdots 2\text{Cl}^-$. Atoms color: H = silver; C = black; N = blue; O = red; F = pink; and Cl = green.

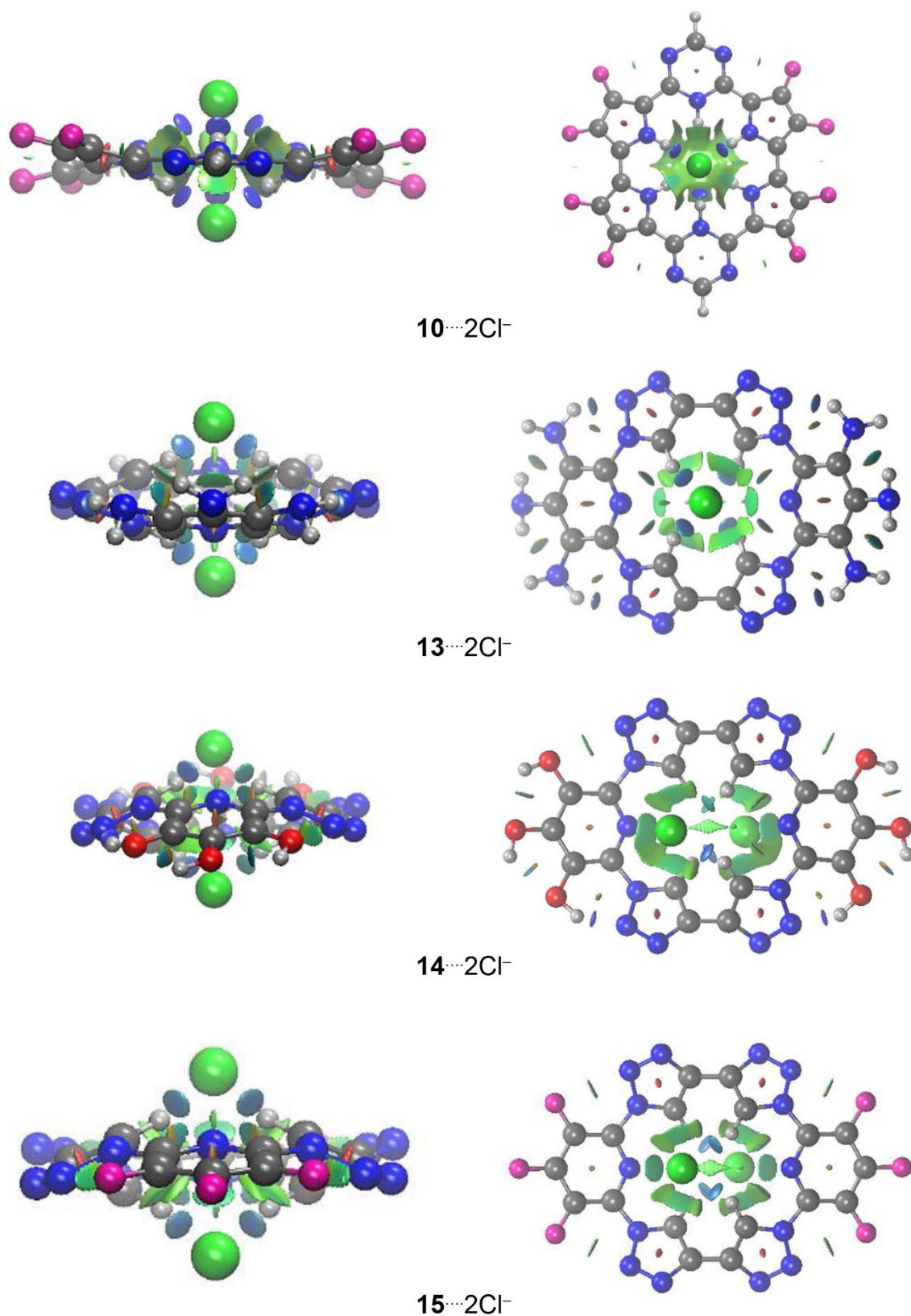


Figure S5. Front (left) and top (right) views of the NCI topology for the systems: (**10**, **13**, **14** and **15**) $\cdots 2\text{Cl}^-$. Atoms color: H = silver; C = black; N = blue; O = red; F = pink; and Cl = green.

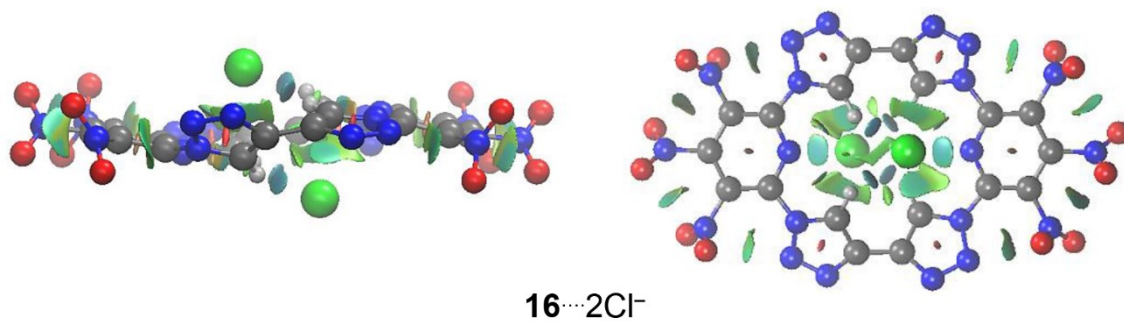


Figure S6. Front (left) and top (right) views of the NCI topology for the system: $16 \cdots 2\text{Cl}^-$. Atoms color: H = silver; C = black; N = blue; O = red; and Cl = green.

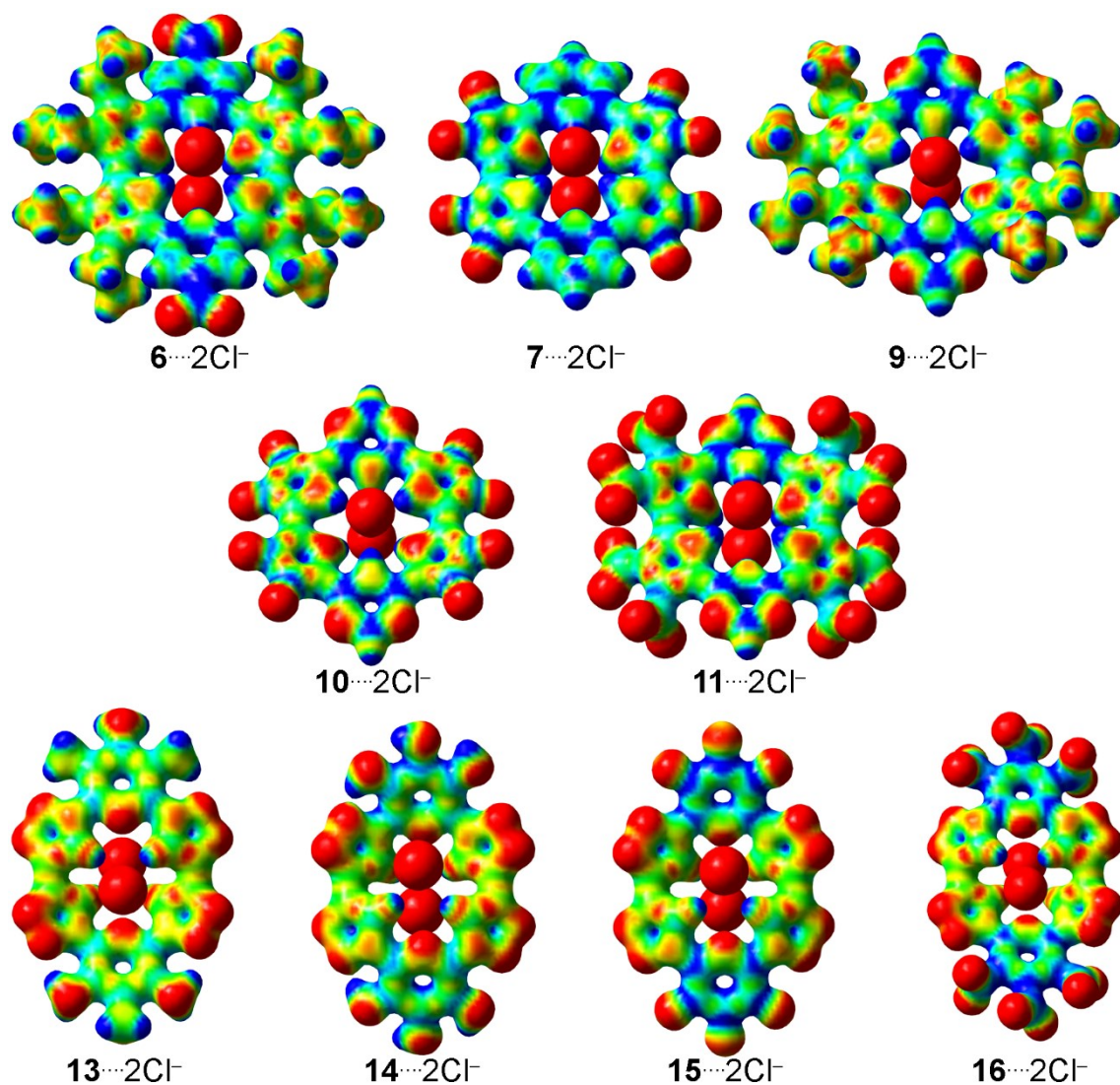


Figure S7. MEP surfaces for the complexes analyzed in this study. The isovalue used to represent the surfaces is equal to 0.050 a.u., while that the values of the scales (red – blue a.u.) are: (6, 7 and 9)...2Cl⁻ (0.100 – 0.250 a.u.); 10...2Cl⁻ (0.150 – 0.300 a.u.); 11...2Cl⁻ (0.200 – 0.350 a.u.); (14 and 15)...2Cl⁻ (–0.100 – 0.100 a.u.); and 16...2Cl⁻ (0.050 – 0.150 a.u.).

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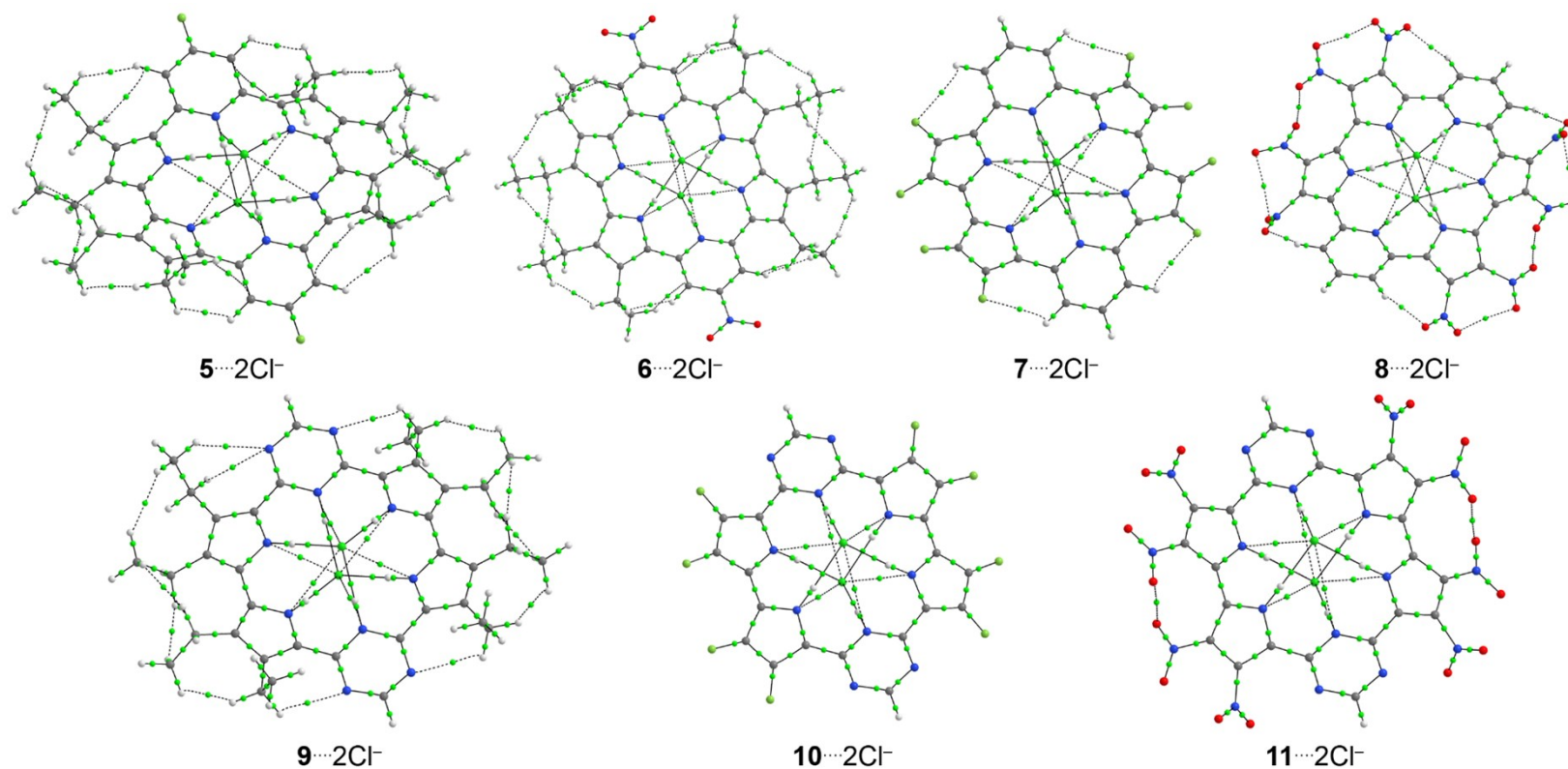


Figure S8. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (light green points) for the structures (5–11) $\cdots 2\text{Cl}^-$. Atoms color: H = white; C = gray; N = blue; O = red; F = green; and Cl = light green.

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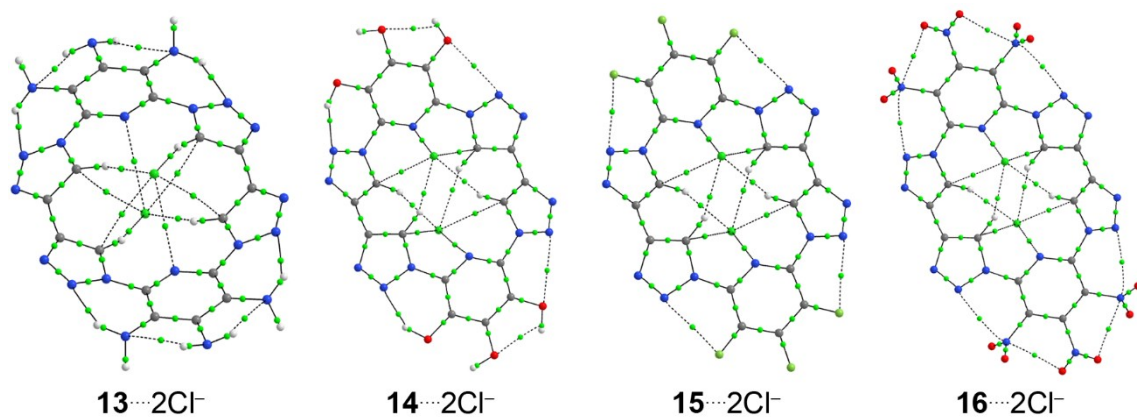


Figure S9. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (light green points) for the structures (13–16)...2Cl⁻. Atoms color: H = white; C = gray; N = blue; O = red; F = green; and Cl = light green.

Table S2. Electron density, ρ_b , Laplacian of ρ_b , $\nabla^2\rho_b$, and $-G_b/V_b$, at BCPs of **(1–3)**··· 2Cl^- . The values of all the parameters are in a.u.

Complex	BCP	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$
1 ··· 2Cl^-	N–H···Cl [−]	0.035	0.067	0.893
		0.035	0.067	0.893
		0.035	0.067	0.892
		0.035	0.067	0.893
	N···Cl [−]	0.009	0.028	1.108
		0.009	0.028	1.108
		0.001	0.008	1.687
		0.001	0.007	1.709
2a ··· 2Cl^-	N–H···Cl [−]	0.033	0.067	0.911
		0.033	0.068	0.911
		0.033	0.067	0.912
		0.033	0.068	0.911
	B–H···Cl [−]	0.004	0.013	1.338
		0.004	0.013	1.356
	B···Cl [−]	0.012	0.025	0.966
		0.012	0.025	0.951
2b ··· 2Cl^-	N–H···Cl [−]	0.014	0.030	0.918
		0.014	0.029	0.919
		0.029	0.055	0.909
		0.028	0.054	0.910
		0.028	0.054	0.910
		0.028	0.054	0.910
		0.005	0.018	1.277
		0.005	0.019	1.267
	N···Cl [−]	0.005	0.018	1.270
		0.005	0.018	1.275
		0.008	0.029	1.192
		0.008	0.029	1.191
		0.033	0.062	0.897
		0.034	0.063	0.894
3 ··· 2Cl^-	N–H···Cl [−]	0.033	0.063	0.895
		0.033	0.063	0.895
		0.006	0.018	1.223
		0.004	0.013	1.335
	N···Cl [−]	0.006	0.018	1.218
		0.009	0.028	1.113
		0.006	0.019	1.217
		0.003	0.013	1.340
		0.005	0.018	1.230
		0.009	0.028	1.113

Table S3. Electron density, ρ_b , Laplacian of ρ_b , $\nabla^2\rho_b$, and $-G_b/V_b$, at BCPs of (4–6)···2Cl[−]. The values of all the parameters are in a.u.^[a]

Complex	BCP	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$
4···2Cl [−]	N–H···Cl [−]	0.033 (0.029)	0.059 (0.063)	0.884 (0.958)
		0.032 (0.028)	0.059 (0.063)	0.885 (0.967)
		0.030 (0.029)	0.059 (0.067)	0.916 (0.961)
		0.030 (0.029)	0.060 (0.068)	0.916 (0.954)
		0.031 (0.030)	0.061 (0.068)	0.915 (0.948)
		0.030 (0.029)	0.060 (0.067)	0.915 (0.954)
	N···Cl [−]	0.009 (0.009)	0.030 (0.031)	1.134 (1.288)
		0.009 (0.009)	0.030 (0.031)	1.129 (1.287)
		0.005 (0.006)	0.022 (0.020)	1.356 (1.441)
		0.010 (0.009)	0.030 (0.031)	1.129 (1.284)
		0.005 (0.006)	0.022 (0.020)	1.353 (1.440)
		0.009 (0.009)	0.029 (0.031)	1.130 (1.292)
5···2Cl [−]	N–H···Cl [−]	0.033	0.060	0.883
		0.033	0.059	0.883
		0.030	0.059	0.916
		0.030	0.060	0.915
		0.031	0.061	0.915
		0.030	0.060	0.915
	N···Cl [−]	0.009	0.030	1.132
		0.005	0.022	1.350
		0.009	0.030	1.129
		0.010	0.030	1.128
		0.006	0.023	1.347
		0.009	0.029	1.130
6···2Cl [−]	N–H···Cl [−]	0.034	0.061	0.879
		0.034	0.061	0.880
		0.030	0.060	0.915
		0.030	0.061	0.915
		0.031	0.061	0.915
		0.030	0.060	0.915
	N···Cl [−]	0.010	0.030	1.133
		0.010	0.031	1.130
		0.006	0.023	1.345
		0.010	0.031	1.128
		0.006	0.023	1.342
		0.009	0.030	1.131

^[a] Values in the parenthesis correspond to results obtained using the B97D3/Def2–TZVP computational model.

Table S4. Electron density, ρ_b , Laplacian of ρ_b , $\nabla^2\rho_b$, and $-G_b/V_b$, at BCPs of (7–9)···2Cl[−]. The values of all the parameters are in a.u.

Complex	BCP	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$
7···2Cl [−]	N–H···Cl [−]	0.030	0.054	0.889
		0.034	0.066	0.902
		0.034	0.066	0.902
		0.034	0.066	0.902
		0.034	0.066	0.902
		0.030	0.054	0.889
	N···Cl [−]	0.010	0.033	1.133
		0.006	0.025	1.321
		0.010	0.033	1.133
		0.010	0.033	1.133
		0.006	0.025	1.321
		0.010	0.033	1.133
8···2Cl [−]	N–H···Cl [−]	0.032	0.056	0.884
		0.034	0.064	0.899
		0.034	0.064	0.899
		0.034	0.064	0.899
		0.034	0.064	0.899
		0.032	0.056	0.884
	N···Cl [−]	0.010	0.031	1.135
		0.005	0.022	1.371
		0.010	0.031	1.135
		0.010	0.031	1.135
		0.005	0.022	1.372
		0.010	0.031	1.135
9···2Cl [−]	N–H···Cl [−]	0.036	0.066	0.874
		0.036	0.066	0.874
		0.032	0.063	0.914
		0.032	0.064	0.913
		0.032	0.064	0.913
		0.032	0.064	0.913
	N···Cl [−]	0.009	0.030	1.140
		0.007	0.026	1.288
		0.010	0.031	1.138
		0.010	0.030	1.137
		0.007	0.026	1.288
		0.009	0.030	1.139

Table S5. Electron density, ρ_b , Laplacian of ρ_b , $\nabla^2\rho_b$, and $-G_b/V_b$, at BCPs of **(10–12)**...2Cl[−]. The values of all the parameters are in a.u.

Complex	BCP	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$
10 ...2Cl [−]	N–H...Cl [−]	0.034	0.061	0.883
		0.035	0.068	0.899
		0.035	0.068	0.899
		0.035	0.068	0.899
		0.035	0.068	0.899
		0.034	0.061	0.883
	N...Cl [−]	0.006	0.025	1.315
		0.010	0.032	1.129
		0.010	0.032	1.129
		0.010	0.032	1.129
		0.006	0.025	1.315
		0.010	0.032	1.129
11 ...2Cl [−]	N–H...Cl [−]	0.038	0.067	0.860
		0.035	0.067	0.897
		0.035	0.067	0.897
		0.035	0.067	0.897
		0.035	0.067	0.897
		0.038	0.067	0.860
	N...Cl [−]	0.009	0.030	1.143
		0.009	0.030	1.143
		0.006	0.026	1.300
		0.009	0.030	1.143
		0.009	0.030	1.142
		0.006	0.026	1.299
12 ...2Cl [−]	C–H...Cl [−]	0.020	0.040	0.898
		0.020	0.040	0.898
		0.020	0.040	0.898
		0.020	0.040	0.898
	C...Cl [−]	0.007	0.019	1.283
		0.007	0.019	1.283
		0.007	0.019	1.284
		0.007	0.019	1.283
	N...Cl [−]	0.009	0.024	1.118
		0.009	0.024	1.118

Table S6. Electron density, ρ_b , Laplacian of ρ_b , $\nabla^2\rho_b$, and $-G_b/V_b$, at BCPs of **(13–16)**... 2Cl^- . The values of all the parameters are in a.u.

Complex	BCP	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$
13 ... 2Cl^-	C–H... Cl^-	0.021	0.042	0.898
		0.021	0.042	0.898
		0.022	0.042	0.898
		0.021	0.042	0.898
	C... Cl^-	0.006	0.018	1.310
		0.006	0.018	1.309
		0.006	0.018	1.310
		0.006	0.018	1.309
	N... Cl^-	0.008	0.022	1.140
		0.008	0.022	1.140
14 ... 2Cl^-	C–H... Cl^-	0.024	0.048	0.901
		0.015	0.030	0.915
		0.015	0.030	0.915
		0.024	0.048	0.901
	C... Cl^-	0.006	0.017	1.333
		0.008	0.022	1.228
		0.008	0.022	1.228
		0.006	0.017	1.333
	N... Cl^-	0.009	0.024	1.116
		0.009	0.024	1.116
15 ... 2Cl^-	C–H... Cl^-	0.020	0.040	0.899
		0.020	0.040	0.899
		0.020	0.040	0.899
		0.020	0.040	0.899
	C... Cl^-	0.007	0.020	1.266
		0.007	0.021	1.266
		0.007	0.020	1.266
		0.007	0.021	1.266
	N... Cl^-	0.010	0.027	1.103
		0.010	0.027	1.103
16 ... 2Cl^-	C–H... Cl^-	0.017	0.035	0.908
		0.019	0.039	0.914
		0.017	0.035	0.908
		0.019	0.039	0.914
	C... Cl^-	0.008	0.022	1.238
		0.012	0.034	1.182
		0.008	0.022	1.238
		0.012	0.034	1.182
	N... Cl^-	0.015	0.038	1.071
		0.015	0.038	1.071

Table S7. Calculated ^1H -NMR chemical shift for the inner-hydrogens of the different macrocycles. Ethyl groups were replaced by hydrogen atoms for simplicity. All values in ppm, obtained via secondary reference employing benzene ^1H -NMR as reference ($\delta^{\text{H}} = \delta^{\text{ref}} + \sigma^{\text{ref}} - \sigma^{\text{H}}$).

Compound	Free-Host	Complexed with 2Cl^-
1	3.78	−2.10
2	6.92	−0.48
3	4.27	−2.34
4	4.82	−1.09
7	5.56	−1.54
9	6.73	1.80
12	5.85	−0.44