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On the Recognition of Chloride, Bromide and Nitrate Anions by Anthracene–Squaramide Conjugated Compounds: A Computational Perspective

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Supplementary Material

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Table S1. Optimized Cartesian coordinates to complexes investigated in this study.

Complex	1-Cl ⁻ [B97D3/6-31+G(d)] – PCM – DMSO		
Atom	X	Y	Z
C	-3.905271	-2.732627	-4.263589
C	-4.605072	-1.660825	-3.751756
C	-3.923185	-0.534436	-3.184528
C	-2.467833	-0.512987	-3.160203
C	-1.785953	-1.658839	-3.695796
C	-2.478399	-2.728444	-4.228001
C	-4.640277	0.544018	-2.643169
C	-3.988631	1.647274	-2.067968
C	-2.535546	1.686675	-2.043214
C	-1.795533	0.610131	-2.605393
C	-4.734763	2.732338	-1.501934
C	-4.096024	3.810217	-0.925633
C	-2.669987	3.853918	-0.893400
C	-1.916212	2.830244	-1.434461
C	-0.279260	0.638535	-2.555311
N	0.208736	0.115697	-1.264184
C	0.982064	0.803384	-0.430497
C	1.496128	0.530307	0.881110
C	2.211792	1.840014	0.917791
C	1.661154	2.122020	-0.470904
N	1.292524	-0.558526	1.648501
O	2.939184	2.461235	1.705181
O	1.735928	3.055844	-1.282910
C	1.784315	-0.866406	2.934083
C	1.380882	-2.097696	3.495592
C	1.832118	-2.468532	4.767411
C	2.687352	-1.623854	5.494327
C	3.084379	-0.401001	4.928976
C	2.642115	-0.013926	3.656469
H	-4.434459	-3.585915	-4.689832
H	-5.696701	-1.651517	-3.763261
H	-0.699156	-1.705758	-3.674138
H	-1.927974	-3.584441	-4.621072
H	-5.732174	0.520540	-2.662023
H	-5.824904	2.683218	-1.534850
H	-4.673737	4.628960	-0.494566
H	-2.168054	4.707776	-0.435675
H	-0.832671	2.905575	-1.390696
H	0.157418	0.042470	-3.364610
H	0.112399	1.652066	-2.672833
H	-0.153311	-0.801660	-0.954416
H	0.675119	-1.282461	1.235378
H	0.716615	-2.752895	2.930421
H	1.512439	-3.422510	5.189680
H	3.748445	0.265537	5.482143
H	2.954965	0.937414	3.228571
Cl	-0.664359	-2.672721	0.170622
H	3.038345	-1.914141	6.485306
Complex	1-Cl ⁻ [B97D3/6-31+G(d)]		
Atom	X	Y	Z
C	-3.940736	-2.820793	-3.752838

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C	-4.641365	-1.644150	-3.591536
C	-3.985276	-0.448928	-3.152821
C	-2.552747	-0.470973	-2.903864
C	-1.871434	-1.723354	-3.069465
C	-2.543211	-2.859189	-3.473389
C	-4.700950	0.741144	-2.950084
C	-4.073056	1.908754	-2.490275
C	-2.637871	1.903680	-2.246985
C	-1.892109	0.717727	-2.489026
C	-4.821882	3.107958	-2.257733
C	-4.208438	4.251703	-1.793191
C	-2.805132	4.248244	-1.537050
C	-2.044622	3.117246	-1.758502
C	-0.379446	0.709400	-2.318458
N	0.053663	0.171514	-1.023185
C	0.752550	0.874154	-0.130671
C	1.359948	0.513539	1.111308
C	1.845376	1.914339	1.336577
C	1.208616	2.283438	-0.008183
N	1.401273	-0.705724	1.689814
O	2.479782	2.519997	2.202488
O	1.117675	3.297605	-0.709719
C	1.971008	-1.100892	2.909243
C	1.896618	-2.475253	3.233383
C	2.436439	-2.938900	4.436850
C	3.055495	-2.051712	5.333601
C	3.126448	-0.688661	5.002688
C	2.591749	-0.203014	3.802778
H	-4.455410	-3.729058	-4.073555
H	-5.717122	-1.603795	-3.780496
H	-0.819236	-1.816727	-2.811660
H	-1.999128	-3.801685	-3.545914
H	-5.777608	0.755163	-3.142254
H	-5.897580	3.090313	-2.450869
H	-4.792520	5.156909	-1.613375
H	-2.321526	5.147760	-1.151975
H	-0.981161	3.159587	-1.529847
H	0.076857	0.100223	-3.113171
H	0.034559	1.715480	-2.418660
H	-0.051374	-0.852330	-0.854400
H	0.990340	-1.482044	1.120017
H	1.417384	-3.159445	2.531160
H	2.372047	-4.003409	4.673529
H	3.606403	0.015258	5.686697
H	2.660566	0.855734	3.552375
H	3.476050	-2.416867	6.272899
Cl	0.205064	-2.886677	-0.261519
Complex 1-Cl ⁻ (B97D3/Def2-TZVP) – PCM – DMSO			
Atom	X	Y	Z
C	-3.872694	-2.745776	-4.170457
C	-4.576838	-1.673089	-3.688338
C	-3.906934	-0.534066	-3.147350
C	-2.457962	-0.505460	-3.118636
C	-1.771093	-1.653967	-3.625119
C	-2.452048	-2.733280	-4.131264

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C	-4.626647	0.548696	-2.635643
C	-3.984142	1.663119	-2.088246
C	-2.536863	1.708750	-2.059679
C	-1.794108	0.625700	-2.587731
C	-4.731685	2.755232	-1.553067
C	-4.101643	3.843128	-1.005707
C	-2.681952	3.893652	-0.971567
C	-1.926540	2.865498	-1.480870
C	-0.282743	0.655838	-2.532864
N	0.206596	0.125514	-1.251246
C	0.961171	0.814967	-0.411555
C	1.475765	0.533393	0.891061
C	2.166048	1.853847	0.952489
C	1.609106	2.146866	-0.432502
N	1.289709	-0.568869	1.635071
O	2.874049	2.471138	1.744712
O	1.660902	3.086850	-1.223714
C	1.782485	-0.890623	2.909000
C	1.386535	-2.124676	3.455220
C	1.839977	-2.509158	4.713976
C	2.690100	-1.676223	5.446618
C	3.080024	-0.451285	4.899219
C	2.636101	-0.050751	3.639407
H	-4.393391	-3.608621	-4.577120
H	-5.664403	-1.670555	-3.703838
H	-0.688112	-1.692269	-3.596863
H	-1.898803	-3.592002	-4.502563
H	-5.714343	0.520287	-2.656716
H	-5.817496	2.701483	-1.587423
H	-4.681019	4.667370	-0.598203
H	-2.187521	4.758401	-0.536283
H	-0.846771	2.946057	-1.438131
H	0.148263	0.068643	-3.347385
H	0.103148	1.668441	-2.642519
H	-0.138027	-0.799939	-0.950927
H	0.682551	-1.292226	1.208536
H	0.724737	-2.770396	2.883606
H	1.525622	-3.465890	5.123508
H	3.741052	0.206692	5.458355
H	2.943252	0.904012	3.224337
Cl	-0.611509	-2.653623	0.130189
H	3.043067	-1.977541	6.428965
Complex 1-Br ⁻ [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	-3.708586	-2.860744	-4.020856
C	-4.425905	-1.842498	-3.429877
C	-3.774382	-0.653347	-2.964781
C	-2.337203	-0.508772	-3.133031
C	-1.635156	-1.599687	-3.749122
C	-2.295545	-2.734194	-4.176199
C	-4.504655	0.370393	-2.341036
C	-3.877410	1.524714	-1.843710
C	-2.441125	1.683450	-2.003843
C	-1.695993	0.670077	-2.665912
C	-4.630783	2.547572	-1.180185

C	−4.012141	3.670487	−0.671731
C	−2.600080	3.824671	−0.808761
C	−1.841589	2.866443	−1.453233
C	−0.185481	0.776067	−2.737611
N	0.380099	0.195721	−1.500997
C	1.103083	0.880805	−0.618609
C	1.509221	0.598691	0.726337
C	2.285472	1.871795	0.803901
C	1.834666	2.170342	−0.621729
N	1.166955	−0.454567	1.493952
O	2.987045	2.460762	1.636655
O	1.985076	3.101139	−1.425400
C	1.586328	−0.806113	2.792872
C	0.967724	−1.930837	3.381160
C	1.344157	−2.342691	4.664291
C	2.334817	−1.645107	5.375439
C	2.944409	−0.526620	4.783708
C	2.580835	−0.101631	3.498434
H	−4.213070	−3.764368	−4.365801
H	−5.506510	−1.925387	−3.298113
H	−0.555132	−1.553669	−3.872295
H	−1.728820	−3.548696	−4.629842
H	−5.583825	0.255388	−2.217141
H	−5.709557	2.412744	−1.079937
H	−4.594889	4.439957	−0.163564
H	−2.113191	4.710934	−0.398985
H	−0.768491	3.023667	−1.534994
H	0.218235	0.238936	−3.602829
H	0.161810	1.808254	−2.821857
H	−0.089401	−0.661297	−1.163576
H	0.461119	−1.092551	1.082808
H	0.197709	−2.469682	2.827189
H	0.859488	−3.213344	5.108913
H	3.715241	0.025164	5.324479
H	3.052557	0.772181	3.051793
Br	−1.249152	−2.303017	0.059071
H	2.626992	−1.968247	6.375296
Complex 1-NO ₃ [−] [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	−3.784067	−2.873554	−3.860130
C	−4.494744	−1.804094	−3.358100
C	−3.829180	−0.608890	−2.930700
C	−2.381992	−0.514056	−3.043051
C	−1.686763	−1.658106	−3.564075
C	−2.362626	−2.796165	−3.957975
C	−4.552240	0.468523	−2.395107
C	−3.912049	1.636518	−1.949907
C	−2.465616	1.746784	−2.056540
C	−1.723824	0.673631	−2.621242
C	−4.663279	2.717878	−1.383510
C	−4.035308	3.856351	−0.924037
C	−2.615413	3.966919	−1.014272
C	−1.857442	2.950374	−1.562780
C	−0.209676	0.747463	−2.685068
N	0.370415	0.182580	−1.450249

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C	1.035211	0.894935	−0.544046
C	1.468149	0.588766	0.786172
C	2.118993	1.924779	0.927816
C	1.651191	2.242406	−0.488047
N	1.241654	−0.540861	1.484708
O	2.759936	2.539162	1.790470
O	1.733978	3.212348	−1.254395
C	1.652972	−0.901052	2.783182
C	1.184963	−2.133861	3.287470
C	1.563859	−2.556291	4.566723
C	2.407190	−1.759733	5.358801
C	2.867211	−0.533616	4.851087
C	2.500144	−0.097246	3.570888
H	−4.300537	−3.780500	−4.177194
H	−5.581838	−1.850250	−3.268867
H	−0.601444	−1.647246	−3.643596
H	−1.802362	−3.649239	−4.343384
H	−5.638554	0.391384	−2.310904
H	−5.748251	2.615333	−1.318776
H	−4.616540	4.671232	−0.490383
H	−2.121157	4.866524	−0.644205
H	−0.778526	3.077305	−1.608463
H	0.181217	0.191326	−3.544723
H	0.153290	1.772268	−2.786757
H	0.024663	−0.740643	−1.152342
H	0.642352	−1.232075	1.001258
H	0.529839	−2.754809	2.674659
H	1.195579	−3.511484	4.944029
H	3.522724	0.095684	5.455555
H	2.857588	0.857936	3.189001
N	−1.616550	−2.250713	0.197360
O	−2.047116	−1.185998	0.712123
O	−2.359813	−3.244057	0.007651
O	−0.368934	−2.323416	−0.146489
Complex 2−Cl [−] [B97D3/6−31+G(d)] − PCM − DMSO			
Atom	X	Y	Z
C	−3.896849	−2.713568	−4.298549
C	−4.599160	−1.640225	−3.793408
C	−3.920213	−0.515880	−3.218759
C	−2.465232	−0.498228	−3.179393
C	−1.780710	−1.645318	−3.708744
C	−2.470433	−2.712882	−4.248558
C	−4.639950	0.564316	−2.684382
C	−3.991500	1.665614	−2.101970
C	−2.538617	1.701125	−2.061733
C	−1.795960	0.622826	−2.616848
C	−4.740817	2.752340	−1.543401
C	−4.105524	3.828194	−0.959632
C	−2.679819	3.868027	−0.911975
C	−1.922998	2.842685	−1.445505
C	−0.280400	0.645817	−2.550665
N	0.191113	0.110887	−1.257711
C	0.959044	0.785747	−0.411087
C	1.461741	0.501915	0.900635
C	2.182131	1.805147	0.960503

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C	1.644531	2.105500	-0.432497
N	1.246810	-0.597389	1.657303
O	2.904176	2.413331	1.761479
O	1.728983	3.044896	-1.232826
C	1.724068	-0.913625	2.936461
C	1.315557	-2.148283	3.489207
C	1.750483	-2.530387	4.758519
C	2.596177	-1.685019	5.498484
C	3.006563	-0.457564	4.944428
C	2.577566	-0.066958	3.675125
H	-4.423763	-3.565341	-4.730558
H	-5.690570	-1.628085	-3.816116
H	-0.694290	-1.694945	-3.676583
H	-1.918147	-3.569888	-4.636756
H	-5.731639	0.543687	-2.714437
H	-5.830646	2.706081	-1.588110
H	-4.685634	4.648263	-0.534396
H	-2.180546	4.720257	-0.448386
H	-0.839839	2.915456	-1.389867
H	0.163349	0.053130	-3.358488
H	0.116812	1.658314	-2.656593
H	-0.176004	-0.808915	-0.960355
H	0.630605	-1.316739	1.229850
H	0.655665	-2.801074	2.917571
H	1.426080	-3.485091	5.168965
H	3.665360	0.203689	5.506908
H	2.897003	0.887762	3.260056
Cl	-0.683853	-2.685199	0.158092
C	3.113335	-2.095513	6.844534
F	3.114885	-1.060636	7.747599
F	2.393392	-3.109353	7.412533
F	4.420666	-2.539679	6.791982
Complex 2-Cl ⁻ (B97D3/Def2-TZVP) – PCM – DMSO			
Atom	X	Y	Z
C	-3.854520	-2.737760	-4.191786
C	-4.564947	-1.664351	-3.720575
C	-3.902019	-0.523395	-3.175206
C	-2.453587	-0.493571	-3.130418
C	-1.759999	-1.642710	-3.626019
C	-2.434433	-2.723953	-4.136766
C	-4.628076	0.560219	-2.674313
C	-3.992599	1.676277	-2.122150
C	-2.545728	1.722955	-2.077078
C	-1.796706	0.639428	-2.594894
C	-4.746993	2.768896	-1.597738
C	-4.124072	3.858132	-1.044991
C	-2.704907	3.909487	-0.994179
C	-1.943015	2.881005	-1.492968
C	-0.286136	0.669998	-2.524289
N	0.189425	0.131078	-1.240553
C	0.936247	0.811453	-0.388881
C	1.440344	0.521223	0.914125
C	2.131034	1.837510	0.997532
C	1.586109	2.146264	-0.391691
N	1.246934	-0.591460	1.647767

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O	2.832186	2.444366	1.802531
O	1.645051	3.091570	-1.172101
C	1.726032	-0.919389	2.916095
C	1.335295	-2.162529	3.449419
C	1.773377	-2.555231	4.705670
C	2.604373	-1.715386	5.457331
C	2.996641	-0.482067	4.924370
C	2.564012	-0.078933	3.666697
H	-4.369889	-3.602167	-4.601879
H	-5.652262	-1.662752	-3.748289
H	-0.677350	-1.680038	-3.585710
H	-1.876398	-3.583207	-4.499541
H	-5.715438	0.531049	-2.707578
H	-5.832281	2.714368	-1.644660
H	-4.708615	4.682761	-0.645777
H	-2.216110	4.775151	-0.554410
H	-0.863922	2.962318	-1.437280
H	0.153776	0.086849	-3.336893
H	0.101180	1.682942	-2.624004
H	-0.155739	-0.798181	-0.951856
H	0.644245	-1.312760	1.206798
H	0.685442	-2.810452	2.867828
H	1.462554	-3.516106	5.103128
H	3.643363	0.175866	5.496416
H	2.868698	0.883203	3.267222
Cl	-0.620930	-2.658384	0.120766
C	3.122833	-2.163472	6.790161
F	3.378891	-1.124957	7.632546
F	2.259562	-2.992972	7.439107
F	4.302049	-2.858966	6.680910
Complex 2-Br ⁻ [B97D3/6-31+G(d)] - PCM - DMSO			
Atom	X	Y	Z
C	-3.710347	-2.861599	-3.985391
C	-4.425944	-1.843198	-3.392585
C	-3.774189	-0.649948	-2.938579
C	-2.338318	-0.503104	-3.115807
C	-1.638405	-1.593581	-3.735095
C	-2.299450	-2.730459	-4.154872
C	-4.504771	0.379893	-2.325246
C	-3.879697	1.543865	-1.848421
C	-2.443577	1.702652	-2.011395
C	-1.697469	0.680222	-2.658538
C	-4.635313	2.576390	-1.202516
C	-4.019154	3.709367	-0.713935
C	-2.607454	3.864105	-0.853877
C	-1.846785	2.896595	-1.481651
C	-0.186473	0.782468	-2.728378
N	0.376462	0.196922	-1.493010
C	1.085238	0.878253	-0.599266
C	1.497834	0.587277	0.740264
C	2.245947	1.872374	0.842883
C	1.791898	2.185533	-0.580735
N	1.177474	-0.489546	1.491859
O	2.934244	2.460552	1.686168
O	1.925880	3.128465	-1.369082

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C	1.590413	−0.840733	2.783388
C	1.031054	−2.012697	3.340860
C	1.399793	−2.425864	4.620863
C	2.329880	−1.677293	5.364863
C	2.890316	−0.513827	4.804984
C	2.528146	−0.092020	3.525026
H	−4.214973	−3.767767	−4.323337
H	−5.505419	−1.927902	−3.253181
H	−0.559887	−1.544366	−3.869041
H	−1.734739	−3.543321	−4.613848
H	−5.583315	0.264080	−2.196920
H	−5.713776	2.440953	−1.100075
H	−4.603509	4.486503	−0.219503
H	−2.122485	4.758802	−0.460496
H	−0.774295	3.055837	−1.566485
H	0.217991	0.245436	−3.593149
H	0.164852	1.813273	−2.808798
H	−0.061299	−0.686439	−1.180599
H	0.504170	−1.150240	1.058330
H	0.305772	−2.588014	2.764912
H	0.959348	−3.330160	5.037754
H	3.614568	0.071867	5.370186
H	2.957413	0.817155	3.107221
Br	−1.076948	−2.450120	−0.007011
C	2.779196	−2.142075	6.717637
F	3.011516	−1.104903	7.584939
F	1.876875	−2.969592	7.328251
F	3.964692	−2.850848	6.662382
Complex 2 −NO ₃ [−] [B97D3/6−31+G(d)] − PCM − DMSO			
Atom	X	Y	Z
C	−3.785525	−2.870836	−3.857244
C	−4.495549	−1.799505	−3.358316
C	−3.829061	−0.604310	−2.932471
C	−2.381601	−0.511659	−3.042653
C	−1.687059	−1.657510	−3.560577
C	−2.363883	−2.795392	−3.953362
C	−4.551481	0.475185	−2.400247
C	−3.910655	1.643505	−1.956918
C	−2.463911	1.751741	−2.061318
C	−1.722801	0.676055	−2.621981
C	−4.661627	2.727014	−1.394347
C	−4.033180	3.865853	−0.936512
C	−2.613053	3.974673	−1.024868
C	−1.855372	2.955958	−1.569668
C	−0.208454	0.746612	−2.681277
N	0.364683	0.178918	−1.443975
C	1.032165	0.884254	−0.536740
C	1.464717	0.576958	0.791428
C	2.122937	1.905854	0.939609
C	1.654983	2.232273	−0.477046
N	1.232289	−0.557494	1.488483
O	2.768069	2.512136	1.803617
O	1.741246	3.201613	−1.239358
C	1.640458	−0.916372	2.778851
C	1.192646	−2.159438	3.277932

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C	1.567243	-2.583452	4.553561
C	2.389558	-1.770457	5.352518
C	2.836220	-0.531571	4.853638
C	2.469526	-0.100904	3.578460
H	-4.302683	-3.777720	-4.173304
H	-5.582822	-1.844019	-3.270663
H	-0.601651	-1.648188	-3.639306
H	-1.804195	-3.649762	-4.336686
H	-5.637983	0.399515	-2.317344
H	-5.746806	2.625838	-1.331303
H	-4.614163	4.682442	-0.505801
H	-2.118392	4.874745	-0.656543
H	-0.776381	3.082160	-1.614529
H	0.184909	0.189174	-3.538819
H	0.158015	1.770267	-2.780992
H	0.018317	-0.745610	-1.150522
H	0.630477	-1.246136	1.000675
H	0.552762	-2.792034	2.662546
H	1.213875	-3.544710	4.921896
H	3.475792	0.105679	5.464262
H	2.814273	0.862666	3.206458
N	-1.625852	-2.237671	0.207002
O	-2.047805	-1.170093	0.722014
O	-2.376540	-3.223020	0.010143
O	-0.375894	-2.321448	-0.130884
C	2.832014	-2.209585	6.716330
F	2.635526	-1.238360	7.670378
F	2.187025	-3.328362	7.160713
F	4.181032	-2.498774	6.761757
Complex 3-Cl ⁻ [B97D3/6-31+G(d)] - PCM - DMSO			
Atom	X	Y	Z
C	-3.886412	-2.709618	-4.294140
C	-4.591208	-1.634451	-3.796313
C	-3.914878	-0.506361	-3.226034
C	-2.460128	-0.486797	-3.183725
C	-1.772878	-1.635610	-3.705580
C	-2.460129	-2.706934	-4.241115
C	-4.636781	0.575812	-2.698564
C	-3.990748	1.680330	-2.119614
C	-2.537915	1.717462	-2.075806
C	-1.793283	0.637644	-2.625127
C	-4.742582	2.768665	-1.567595
C	-4.109910	3.847389	-0.986336
C	-2.684392	3.888481	-0.934514
C	-1.925109	2.861840	-1.461983
C	-0.277911	0.660852	-2.556894
N	0.191904	0.115105	-1.267574
C	0.951291	0.784553	-0.409915
C	1.448452	0.488153	0.899902
C	2.162662	1.791113	0.982623
C	1.631912	2.109073	-0.410408
N	1.236735	-0.621859	1.642909
O	2.877661	2.387223	1.799225
O	1.717098	3.057793	-1.197659
C	1.712230	-0.940875	2.919389

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C	1.318727	-2.187071	3.458315
C	1.763273	-2.564923	4.725859
C	2.597660	-1.726586	5.486646
C	2.976730	-0.496566	4.938165
C	2.546552	-0.091259	3.665905
H	-4.411319	-3.564340	-4.722733
H	-5.682571	-1.623769	-3.821553
H	-0.686439	-1.683427	-3.671071
H	-1.905984	-3.565318	-4.623548
H	-5.728371	0.554072	-2.731066
H	-5.832227	2.721206	-1.615167
H	-4.691912	4.668658	-0.566053
H	-2.187173	4.742735	-0.472459
H	-0.842195	2.935804	-1.402795
H	0.167132	0.074153	-3.368385
H	0.119879	1.673863	-2.654025
H	-0.170603	-0.809642	-0.981093
H	0.627412	-1.343477	1.205558
H	0.672112	-2.840066	2.875163
H	2.853046	0.871650	3.257540
Cl	-0.655349	-2.703752	0.142560
H	2.938562	-2.029027	6.473162
C	3.867707	0.448313	5.709077
F	3.244416	1.644952	5.960537
F	4.262340	-0.049431	6.914843
F	5.010208	0.754246	5.014241
C	1.340701	-3.885056	5.323633
F	0.556490	-3.710022	6.437521
F	0.629068	-4.663233	4.461800
F	2.418586	-4.628165	5.732414
Complex 3-Br ⁻ [B97D3/6-31+G(d)] - PCM - DMSO			
Atom	X	Y	Z
C	-3.653689	-2.877594	-3.986793
C	-4.379411	-1.877320	-3.375690
C	-3.742943	-0.677035	-2.918621
C	-2.312379	-0.502965	-3.113388
C	-1.601204	-1.575635	-3.750671
C	-2.247542	-2.720228	-4.172411
C	-4.483335	0.333869	-2.285897
C	-3.872147	1.502921	-1.803573
C	-2.441207	1.688453	-1.983005
C	-1.686262	0.686461	-2.651476
C	-4.636894	2.514452	-1.135623
C	-4.033991	3.652084	-0.641380
C	-2.627078	3.832767	-0.797288
C	-1.858170	2.886005	-1.446273
C	-0.177986	0.813920	-2.737167
N	0.405277	0.219548	-1.515042
C	1.105118	0.898798	-0.613056
C	1.515173	0.595127	0.722840
C	2.254027	1.880568	0.848233
C	1.799455	2.214440	-0.572677
N	1.202485	-0.495287	1.458408
O	2.937823	2.454109	1.705398
O	1.925491	3.169830	-1.345149

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C	1.607302	−0.849594	2.749108
C	1.061604	−2.036807	3.284304
C	1.433115	−2.454286	4.564374
C	2.337769	−1.708836	5.339200
C	2.869065	−0.534855	4.791374
C	2.518233	−0.093572	3.507747
H	−4.146583	−3.789476	−4.326640
H	−5.455352	−1.982373	−3.223490
H	−0.525567	−1.506165	−3.898182
H	−1.674374	−3.519041	−4.645359
H	−5.557913	0.197891	−2.144828
H	−5.711438	2.359145	−1.021012
H	−4.625101	4.413064	−0.130164
H	−2.152424	4.730932	−0.399296
H	−0.789785	3.064940	−1.542868
H	0.225752	0.294686	−3.612949
H	0.156979	1.850933	−2.806580
H	−0.018713	−0.673285	−1.211538
H	0.537168	−1.159437	1.014714
H	0.354957	−2.613556	2.689014
H	2.934814	0.828172	3.102453
Br	−1.005788	−2.467847	−0.029244
H	2.619678	−2.037278	6.335319
C	3.838754	0.310111	5.583109
F	3.326844	1.555473	5.851112
F	4.176080	−0.240935	6.782996
F	5.009872	0.520223	4.900952
C	0.800408	−3.691960	5.153460
F	−0.325850	−3.386475	5.881513
F	0.411924	−4.591486	4.203533
F	1.640100	−4.352086	6.006317
Complex 3 –NO ₃ [−] [B97D3/6–31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	−3.780984	−2.866852	−3.854904
C	−4.490285	−1.796074	−3.353774
C	−3.823310	−0.600710	−2.929237
C	−2.376220	−0.507269	−3.043052
C	−1.682393	−1.652370	−3.563585
C	−2.359690	−2.790450	−3.955007
C	−4.544866	0.478139	−2.394523
C	−3.903573	1.646496	−1.951995
C	−2.457118	1.755482	−2.059676
C	−1.717071	0.680461	−2.622964
C	−4.653756	2.729134	−1.386724
C	−4.024795	3.867810	−0.929223
C	−2.604936	3.977342	−1.020722
C	−1.848061	2.959518	−1.568267
C	−0.202880	0.750803	−2.684766
N	0.371093	0.177636	−1.450116
C	1.038496	0.877330	−0.539422
C	1.469946	0.562561	0.786152
C	2.131841	1.885929	0.945173
C	1.663965	2.225767	−0.469710
N	1.238088	−0.576708	1.477165
O	2.780045	2.479388	1.816123

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O	1.751782	3.199365	-1.224350
C	1.641460	-0.928852	2.768500
C	1.212253	-2.182206	3.260238
C	1.588657	-2.590406	4.540262
C	2.389847	-1.775206	5.359333
C	2.804872	-0.536846	4.857674
C	2.442911	-0.101848	3.574154
H	-4.298438	-3.773947	-4.169830
H	-5.577286	-1.841205	-3.263240
H	-0.597236	-1.642332	-3.645935
H	-1.800579	-3.644241	-4.340433
H	-5.631095	0.401837	-2.308815
H	-5.738731	2.627392	-1.321320
H	-4.605132	4.683729	-0.496410
H	-2.109813	4.877269	-0.652699
H	-0.769270	3.086508	-1.615521
H	0.189395	0.196146	-3.544531
H	0.164403	1.774484	-2.780665
H	0.026698	-0.749070	-1.161785
H	0.637438	-1.266060	0.985973
H	0.592795	-2.822172	2.635405
H	2.771965	0.868996	3.204094
N	-1.613491	-2.242076	0.206753
O	-2.032857	-1.174948	0.723961
O	-2.365676	-3.224054	0.003239
O	-0.361494	-2.328665	-0.127642
F	3.663282	0.383493	5.693019
F	3.044559	1.586027	5.924538
F	3.978871	-0.137133	6.912111
F	4.849080	0.679985	5.070248
C	1.135158	-3.923328	5.084938
F	0.354952	-3.775425	6.204431
F	0.408009	-4.650385	4.192136
F	2.196808	-4.705625	5.463102
H	2.677902	-2.101584	6.355016
Complex 4-Cl ⁻ [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	-3.893934	-2.729295	-4.258361
C	-4.597577	-1.653737	-3.759821
C	-3.919805	-0.523283	-3.196020
C	-2.464862	-0.501678	-3.160847
C	-1.778833	-1.650969	-3.683174
C	-2.467440	-2.724476	-4.212566
C	-4.640714	0.559264	-2.668001
C	-3.993673	1.666656	-2.095794
C	-2.540775	1.706223	-2.059556
C	-1.797289	0.625467	-2.608594
C	-4.744536	2.755471	-1.543464
C	-4.110745	3.837270	-0.969214
C	-2.685067	3.881176	-0.925413
C	-1.926887	2.853936	-1.453268
C	-0.281849	0.652300	-2.546949
N	0.192772	0.120227	-1.252985
C	0.965742	0.791118	-0.411998
C	1.478406	0.511881	0.895728

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C	2.200805	1.811716	0.954885
C	1.653482	2.115102	-0.438011
N	1.267414	-0.591130	1.656193
O	2.927471	2.417433	1.750627
O	1.732546	3.051335	-1.237118
C	1.746630	-0.904906	2.923028
C	1.343509	-2.148978	3.474792
C	1.781159	-2.533708	4.734848
C	2.630354	-1.676492	5.461628
C	3.037506	-0.439806	4.925492
C	2.600802	-0.052431	3.663408
N	3.090301	-2.072176	6.777120
O	3.839388	-1.295647	7.408556
O	2.721361	-3.176108	7.233389
H	-4.419829	-3.585806	-4.682109
H	-5.689048	-1.644414	-3.779621
H	-0.692183	-1.697564	-3.654388
H	-1.914041	-3.582984	-4.595778
H	-5.732405	0.535586	-2.694811
H	-5.834309	2.705956	-1.585237
H	-4.691923	4.658947	-0.548641
H	-2.186864	4.738092	-0.469437
H	-0.843863	2.930442	-1.400867
H	0.161982	0.056810	-3.352472
H	0.113928	1.664798	-2.656613
H	-0.170353	-0.801960	-0.954674
H	0.648726	-1.311731	1.227389
H	0.685678	-2.801077	2.900642
H	1.473466	-3.485821	5.159554
H	3.693443	0.209211	5.500481
H	2.914016	0.903993	3.247741
Cl	-0.649115	-2.665722	0.172680
Complex 4-Cl ⁻ (B97D3/Def2-TZVP) – PCM – DMSO			
Atom	X	Y	Z
C	-3.862756	-2.744953	-4.160068
C	-4.570283	-1.666984	-3.694949
C	-3.904122	-0.523733	-3.158552
C	-2.455620	-0.496430	-3.116502
C	-1.765048	-1.650093	-3.605611
C	-2.442591	-2.733432	-4.107774
C	-4.627158	0.564645	-2.663626
C	-3.988800	1.683197	-2.120028
C	-2.541781	1.727482	-2.077614
C	-1.796070	0.639022	-2.589605
C	-4.740419	2.780523	-1.601553
C	-4.114713	3.872183	-1.056870
C	-2.695400	3.921325	-1.008722
C	-1.936231	2.888270	-1.502083
C	-0.285558	0.667139	-2.522081
N	0.190140	0.130779	-1.236430
C	0.945366	0.805271	-0.391456
C	1.458232	0.519025	0.908007
C	2.157387	1.828834	0.988053
C	1.604138	2.140812	-0.401124
N	1.263545	-0.594926	1.647225

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O	2.866508	2.431311	1.786793
O	1.662237	3.081749	-1.181774
C	1.743398	-0.920494	2.904343
C	1.354573	-2.170131	3.438081
C	1.794678	-2.565771	4.686594
C	2.631269	-1.715892	5.421831
C	3.023712	-0.474866	4.905461
C	2.585400	-0.075265	3.654886
N	3.096750	-2.126950	6.734135
O	3.833001	-1.358358	7.367866
O	2.739493	-3.230517	7.168933
H	-4.380473	-3.611134	-4.563347
H	-5.657616	-1.663385	-3.720781
H	-0.682366	-1.689359	-3.567562
H	-1.886855	-3.596086	-4.465934
H	-5.714616	0.537226	-2.694671
H	-5.825846	2.727625	-1.646501
H	-4.697074	4.700463	-0.662126
H	-2.204307	4.788981	-0.575551
H	-0.856995	2.968437	-1.448925
H	0.152659	0.078648	-3.331517
H	0.104399	1.678449	-2.626398
H	-0.156176	-0.798185	-0.945056
H	0.654890	-1.315739	1.206427
H	0.704811	-2.816347	2.854943
H	1.499203	-3.522575	5.099716
H	3.671193	0.167665	5.490160
H	2.887016	0.886730	3.252859
Cl	-0.602156	-2.645673	0.140858
Complex 4-Br ⁻ [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	-3.688401	-2.872286	-3.979027
C	-4.417037	-1.848586	-3.411759
C	-3.776232	-0.648973	-2.959182
C	-2.337995	-0.500368	-3.113224
C	-1.624151	-1.596136	-3.706594
C	-2.274786	-2.740196	-4.123105
C	-4.518748	0.383225	-2.364354
C	-3.903472	1.549777	-1.881110
C	-2.465505	1.711297	-2.023050
C	-1.708202	0.688556	-2.655975
C	-4.670806	2.582176	-1.249099
C	-4.064220	3.717011	-0.752994
C	-2.650695	3.873694	-0.870735
C	-1.878868	2.906495	-1.485108
C	-0.197261	0.795902	-2.706360
N	0.345660	0.217484	-1.458413
C	1.088743	0.879932	-0.583313
C	1.512020	0.591771	0.752104
C	2.304605	1.848642	0.837018
C	1.837917	2.169058	-0.585699
N	1.163021	-0.470078	1.520777
O	3.024338	2.417338	1.664584
O	1.986574	3.099126	-1.381035
C	1.595507	-0.833914	2.790254

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C	1.002654	−1.987070	3.366237
C	1.389783	−2.417594	4.628110
C	2.376497	−1.698664	5.330650
C	2.971259	−0.551726	4.770138
C	2.585375	−0.119003	3.506482
N	2.784186	−2.144908	6.647455
O	3.663817	−1.496069	7.254107
O	2.241296	−3.162792	7.129118
H	−4.184634	−3.783717	−4.315129
H	−5.498629	−1.934419	−3.290868
H	−0.543425	−1.545952	−3.821509
H	−1.699653	−3.557753	−4.560268
H	−5.598933	0.265771	−2.252646
H	−5.750441	2.444968	−1.162966
H	−4.657401	4.493971	−0.268988
H	−2.173373	4.769377	−0.470427
H	−0.805216	3.066953	−1.552883
H	0.221618	0.254459	−3.561558
H	0.152623	1.827142	−2.787678
H	−0.117208	−0.648708	−1.131744
H	0.448242	−1.102016	1.105098
H	0.240018	−2.531234	2.809076
H	0.938119	−3.300537	5.073080
H	3.730525	−0.008131	5.326881
H	3.035658	0.773087	3.074527
Br	−1.201798	−2.317873	0.093485
Complex			
4-NO ₃ [−] [B97D3/6−31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	−3.777063	−2.881065	−3.839476
C	−4.489326	−1.810740	−3.341654
C	−3.825751	−0.611836	−2.921934
C	−2.378980	−0.514483	−3.036546
C	−1.681962	−1.659232	−3.553479
C	−2.356098	−2.800578	−3.940847
C	−4.550405	0.466878	−2.391227
C	−3.912758	1.639105	−1.953765
C	−2.466712	1.752135	−2.062085
C	−1.723608	0.676815	−2.620778
C	−4.666368	2.721590	−1.392862
C	−4.041067	3.864224	−0.940268
C	−2.621661	3.978040	−1.032836
C	−1.861651	2.960299	−1.576184
C	−0.209652	0.751221	−2.680899
N	0.361674	0.186195	−1.440725
C	1.033244	0.886880	−0.537030
C	1.471183	0.584049	0.789203
C	2.132289	1.908975	0.939147
C	1.658754	2.239049	−0.479059
N	1.237030	−0.553404	1.489575
O	2.780334	2.512518	1.800328
O	1.742097	3.205539	−1.239703
C	1.645353	−0.910914	2.768410
C	1.203326	−2.164913	3.263702
C	1.577410	−2.591587	4.530781
C	2.398614	−1.764916	5.321850

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C	2.842254	−0.517293	4.843266
C	2.470616	−0.089446	3.573566
N	2.791733	−2.204598	6.645688
O	3.519461	−1.456399	7.333156
O	2.388662	−3.316023	7.051188
H	−4.291897	−3.790803	−4.151005
H	−5.576132	−1.858771	−3.250462
H	−0.596902	−1.646319	−3.636645
H	−1.794619	−3.653841	−4.323963
H	−5.636325	0.387427	−2.304667
H	−5.750981	2.616592	−1.326940
H	−4.623923	4.680079	−0.510783
H	−2.129367	4.881301	−0.669265
H	−0.783487	3.091218	−1.625227
H	0.186757	0.191460	−3.535279
H	0.155593	1.775029	−2.782230
H	0.021685	−0.742161	−1.149932
H	0.632632	−1.241389	0.998356
H	0.568903	−2.797420	2.643339
H	1.240689	−3.552138	4.912080
H	3.474884	0.108362	5.468016
H	2.808073	0.877291	3.203314
N	−1.615666	−2.211168	0.220251
O	−2.029296	−1.141355	0.736079
O	−2.371644	−3.190002	0.018422
O	−0.363590	−2.303491	−0.114830
Complex 5-Cl [−] [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	−3.860464	−2.702318	−4.324593
C	−4.571583	−1.626428	−3.837458
C	−3.902651	−0.497811	−3.259622
C	−2.448603	−0.478470	−3.197877
C	−1.754653	−1.627800	−3.709634
C	−2.435029	−2.699632	−4.252933
C	−4.631340	0.585072	−2.743064
C	−3.993086	1.690220	−2.156779
C	−2.541004	1.727107	−2.093235
C	−1.789407	0.646460	−2.631234
C	−4.752215	2.779164	−1.616110
C	−4.127366	3.858313	−1.027251
C	−2.702697	3.899235	−0.956096
C	−1.936506	2.871979	−1.472236
C	−0.275356	0.668738	−2.540756
N	0.173367	0.124318	−1.242912
C	0.924373	0.790092	−0.376530
C	1.402140	0.495173	0.939415
C	2.122846	1.791044	1.033819
C	1.613001	2.113306	−0.368469
N	1.173185	−0.614278	1.682182
O	2.829440	2.379457	1.862095
O	1.713196	3.059632	−1.153991
C	1.625351	−0.930193	2.961736
C	1.218585	−2.171398	3.499605
C	1.648346	−2.530641	4.777390
C	2.469674	−1.717161	5.562908

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C	2.848761	-0.498037	4.995428
C	2.453714	-0.079093	3.722105
H	-4.379776	-3.557473	-4.759057
H	-5.662499	-1.615539	-3.877216
H	-0.668699	-1.675612	-3.661832
H	-1.875970	-3.558303	-4.627461
H	-5.722389	0.563345	-2.790049
H	-5.841102	2.731823	-1.678521
H	-4.714877	4.680069	-0.615716
H	-2.211637	4.753876	-0.488244
H	-0.854523	2.946089	-1.398464
H	0.181983	0.079670	-3.343514
H	0.125342	1.680985	-2.633417
H	-0.197349	-0.797975	-0.959425
H	0.565136	-1.335441	1.236903
H	0.578899	-2.836944	2.924398
H	2.778832	0.883930	3.329748
Cl	-0.693422	-2.685014	0.186793
H	2.792718	-2.014605	6.553811
N	3.718933	0.400439	5.791637
O	4.047319	1.484315	5.291556
O	4.071346	0.018190	6.916590
N	1.213606	-3.834526	5.328189
O	1.600166	-4.140718	6.464738
O	0.487290	-4.549206	4.624139
Complex 5-Br ⁻ [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	-3.649531	-2.867746	-3.990132
C	-4.374102	-1.874105	-3.366961
C	-3.737871	-0.675619	-2.905018
C	-2.309304	-0.495792	-3.108606
C	-1.599096	-1.561859	-3.757810
C	-2.245088	-2.705077	-4.183655
C	-4.475983	0.327244	-2.256968
C	-3.864863	1.494660	-1.770593
C	-2.436384	1.687349	-1.961687
C	-1.684016	0.692984	-2.644117
C	-4.627252	2.497448	-1.086985
C	-4.024036	3.632854	-0.588052
C	-2.619285	3.820243	-0.755139
C	-1.852916	2.882303	-1.419715
C	-0.176998	0.825241	-2.740715
N	0.414497	0.217570	-1.528942
C	1.128601	0.881390	-0.628551
C	1.553222	0.561707	0.697717
C	2.307827	1.834218	0.830329
C	1.836089	2.192723	-0.581345
N	1.237266	-0.534199	1.428088
O	3.009277	2.386650	1.686208
O	1.958868	3.155080	-1.342679
C	1.654156	-0.902300	2.704772
C	1.115258	-2.095848	3.233955
C	1.509548	-2.509947	4.506018
C	2.420971	-1.798162	5.291369
C	2.930311	-0.624017	4.731128

C	2.575811	-0.153089	3.463911
H	-4.142052	-3.778510	-4.333459
H	-5.448583	-1.983639	-3.207873
H	-0.524582	-1.488497	-3.911614
H	-1.672830	-3.498982	-4.665846
H	-5.548821	0.186398	-2.107736
H	-5.700120	2.337118	-0.964029
H	-4.613211	4.387037	-0.064707
H	-2.144314	4.716516	-0.353320
H	-0.786071	3.066178	-1.524302
H	0.221638	0.316092	-3.624697
H	0.155868	1.863454	-2.800785
H	-0.009666	-0.677191	-1.230597
H	0.559485	-1.189477	0.985730
H	0.401694	-2.678673	2.655127
H	2.994881	0.775929	3.079896
Br	-0.988935	-2.471569	-0.041924
H	2.715258	-2.137567	6.277751
N	3.899871	0.165673	5.527518
O	4.205869	-0.255719	6.652003
O	4.352505	1.204251	5.027841
N	0.935834	-3.762023	5.049526
O	0.129129	-4.383953	4.344820
O	1.293321	-4.120238	6.180378
Complex 5-NO₃⁻ [B97D3/6-31+G(d)] - PCM - DMSO			
Atom	X	Y	Z
C	-3.749067	-2.859354	-3.903602
C	-4.468235	-1.790062	-3.413402
C	-3.810107	-0.594798	-2.975105
C	-2.361271	-0.500363	-3.062169
C	-1.657056	-1.644118	-3.571472
C	-2.326245	-2.781860	-3.977515
C	-4.541980	0.483062	-2.452615
C	-3.909822	1.651769	-1.998041
C	-2.461772	1.762153	-2.079687
C	-1.710998	0.687697	-2.629549
C	-4.671084	2.733476	-1.446024
C	-4.051581	3.872754	-0.977279
C	-2.630481	3.983900	-1.043737
C	-1.862918	2.966874	-1.577707
C	-0.196182	0.758737	-2.663524
N	0.353518	0.184646	-1.417860
C	1.007020	0.881178	-0.496293
C	1.415893	0.568929	0.835743
C	2.077560	1.888196	1.008248
C	1.635245	2.230583	-0.416286
N	1.167338	-0.569520	1.526988
O	2.710413	2.477355	1.892223
O	1.736659	3.202524	-1.168418
C	1.555916	-0.918949	2.817803
C	1.110470	-2.163077	3.314796
C	1.481774	-2.552875	4.602083
C	2.281037	-1.766403	5.435907
C	2.701172	-0.543016	4.907714
C	2.364971	-0.095034	3.627745

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H	-4.260018	-3.766192	-4.229643
H	-5.556669	-1.836160	-3.342910
H	-0.570576	-1.633171	-3.634158
H	-1.759586	-3.634493	-4.354349
H	-5.629499	0.405823	-2.386628
H	-5.756935	2.630656	-1.400065
H	-4.640367	4.688034	-0.554839
H	-2.142966	4.884507	-0.667360
H	-0.783708	3.095506	-1.606536
H	0.212923	0.203938	-3.515193
H	0.173163	1.782314	-2.751719
H	0.004835	-0.742808	-1.137875
H	0.566249	-1.257177	1.029374
H	0.487720	-2.814061	2.706524
H	2.713976	0.873193	3.270901
N	-1.665617	-2.215559	0.222082
O	-2.086545	-1.151965	0.744552
O	-2.421052	-3.186018	-0.016851
O	-0.404966	-2.310192	-0.081125
N	3.552913	0.326535	5.755171
O	3.937520	1.403175	5.280409
O	3.834547	-0.072243	6.894030
N	1.005880	-3.860379	5.108705
O	1.343671	-4.195467	6.252366
O	0.296035	-4.548322	4.362455
H	2.558532	-2.087256	6.433263
Complex 6-Cl ⁻ [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	-3.511740	-2.781913	-4.501838
C	-4.330331	-1.794211	-3.996796
C	-3.782068	-0.632771	-3.360087
C	-2.338081	-0.483516	-3.258963
C	-1.529001	-1.545437	-3.789892
C	-2.094701	-2.653500	-4.389338
C	-4.618853	0.357944	-2.822628
C	-4.098341	1.491185	-2.176637
C	-2.657571	1.657980	-2.073991
C	-1.798055	0.674066	-2.635021
C	-4.966505	2.482330	-1.612473
C	-4.457089	3.587598	-0.963876
C	-3.044176	3.754847	-0.853115
C	-2.175133	2.825132	-1.390795
C	-0.294674	0.827628	-2.506511
N	0.176488	0.249004	-1.232101
C	0.824521	0.934168	-0.298364
C	1.267443	0.615077	1.020244
C	1.811654	1.972696	1.242712
C	1.385144	2.317732	-0.187413
N	1.119155	-0.501002	1.758006
O	2.339986	2.570281	2.186436
O	1.432636	3.306540	-0.924502
C	1.682257	-0.758866	3.012957
C	0.872420	-1.455868	3.937854
C	1.308478	-1.712646	5.236535
C	2.572712	-1.262232	5.662856

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C	3.403974	-0.601646	4.761906
C	2.987847	-0.380493	3.433675
H	-3.939773	-3.663376	-4.980969
H	-5.416344	-1.880850	-4.066526
H	-0.444749	-1.496275	-3.711361
H	-1.450432	-3.443848	-4.777166
H	-5.701943	0.239208	-2.899214
H	-6.044716	2.338185	-1.705035
H	-5.126915	4.333843	-0.534600
H	-2.644611	4.629168	-0.337021
H	-1.106390	2.993228	-1.284294
H	0.228905	0.331058	-3.331353
H	0.014469	1.875279	-2.531048
H	-0.164309	-0.693736	-0.981697
H	0.453558	-1.214870	1.391197
H	-0.125102	-1.758536	3.619255
H	0.653141	-2.243915	5.926784
H	4.401627	-0.282856	5.052724
Cl	-0.823962	-2.492800	0.246561
H	2.911910	-1.443382	6.682014
N	4.006107	0.121115	2.510891
O	3.874882	-0.114700	1.294604
O	5.000599	0.700896	2.986923
Complex 7-Cl ⁻ [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	-3.903709	-2.724267	-4.253652
C	-4.604687	-1.650729	-3.747012
C	-3.923888	-0.520888	-3.185529
C	-2.468718	-0.497749	-3.161737
C	-1.785465	-1.645150	-3.691969
C	-2.476865	-2.718168	-4.218682
C	-4.641757	0.559461	-2.648915
C	-3.991120	1.665722	-2.078486
C	-2.537957	1.706591	-2.053568
C	-1.797523	0.628399	-2.611816
C	-4.738493	2.752207	-1.516835
C	-4.101066	3.832710	-0.944114
C	-2.675100	3.877634	-0.911137
C	-1.920127	2.852821	-1.448284
C	-0.281382	0.655463	-2.561757
N	0.204724	0.116174	-1.276012
C	0.971591	0.792088	-0.429344
C	1.481455	0.503992	0.878031
C	2.195417	1.808548	0.943751
C	1.649562	2.116679	-0.444962
N	1.280518	-0.600415	1.630530
O	2.919323	2.410328	1.748162
O	1.725666	3.061021	-1.239662
C	1.759620	-0.909325	2.911201
C	1.382915	-2.158722	3.458543
C	1.821722	-2.536549	4.731288
C	2.640546	-1.689500	5.488359
C	2.998361	-0.457179	4.923475
C	2.580422	-0.042404	3.653503
H	-4.431990	-3.580305	-4.675440

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H	−5.696312	−1.642691	−3.758321
H	−0.698577	−1.690415	−3.670972
H	−1.925558	−3.575313	−4.607954
H	−5.733623	0.534874	−2.667314
H	−5.828550	2.701901	−1.550092
H	−4.679672	4.652513	−0.516329
H	−2.174104	4.733384	−0.455975
H	−0.836716	2.929619	−1.403605
H	0.155273	0.066989	−3.376529
H	0.112388	1.669222	−2.667570
H	−0.153260	−0.807805	−0.981160
H	0.672697	−1.327440	1.202667
H	0.745149	−2.824100	2.876194
H	1.521721	−3.502112	5.137471
Cl	−0.626840	−2.697987	0.140195
H	2.989220	−1.968651	6.478453
H	2.885175	0.923929	3.256313
N	3.858204	0.454256	5.703198
O	4.243707	0.081851	6.824313
O	4.158261	1.551829	5.206669
Complex			
8-Cl [−] [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	−3.880819	−2.732276	−4.273905
C	−4.586492	−1.658740	−3.773854
C	−3.910962	−0.528307	−3.207222
C	−2.456030	−0.504541	−3.170988
C	−1.767853	−1.651919	−3.694925
C	−2.454333	−2.725524	−4.226849
C	−4.633895	0.552074	−2.677530
C	−3.988701	1.659074	−2.102365
C	−2.535866	1.700549	−2.064984
C	−1.790159	0.622316	−2.616054
C	−4.741314	2.745721	−1.548093
C	−4.109260	3.827000	−0.970891
C	−2.683644	3.872551	−0.925741
C	−1.923682	2.847544	−1.455441
C	−0.274602	0.650799	−2.553037
N	0.201193	0.117827	−1.260792
C	0.965007	0.796412	−0.413378
C	1.467672	0.512259	0.897761
C	2.182177	1.817685	0.962042
C	1.644762	2.119577	−0.431043
N	1.256738	−0.590239	1.650154
O	2.900603	2.425090	1.767168
O	1.725945	3.060986	−1.228939
C	1.734758	−0.904853	2.929621
C	1.334696	−2.141280	3.473159
C	1.790159	−2.494430	4.746526
C	2.630383	−1.668764	5.507562
C	3.015590	−0.444644	4.947778
C	2.580729	−0.054379	3.674739
H	−4.405124	−3.588786	−4.699663
H	−5.677983	−1.651161	−3.794425
H	−0.681150	−1.696751	−3.665042
H	−1.899362	−3.582607	−4.611011

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H	-5.725546	0.526967	-2.705307
H	-5.831023	2.694928	-1.590643
H	-4.691851	4.646944	-0.548822
H	-2.186937	4.728955	-0.467111
H	-0.840715	2.924785	-1.401625
H	0.169620	0.059160	-3.361384
H	0.119190	1.664482	-2.659989
H	-0.161340	-0.803270	-0.963048
H	0.644236	-1.312985	1.220735
H	0.683392	-2.808032	2.912880
Cl	-0.651168	-2.686883	0.173031
H	2.965002	-1.976159	6.494207
H	2.891153	0.903364	3.258318
H	3.668058	0.220832	5.512835
N	1.364853	-3.790364	5.305582
O	0.623596	-4.513755	4.620279
O	1.767799	-4.100786	6.438919
Complex 9-Cl ⁻ [B97D3/6-31+G(d)] – PCM – DMSO			
Atom	X	Y	Z
C	-3.143127	-2.679315	-5.407122
C	-3.744391	-1.553602	-4.886044
C	-2.970019	-0.527424	-4.251464
C	-1.523410	-0.666555	-4.168030
C	-0.946873	-1.863694	-4.715105
C	-1.727271	-2.833377	-5.312885
C	-3.589596	0.604860	-3.699668
C	-2.848819	1.611175	-3.058448
C	-1.402628	1.490856	-2.975545
C	-0.759541	0.358515	-3.546635
C	-3.497225	2.752176	-2.482146
C	-2.771172	3.734652	-1.842218
C	-1.351314	3.621629	-1.753210
C	-0.690200	2.539764	-2.301893
C	0.747378	0.225862	-3.438769
N	1.126169	-0.351530	-2.133497
C	1.998864	0.201887	-1.306667
C	2.509472	-0.148013	-0.018210
C	3.419994	1.022820	0.016438
C	2.854291	1.431400	-1.344507
N	2.311392	-1.239546	0.760410
O	4.280304	1.466535	0.784005
O	3.037181	2.346960	-2.150156
C	2.654481	-1.315132	2.113661
C	3.037705	-2.528426	2.760040
C	3.349642	-2.547938	4.134671
C	3.295558	-1.379431	4.886447
C	2.931642	-0.171401	4.259455
C	2.614378	-0.143710	2.903912
N	3.183029	-3.777884	2.033259
O	3.802078	-4.714855	2.575846
O	2.693931	-3.865921	0.887331
H	-3.742385	-3.455515	-5.884806
H	-4.826954	-1.424028	-4.941298
H	0.126187	-2.031339	-4.649542
H	-1.256332	-3.732385	-5.713108

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H	−4.675828	0.700981	−3.762459
H	−4.583877	2.823616	−2.559334
H	−3.275015	4.597170	−1.404002
H	−0.780296	4.400620	−1.245708
H	0.392274	2.494505	−2.213898
H	1.150428	−0.411409	−4.233712
H	1.247815	1.193010	−3.535903
H	0.607687	−1.190868	−1.807066
H	1.796863	−2.034318	0.358157
H	3.629978	−3.494812	4.588664
H	3.525104	−1.405419	5.950814
H	2.871658	0.750054	4.838710
H	2.298675	0.786057	2.438180
Cl	−0.314858	−2.792934	−0.691820
Complex 1-Cl [−] [ZORA-BLYP-D3(BJ)/TZ2P] – COSMO – DMSO			
Atom	X	Y	Z
C	−3.895103	−2.766347	−4.127109
C	−4.603744	−1.658833	−3.727021
C	−3.937784	−0.510656	−3.188955
C	−2.487139	−0.508497	−3.084941
C	−1.796761	−1.695334	−3.501607
C	−2.474823	−2.782971	−4.002911
C	−4.661979	0.606060	−2.752262
C	−4.024403	1.726371	−2.202952
C	−2.574090	1.749748	−2.107402
C	−1.826232	0.637272	−2.571760
C	−4.778405	2.848839	−1.731518
C	−4.153958	3.941804	−1.179852
C	−2.731947	3.969957	−1.077960
C	−1.968963	2.915816	−1.528580
C	−0.309230	0.661264	−2.492333
N	0.173931	0.139840	−1.191926
C	0.916528	0.836705	−0.341951
C	1.452582	0.543739	0.957247
C	2.096878	1.886252	1.039313
C	1.530258	2.186481	−0.338436
N	1.314842	−0.582899	1.680070
O	2.791441	2.518341	1.850986
O	1.557655	3.150713	−1.120361
C	1.843428	−0.929778	2.943018
C	1.502250	−2.200697	3.448818
C	1.993912	−2.615920	4.687874
C	2.827386	−1.775173	5.438428
C	3.161973	−0.512518	4.930735
C	2.678284	−0.081511	3.690818
H	−4.411412	−3.634729	−4.531125
H	−5.689568	−1.634677	−3.806083
H	−0.717468	−1.754774	−3.405773
H	−1.922228	−3.670957	−4.303521
H	−5.748515	0.598644	−2.831734
H	−5.863466	2.812476	−1.816889
H	−4.737421	4.786621	−0.819175
H	−2.244394	4.837821	−0.638046
H	−0.889807	2.979984	−1.436017
H	0.128624	0.057517	−3.291951

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H	0.081168	1.672114	-2.609581
H	-0.134395	-0.806907	-0.911672
H	0.735143	-1.321272	1.239961
H	0.855772	-2.851732	2.863637
H	1.723851	-3.599775	5.066855
H	3.808701	0.148726	5.504386
H	2.941712	0.899569	3.305907
Cl	-0.518707	-2.723958	0.110582
H	3.210592	-2.099468	6.403509
Complex			
1-Cl ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.975324	-2.828773	-3.583948
C	-4.658661	-1.635962	-3.558685
C	-4.009989	-0.422703	-3.165456
C	-2.599648	-0.451177	-2.812501
C	-1.934552	-1.721251	-2.847248
C	-2.600721	-2.868209	-3.213615
C	-4.707100	0.791022	-3.112702
C	-4.089335	1.976262	-2.696856
C	-2.679756	1.961528	-2.333340
C	-1.946994	0.750239	-2.430740
C	-4.818721	3.206075	-2.625378
C	-4.216372	4.365113	-2.199938
C	-2.843486	4.351277	-1.816559
C	-2.100249	3.194583	-1.880358
C	-0.443499	0.737625	-2.175168
N	-0.054711	0.196017	-0.859488
C	0.609407	0.903320	0.057440
C	1.250965	0.516710	1.270962
C	1.652471	1.932939	1.573830
C	0.980023	2.332767	0.243976
N	1.387379	-0.731784	1.769658
O	2.255332	2.525002	2.467466
O	0.832590	3.368718	-0.411011
C	2.043284	-1.170607	2.931367
C	2.087887	-2.565708	3.148683
C	2.724114	-3.075540	4.279962
C	3.323907	-2.215262	5.211187
C	3.275952	-0.832318	4.989208
C	2.642888	-0.300074	3.862454
H	-4.484342	-3.747692	-3.871853
H	-5.714621	-1.592997	-3.824926
H	-0.903137	-1.818566	-2.522805
H	-2.071277	-3.818221	-3.189035
H	-5.761379	0.810857	-3.391355
H	-5.870861	3.197373	-2.909963
H	-4.784827	5.292503	-2.144666
H	-2.374603	5.264919	-1.455955
H	-1.066399	3.228847	-1.547123
H	0.042084	0.124132	-2.945834
H	-0.029497	1.742028	-2.259709
H	-0.068858	-0.841934	-0.736166
H	1.022180	-1.499641	1.153523
H	1.626240	-3.226162	2.416277
H	2.753282	-4.153692	4.433259

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H	3.739875	−0.151570	5.702279
H	2.619392	0.774434	3.694196
H	3.821808	−2.616431	6.092344
Cl	0.342830	−2.864725	−0.284951
Complex $1-\text{Br}^- [\text{ZORA-BLYP-D3(BJ)}/\text{TZ2P}]$			
Atom	X	Y	Z
C	−3.961279	−2.814342	−3.659531
C	−4.655196	−1.638631	−3.500046
C	−3.989002	−0.436720	−3.101149
C	−2.550924	−0.456700	−2.886342
C	−1.876628	−1.711526	−3.053678
C	−2.557890	−2.848746	−3.421155
C	−4.696476	0.755760	−2.905326
C	−4.057970	1.930778	−2.491348
C	−2.618582	1.927346	−2.275786
C	−1.882936	0.734324	−2.498467
C	−4.796123	3.138747	−2.275564
C	−4.170101	4.288875	−1.859567
C	−2.763119	4.287330	−1.631965
C	−2.013171	3.151326	−1.832892
C	−0.367126	0.723602	−2.332266
N	0.073778	0.175415	−1.035632
C	0.729841	0.883629	−0.114524
C	1.322351	0.518403	1.130374
C	1.764151	1.929924	1.396747
C	1.140512	2.306510	0.037921
N	1.394163	−0.710347	1.688175
O	2.363535	2.531308	2.286066
O	1.038967	3.324218	−0.652384
C	1.965346	−1.120705	2.905497
C	1.915777	−2.501511	3.198125
C	2.455871	−2.981950	4.390660
C	3.053164	−2.105407	5.308163
C	3.100700	−0.736842	5.009963
C	2.564746	−0.233952	3.820549
H	−4.482525	−3.725465	−3.950130
H	−5.732414	−1.601272	−3.661261
H	−0.818743	−1.803129	−2.832638
H	−2.017228	−3.789567	−3.496591
H	−5.774430	0.767050	−3.070542
H	−5.872551	3.120860	−2.445253
H	−4.744151	5.199684	−1.694850
H	−2.271539	5.194034	−1.284267
H	−0.949203	3.194823	−1.619890
H	0.081989	0.115201	−3.127222
H	0.044276	1.728276	−2.427422
H	0.000424	−0.854013	−0.893197
H	1.020046	−1.489676	1.100649
H	1.455819	−3.176379	2.477903
H	2.410130	−4.049422	4.602458
H	3.563806	−0.044115	5.711805
H	2.613221	0.828887	3.594919
H	3.474161	−2.482631	6.238464
Br	0.297499	−3.049968	−0.376812
Complex $1-\text{NO}_3^- [\text{ZORA-BLYP-D3(BJ)}/\text{TZ2P}]$			

Atom	X	Y	Z
C	-3.818957	-2.882542	-3.430950
C	-4.520254	-1.765032	-3.050941
C	-3.851564	-0.532828	-2.766978
C	-2.408425	-0.458373	-2.905333
C	-1.724642	-1.651683	-3.310169
C	-2.402235	-2.822402	-3.554789
C	-4.557076	0.592769	-2.326601
C	-3.906099	1.787539	-1.996213
C	-2.459989	1.874923	-2.124068
C	-1.735739	0.750399	-2.594675
C	-4.635772	2.920424	-1.515035
C	-3.993195	4.082647	-1.161236
C	-2.575802	4.170493	-1.272699
C	-1.834857	3.107455	-1.737915
C	-0.217679	0.792402	-2.678675
N	0.390789	0.204983	-1.467408
C	0.975493	0.938554	-0.517394
C	1.396478	0.605721	0.799660
C	1.950482	1.983781	1.033165
C	1.483852	2.331938	-0.401554
N	1.245841	-0.584360	1.424955
O	2.523676	2.579271	1.942457
O	1.503880	3.317289	-1.141505
C	1.624403	-0.972755	2.719673
C	1.319092	-2.294310	3.111249
C	1.664369	-2.744401	4.385138
C	2.317235	-1.893792	5.288651
C	2.617913	-0.583138	4.894057
C	2.280591	-0.112994	3.622030
H	-4.336389	-3.822121	-3.615782
H	-5.602593	-1.802377	-2.931314
H	-0.642316	-1.655830	-3.385793
H	-1.847839	-3.720299	-3.818960
H	-5.639775	0.529742	-2.213851
H	-5.718371	2.833649	-1.423565
H	-4.560670	4.933394	-0.786459
H	-2.066872	5.085518	-0.975060
H	-0.755717	3.215140	-1.784073
H	0.130151	0.231872	-3.553794
H	0.158584	1.810318	-2.781352
H	0.107241	-0.756861	-1.193192
H	0.750152	-1.308012	0.860949
H	0.812069	-2.953608	2.409087
H	1.419771	-3.765775	4.672793
H	3.123067	0.089849	5.585813
H	2.516041	0.907136	3.326547
H	2.584034	-2.246347	6.283423
N	-1.249347	-2.632683	-0.111659
O	-1.999125	-1.649554	0.142516
O	-1.657487	-3.818806	-0.135543
O	0.031947	-2.395562	-0.372134
Complex	2-Cl ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]		
Atom	X	Y	Z
C	-3.981766	-2.821992	-3.620932

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C	-4.649941	-1.621090	-3.650882
C	-4.003140	-0.407233	-3.256526
C	-2.610929	-0.444501	-2.838708
C	-1.961235	-1.722813	-2.818647
C	-2.625221	-2.869374	-3.190412
C	-4.685008	0.816126	-3.266501
C	-4.069144	2.004637	-2.857854
C	-2.677905	1.981674	-2.429065
C	-1.960094	0.757636	-2.455678
C	-4.782885	3.245480	-2.858125
C	-4.182764	4.409954	-2.445063
C	-2.828793	4.390258	-2.000869
C	-2.101132	3.221769	-1.992324
C	-0.469865	0.731894	-2.131645
N	-0.139464	0.206964	-0.790843
C	0.513662	0.914403	0.131700
C	1.128689	0.544945	1.363855
C	1.541165	1.957083	1.654545
C	0.895375	2.347186	0.305807
N	1.248230	-0.699206	1.890034
O	2.136591	2.552691	2.549714
O	0.770288	3.372175	-0.365178
C	1.872946	-1.118981	3.065966
C	1.899906	-2.511722	3.314665
C	2.501027	-3.009501	4.465182
C	3.085425	-2.135712	5.398917
C	3.063114	-0.752152	5.146599
C	2.465260	-0.239241	3.998110
H	-4.489289	-3.740668	-3.911882
H	-5.692325	-1.570907	-3.965385
H	-0.944538	-1.824442	-2.452285
H	-2.108825	-3.824596	-3.126471
H	-5.725319	0.842012	-3.593170
H	-5.821155	3.241515	-3.189825
H	-4.738949	5.346219	-2.446518
H	-2.362375	5.309901	-1.652432
H	-1.082987	3.252821	-1.614981
H	0.041862	0.099471	-2.869262
H	-0.039955	1.729300	-2.215005
H	-0.173024	-0.828755	-0.651184
H	0.885641	-1.475980	1.277353
H	1.446683	-3.183257	2.587436
H	2.513451	-4.081733	4.641571
H	3.516050	-0.066139	5.858672
H	2.459577	0.832818	3.812065
C	3.780835	-2.663956	6.616855
F	3.595118	-1.866275	7.730719
F	3.369829	-3.931436	6.970082
F	5.161563	-2.750399	6.455908
Cl	0.218723	-2.837647	-0.126159
Complex			2-Br ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	-3.999675	-2.784298	-3.762429
C	-4.662074	-1.579971	-3.769292
C	-4.016817	-0.380904	-3.329533

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C	-2.632357	-0.436283	-2.888109
C	-1.988863	-1.717513	-2.895848
C	-2.650667	-2.850061	-3.311453
C	-4.693114	0.845242	-3.317850
C	-4.078460	2.019762	-2.868742
C	-2.695251	1.978545	-2.416490
C	-1.983300	0.751149	-2.458292
C	-4.785663	3.264220	-2.852215
C	-4.185994	4.415867	-2.404212
C	-2.839179	4.378573	-1.940258
C	-2.118531	3.205650	-1.944960
C	-0.500254	0.710875	-2.103943
N	-0.198018	0.187524	-0.752857
C	0.489469	0.879310	0.158717
C	1.118829	0.516880	1.386925
C	1.557025	1.928013	1.649877
C	0.898838	2.307373	0.306575
N	1.236048	-0.715982	1.941272
O	2.172318	2.529156	2.527053
O	0.781323	3.324089	-0.377523
C	1.889516	-1.117767	3.111389
C	1.914042	-2.506584	3.388100
C	2.541349	-2.983419	4.532157
C	3.160298	-2.094547	5.432374
C	3.139179	-0.719026	5.152683
C	2.512471	-0.225751	4.007870
H	-4.506115	-3.691863	-4.087825
H	-5.698597	-1.515658	-4.100177
H	-0.977765	-1.832179	-2.518432
H	-2.138950	-3.808851	-3.266827
H	-5.727519	0.885004	-3.661380
H	-5.818062	3.273672	-3.201517
H	-4.736722	5.355296	-2.394580
H	-2.371881	5.288252	-1.567926
H	-1.103977	3.223876	-1.557769
H	0.021725	0.072788	-2.828950
H	-0.059632	1.704150	-2.179562
H	-0.263017	-0.842909	-0.614292
H	0.854746	-1.500939	1.360195
H	1.439027	-3.191271	2.687457
H	2.551055	-4.053027	4.729285
H	3.616755	-0.021606	5.835408
H	2.510707	0.842122	3.800718
C	3.846090	-2.637572	6.651565
F	4.273835	-1.659381	7.519022
F	3.033777	-3.484670	7.389862
F	4.970686	-3.395230	6.344610
Br	0.104325	-3.030901	-0.087919
Complex 2-NO ₃ ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-4.235449	-2.653571	-3.467735
C	-4.845590	-1.424122	-3.535618
C	-4.135777	-0.228693	-3.197090
C	-2.739429	-0.317273	-2.802349
C	-2.151589	-1.624482	-2.746440

ARTICLE			Journal Name
C	-2.875713	-2.752463	-3.056934
C	-4.759853	1.024488	-3.238154
C	-4.083317	2.195925	-2.878695
C	-2.687611	2.122294	-2.470638
C	-2.028092	0.865469	-2.470864
C	-4.740620	3.467675	-2.905692
C	-4.082754	4.615089	-2.534329
C	-2.724548	4.546313	-2.108453
C	-2.049645	3.347042	-2.077790
C	-0.536486	0.775613	-2.168710
N	-0.212711	0.230235	-0.832884
C	0.468893	0.914375	0.089897
C	1.055568	0.546602	1.336373
C	1.530380	1.950805	1.590640
C	0.913640	2.330162	0.227461
N	1.103655	-0.681135	1.911229
O	2.143213	2.547570	2.471263
O	0.838686	3.340652	-0.471480
C	1.730053	-1.085254	3.098423
C	1.639980	-2.455002	3.436419
C	2.251747	-2.931606	4.591499
C	2.957262	-2.058320	5.437566
C	3.039419	-0.696575	5.100324
C	2.434088	-0.204723	3.945773
H	-4.791173	-3.557411	-3.712686
H	-5.889564	-1.335497	-3.836003
H	-1.128418	-1.762939	-2.412369
H	-2.402817	-3.724758	-2.950702
H	-5.803528	1.088126	-3.548247
H	-5.783028	3.501297	-3.222203
H	-4.596187	5.575189	-2.554260
H	-2.213022	5.453289	-1.791270
H	-1.026128	3.341507	-1.714242
H	-0.061691	0.126965	-2.916998
H	-0.063648	1.753217	-2.247742
H	-0.309529	-0.788537	-0.695363
H	0.709411	-1.456428	1.328031
H	1.077828	-3.127319	2.788859
H	2.174380	-3.986710	4.839961
H	3.580819	-0.010932	5.747397
H	2.504473	0.852032	3.697838
C	3.671599	-2.575707	6.650288
F	3.693442	-1.666749	7.689759
F	3.118431	-3.734284	7.152586
F	5.006950	-2.878805	6.397931
N	-0.390602	-3.581074	0.118185
O	-0.404413	-4.074722	1.280284
O	-0.885510	-4.166419	-0.876992
O	0.180902	-2.403725	-0.058357
Complex			3-Cl ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	-4.099236	-2.795998	-3.549600
C	-4.736862	-1.579212	-3.590648
C	-4.053092	-0.375489	-3.228705
C	-2.655219	-0.441397	-2.834455

Journal Name			ARTICLE
C	-2.038224	-1.735772	-2.801358
C	-2.737460	-2.871244	-3.140194
C	-4.703741	0.864641	-3.247638
C	-4.051109	2.043787	-2.869561
C	-2.653591	1.992551	-2.464841
C	-1.968002	0.750085	-2.483871
C	-4.733496	3.302350	-2.877178
C	-4.097238	4.457499	-2.492422
C	-2.736431	4.410475	-2.071844
C	-2.038380	3.224118	-2.057953
C	-0.475067	0.689906	-2.180061
N	-0.145282	0.184700	-0.831834
C	0.529138	0.892946	0.072753
C	1.127875	0.537483	1.315481
C	1.594242	1.937228	1.569832
C	0.964206	2.316768	0.209071
N	1.190460	-0.692652	1.884220
O	2.212057	2.528256	2.452591
O	0.874490	3.325923	-0.488255
C	1.820811	-1.099330	3.059268
C	1.748197	-2.479278	3.372238
C	2.354653	-2.960799	4.528175
C	3.050300	-2.101470	5.397009
C	3.115742	-0.742488	5.076462
C	2.511227	-0.227070	3.922034
H	-4.634598	-3.706406	-3.815233
H	-5.782709	-1.508002	-3.888887
H	-1.018234	-1.855528	-2.450683
H	-2.245895	-3.838701	-3.066423
H	-5.748690	0.911806	-3.556437
H	-5.777210	3.319749	-3.190739
H	-4.629592	5.407424	-2.498625
H	-2.241151	5.323315	-1.745994
H	-1.012763	3.235348	-1.700456
H	0.009894	0.027727	-2.909392
H	-0.017567	1.672570	-2.289112
H	-0.230864	-0.842387	-0.656728
H	0.780144	-1.473921	1.302574
H	1.218863	-3.144146	2.693540
H	2.572934	0.835032	3.686257
H	3.523504	-2.483937	6.294114
C	3.853223	0.221165	5.982089
F	3.027909	1.212260	6.465514
F	4.407907	-0.396447	7.082081
F	4.886329	0.859337	5.333065
C	2.283762	-4.429781	4.878675
F	1.722874	-4.632961	6.128166
F	1.551199	-5.167598	3.993779
F	3.540814	-5.007049	4.934971
Cl	0.051090	-2.841880	-0.016691
Complex 3-Br [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-4.205307	-2.741919	-3.462816
C	-4.804100	-1.510055	-3.576456
C	-4.095230	-0.311681	-3.245661

ARTICLE			Journal Name
C	-2.715659	-0.400671	-2.796330
C	-2.136745	-1.708585	-2.700279
C	-2.857960	-2.837566	-3.012990
C	-4.702633	0.945597	-3.352907
C	-4.024401	2.121360	-3.011890
C	-2.650723	2.046397	-2.535010
C	-2.007388	0.783004	-2.459548
C	-4.658442	3.400222	-3.128144
C	-3.999147	4.554002	-2.780280
C	-2.665894	4.484588	-2.281847
C	-2.014462	3.278376	-2.162429
C	-0.532410	0.690655	-2.082028
N	-0.266442	0.185092	-0.716164
C	0.405021	0.879730	0.204570
C	1.014126	0.512104	1.438946
C	1.455070	1.915874	1.718122
C	0.821633	2.307280	0.362266
N	1.121730	-0.726366	1.985420
O	2.060624	2.501753	2.611713
O	0.729009	3.323507	-0.322855
C	1.808214	-1.145142	3.128014
C	1.863353	-2.540902	3.360176
C	2.546192	-3.034605	4.469072
C	3.179003	-2.168373	5.376394
C	3.114946	-0.792094	5.137423
C	2.439817	-0.266380	4.028077
H	-4.759817	-3.647233	-3.705585
H	-5.837111	-1.421358	-3.912643
H	-1.126988	-1.845734	-2.327129
H	-2.392667	-3.812798	-2.887843
H	-5.731696	1.010186	-3.708372
H	-5.682948	3.434258	-3.498135
H	-4.493107	5.519910	-2.873496
H	-2.155278	5.397512	-1.980597
H	-1.012932	3.274315	-1.742952
H	-0.028206	0.012074	-2.782748
H	-0.048628	1.661471	-2.175487
H	-0.333584	-0.842956	-0.568819
H	0.741666	-1.507471	1.394768
H	1.382616	-3.211301	2.650587
H	2.413340	0.807937	3.848553
H	3.712185	-2.558284	6.235638
C	3.810124	0.176130	6.071287
F	2.964494	1.163972	6.519683
F	4.326158	-0.438203	7.191639
F	4.866982	0.816756	5.460412
C	2.587320	-4.524618	4.731674
F	1.666245	-4.904433	5.694474
F	2.322668	-5.275897	3.621896
F	3.818026	-4.933570	5.208174
Br	0.031483	-3.042359	-0.019389
Complex			3-NO ₃ ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	-4.282882	-2.619124	-3.436419
C	-4.883932	-1.385675	-3.511188

Journal Name	ARTICLE		
C	-4.162662	-0.192770	-3.188176
C	-2.765064	-0.288620	-2.800042
C	-2.186039	-1.599591	-2.739702
C	-2.920588	-2.724651	-3.035880
C	-4.776849	1.064964	-3.238855
C	-4.089776	2.234364	-2.893361
C	-2.693892	2.153278	-2.487392
C	-2.044151	0.891377	-2.479681
C	-4.736817	3.511179	-2.931684
C	-4.069362	4.656552	-2.571520
C	-2.711790	4.580452	-2.145013
C	-2.046459	3.376298	-2.104674
C	-0.552618	0.792372	-2.181066
N	-0.228531	0.237816	-0.848839
C	0.445416	0.915464	0.082812
C	1.025565	0.537776	1.328233
C	1.500866	1.936258	1.599525
C	0.889458	2.332070	0.237060
N	1.066075	-0.695008	1.897028
O	2.113096	2.518389	2.489978
O	0.816719	3.348873	-0.450272
C	1.702279	-1.101797	3.076674
C	1.581505	-2.467114	3.431059
C	2.209024	-2.937019	4.582631
C	2.963470	-2.081719	5.403139
C	3.065003	-0.734765	5.045738
C	2.444257	-0.231311	3.894916
H	-4.847090	-3.520833	-3.669292
H	-5.929057	-1.291603	-3.805656
H	-1.160222	-1.742962	-2.416037
H	-2.453590	-3.699574	-2.927529
H	-5.821112	1.133894	-3.545695
H	-5.779122	3.550325	-3.247751
H	-4.574740	5.620639	-2.600157
H	-2.193306	5.485892	-1.834857
H	-1.023702	3.365629	-1.739587
H	-0.082395	0.144132	-2.932472
H	-0.074387	1.767496	-2.256421
H	-0.319463	-0.782581	-0.718913
H	0.679198	-1.467694	1.301208
H	0.989386	-3.130193	2.800942
H	2.530154	0.823135	3.635510
C	3.900908	0.212784	5.878718
F	3.263354	1.404299	6.116729
F	4.235582	-0.310633	7.109154
F	5.094574	0.526238	5.256748
C	2.091310	-4.390354	4.986967
F	1.520260	-4.527053	6.241517
F	1.344641	-5.137640	4.127934
F	3.333380	-4.998085	5.075577
H	3.450951	-2.457321	6.295860
N	-0.417391	-3.549143	0.116255
O	-0.456307	-4.004081	1.293366
O	-0.921763	-4.147119	-0.864290
O	0.194166	-2.394936	-0.089961

Complex		4-Cl ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]		
Atom	X	Y	Z	
C	-3.935117	-2.862421	-3.484693	
C	-4.636351	-1.685187	-3.377274	
C	-3.976508	-0.461563	-3.038774	
C	-2.538125	-0.462070	-2.827017	
C	-1.855048	-1.718092	-2.941222	
C	-2.530038	-2.875362	-3.252974	
C	-4.690499	0.735499	-2.902662	
C	-4.058683	1.933626	-2.550253	
C	-2.619454	1.948934	-2.332053	
C	-1.877844	0.750319	-2.496737	
C	-4.804047	3.146827	-2.401406	
C	-4.186209	4.320812	-2.044868	
C	-2.780479	4.338300	-1.810103	
C	-2.023727	3.197548	-1.948339	
C	-0.360991	0.754355	-2.339627	
N	0.097901	0.207418	-1.047572	
C	0.716306	0.922259	-0.113268	
C	1.301379	0.560118	1.134802	
C	1.709101	1.969894	1.434238	
C	1.092069	2.360270	0.068626	
N	1.398618	-0.684828	1.668620	
O	2.285492	2.565229	2.340091	
O	0.978628	3.381945	-0.604907	
C	1.911008	-1.094684	2.891412	
C	1.891177	-2.489741	3.156839	
C	2.366148	-2.980745	4.361409	
C	2.869611	-2.088016	5.324235	
C	2.901987	-0.706369	5.069809	
C	2.428969	-0.205894	3.864085	
N	3.360031	-2.601862	6.598858	
O	3.789107	-1.782270	7.449438	
O	3.331809	-3.843336	6.792921	
H	-4.450753	-3.789397	-3.731012	
H	-5.714132	-1.662170	-3.536651	
H	-0.794590	-1.793157	-2.725948	
H	-1.982526	-3.814375	-3.293806	
H	-5.768325	0.732622	-3.068278	
H	-5.879544	3.113898	-2.573811	
H	-4.765427	5.235989	-1.931603	
H	-2.296237	5.264419	-1.505723	
H	-0.962646	3.256172	-1.726911	
H	0.087344	0.146307	-3.135246	
H	0.041487	1.761725	-2.440888	
H	0.058733	-0.829732	-0.905624	
H	1.058451	-1.464403	1.040838	
H	1.495956	-3.160790	2.396431	
H	2.353977	-4.043940	4.576960	
H	3.300965	-0.040175	5.827692	
H	2.462341	0.862042	3.659824	
Cl	0.431674	-2.817439	-0.355499	
Complex		4-Br ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]		
Atom	X	Y	Z	
C	-3.956406	-2.826468	-3.634845	

Journal Name			ARTICLE
C	-4.650919	-1.651367	-3.475584
C	-3.982803	-0.445108	-3.093724
C	-2.542682	-0.460226	-2.893687
C	-1.867333	-1.714150	-3.062796
C	-2.549909	-2.855220	-3.414990
C	-4.690693	0.747382	-2.900426
C	-4.050970	1.927898	-2.504858
C	-2.609685	1.929749	-2.303131
C	-1.874870	0.735215	-2.519735
C	-4.790459	3.135850	-2.294155
C	-4.163898	4.292261	-1.897378
C	-2.754435	4.297388	-1.686223
C	-2.003751	3.161051	-1.881952
C	-0.359216	0.726268	-2.359299
N	0.084076	0.179011	-1.060342
C	0.733541	0.883139	-0.138515
C	1.309867	0.534214	1.117571
C	1.767294	1.937858	1.376758
C	1.159738	2.311092	0.004132
N	1.365297	-0.693613	1.696223
O	2.365531	2.538722	2.264191
O	1.075657	3.317254	-0.695871
C	1.888448	-1.082922	2.923597
C	1.819359	-2.465085	3.239742
C	2.308256	-2.932544	4.448502
C	2.873192	-2.027935	5.364180
C	2.951832	-0.658484	5.060131
C	2.466197	-0.182107	3.849483
N	3.380911	-2.516861	6.643042
O	3.850261	-1.683602	7.457477
O	3.326138	-3.750525	6.874574
H	-4.478530	-3.740912	-3.912399
H	-5.729832	-1.617431	-3.624779
H	-0.805532	-1.800079	-2.859570
H	-2.008012	-3.794873	-3.495106
H	-5.770294	0.754567	-3.053632
H	-5.868341	3.112958	-2.452663
H	-4.738558	5.203116	-1.736470
H	-2.261914	5.210329	-1.356669
H	-0.937670	3.210430	-1.684307
H	0.089736	0.113671	-3.150481
H	0.053901	1.729646	-2.457522
H	-0.011520	-0.848660	-0.905065
H	0.989639	-1.479703	1.107660
H	1.378323	-3.147753	2.515582
H	2.260551	-3.986394	4.701912
H	3.397636	0.017665	5.782426
H	2.535012	0.875912	3.606721
Br	0.260808	-3.012116	-0.315351
Complex			
4-NO ₃ ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.784441	-2.907137	-3.401445
C	-4.500550	-1.783569	-3.070167
C	-3.844925	-0.541020	-2.801088
C	-2.398429	-0.464053	-2.896411

ARTICLE			Journal Name
C	-1.698794	-1.663884	-3.252189
C	-2.364929	-2.843149	-3.487461
C	-4.567947	0.594696	-2.419003
C	-3.932987	1.803418	-2.109461
C	-2.483468	1.892283	-2.187655
C	-1.741030	0.755674	-2.596332
C	-4.683659	2.950000	-1.697880
C	-4.058625	4.127640	-1.365548
C	-2.637958	4.216794	-1.425622
C	-1.877039	3.140320	-1.821625
C	-0.221557	0.799699	-2.625287
N	0.341656	0.228631	-1.383181
C	0.921587	0.958705	-0.435077
C	1.341554	0.635128	0.883364
C	1.899036	2.006190	1.121580
C	1.435259	2.358650	-0.319451
N	1.184863	-0.559369	1.513731
O	2.471911	2.596923	2.031219
O	1.459916	3.337512	-1.059431
C	1.612959	-0.964602	2.769818
C	1.302522	-2.292490	3.162401
C	1.715564	-2.776190	4.392840
C	2.447746	-1.941451	5.254357
C	2.752179	-0.621262	4.882739
C	2.338843	-0.128755	3.652060
N	2.900778	-2.456781	6.544225
O	3.578181	-1.701380	7.284363
O	2.595915	-3.634995	6.855695
H	-4.292685	-3.853064	-3.578162
H	-5.585736	-1.822320	-2.982115
H	-0.614769	-1.664846	-3.301682
H	-1.800174	-3.743971	-3.717170
H	-5.653450	0.530404	-2.339972
H	-5.768533	2.862000	-1.645059
H	-4.641950	4.990257	-1.046934
H	-2.144054	5.145242	-1.144945
H	-0.797463	3.250787	-1.831192
H	0.161283	0.225612	-3.476530
H	0.158188	1.815934	-2.727912
H	0.061964	-0.735454	-1.111138
H	0.674617	-1.279477	0.944971
H	0.742452	-2.929694	2.481404
H	1.486583	-3.790491	4.702026
H	3.313374	0.004472	5.568833
H	2.568813	0.894681	3.363396
N	-1.323638	-2.522817	0.016575
O	-2.025049	-1.502963	0.260190
O	-1.781633	-3.686892	-0.005425
O	-0.025913	-2.343592	-0.236103
Complex			5-Cl ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	-3.997237	-2.803563	-3.592433
C	-4.666812	-1.603110	-3.590613
C	-4.005133	-0.390001	-3.219660
C	-2.596915	-0.427775	-2.860439

Journal Name			ARTICLE
C	-1.945976	-1.705345	-2.873645
C	-2.623257	-2.851262	-3.221204
C	-4.687522	0.832864	-3.194043
C	-4.057042	2.019691	-2.802703
C	-2.650093	1.995753	-2.429799
C	-1.934030	0.772692	-2.494727
C	-4.771766	3.259330	-2.764046
C	-4.157635	4.421041	-2.363919
C	-2.786955	4.399993	-1.973643
C	-2.058341	3.232623	-2.004245
C	-0.436846	0.741955	-2.212257
N	-0.087204	0.211383	-0.879232
C	0.561012	0.912741	0.047006
C	1.135475	0.545772	1.296300
C	1.594355	1.940020	1.580719
C	0.983078	2.340064	0.213516
N	1.181904	-0.692704	1.852723
O	2.196892	2.514407	2.483127
O	0.892025	3.358799	-0.466687
C	1.762256	-1.110922	3.042902
C	1.650465	-2.488720	3.353571
C	2.218186	-2.965964	4.529959
C	2.908388	-2.149615	5.428287
C	2.992265	-0.797810	5.093152
C	2.441416	-0.249946	3.934691
H	-4.515692	-3.722092	-3.863193
H	-5.721555	-1.553346	-3.859820
H	-0.914349	-1.804729	-2.552729
H	-2.104786	-3.806664	-3.182655
H	-5.740566	0.859292	-3.476166
H	-5.822226	3.256556	-3.054340
H	-4.714547	5.356299	-2.334703
H	-2.308734	5.317316	-1.635384
H	-1.025643	3.262364	-1.669128
H	0.056582	0.109205	-2.961488
H	-0.002596	1.737155	-2.299890
H	-0.171728	-0.818502	-0.718436
H	0.787188	-1.469963	1.248711
H	1.130585	-3.159404	2.673660
H	2.537613	0.815055	3.724734
Cl	0.112783	-2.815620	-0.080984
H	3.348990	-2.540944	6.334520
N	3.717109	0.108690	6.037485
O	3.741725	1.321947	5.774764
O	4.256072	-0.410254	7.036750
N	2.079420	-4.417735	4.858031
O	2.656719	-4.835856	5.881773
O	1.396027	-5.123735	4.097323
Complex			5-Br ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	-3.977094	-2.813150	-3.603769
C	-4.665970	-1.634261	-3.447775
C	-3.991088	-0.428441	-3.076581
C	-2.550205	-0.448470	-2.883752
C	-1.880487	-1.705478	-3.051969

ARTICLE

Journal Name

C	-2.569314	-2.846015	-3.393300
C	-4.692601	0.768481	-2.886744
C	-4.046029	1.947885	-2.498905
C	-2.604279	1.943673	-2.300230
C	-1.875981	0.745240	-2.516107
C	-4.779003	3.160482	-2.292069
C	-4.145946	4.315150	-1.900573
C	-2.736342	4.313728	-1.689980
C	-1.991620	3.172930	-1.882451
C	-0.360362	0.728585	-2.359675
N	0.082557	0.168912	-1.066188
C	0.742018	0.860637	-0.141143
C	1.319841	0.494884	1.107115
C	1.794864	1.886022	1.380734
C	1.180789	2.284429	0.015399
N	1.352711	-0.736096	1.682428
O	2.406852	2.459533	2.276967
O	1.094437	3.299798	-0.669694
C	1.911789	-1.143896	2.888522
C	1.768146	-2.512426	3.225177
C	2.311539	-2.976372	4.418297
C	3.004457	-2.155034	5.309454
C	3.119032	-0.812369	4.948665
C	2.594267	-0.277887	3.771455
H	-4.504412	-3.727358	-3.871956
H	-5.745592	-1.597109	-3.590866
H	-0.817205	-1.793490	-2.857806
H	-2.031534	-3.788095	-3.472087
H	-5.772704	0.779969	-3.035955
H	-5.857193	3.142545	-2.449026
H	-4.715632	5.229614	-1.742784
H	-2.239223	5.225144	-1.363152
H	-0.925396	3.216770	-1.683729
H	0.084026	0.120825	-3.157364
H	0.057452	1.730596	-2.450284
H	-0.026043	-0.856864	-0.913838
H	0.950369	-1.515280	1.097731
H	1.243598	-3.187872	2.553267
H	2.712808	0.780800	3.541974
Br	0.216012	-3.027498	-0.288369
H	3.424298	-2.536202	6.229811
N	3.846291	0.099553	5.885447
O	4.371205	-0.410777	6.896536
O	3.886191	1.308500	5.605231
N	2.139540	-4.418300	4.774780
O	1.452206	-5.125923	4.019780
O	2.695102	-4.825513	5.814880
Complex 5-NO ₃ ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.705553	-2.901517	-3.808851
C	-4.415441	-1.854383	-3.276279
C	-3.763854	-0.646713	-2.873811
C	-2.326089	-0.523234	-3.039095
C	-1.630949	-1.649249	-3.591017
C	-2.295175	-2.794129	-3.963794

Journal Name			ARTICLE
C	-4.481450	0.408750	-2.301358
C	-3.851855	1.586569	-1.880997
C	-2.414976	1.727017	-2.043405
C	-1.674954	0.668088	-2.627932
C	-4.595882	2.649568	-1.278282
C	-3.974201	3.796524	-0.846849
C	-2.565468	3.938880	-0.999832
C	-1.812438	2.942498	-1.578188
C	-0.160764	0.755250	-2.715663
N	0.450837	0.159870	-1.503698
C	1.032017	0.890440	-0.551590
C	1.400530	0.590841	0.785490
C	2.010520	1.941801	0.999390
C	1.591486	2.274329	-0.460215
N	1.146184	-0.556961	1.467116
O	2.581766	2.528392	1.912428
O	1.644697	3.239981	-1.215092
C	1.505387	-0.899074	2.762595
C	1.018657	-2.127840	3.269332
C	1.358909	-2.514022	4.561961
C	2.167994	-1.743230	5.398075
C	2.637966	-0.543288	4.863161
C	2.333656	-0.095209	3.579055
H	-4.211532	-3.822231	-4.093349
H	-5.492289	-1.930257	-3.130575
H	-0.551202	-1.618844	-3.696535
H	-1.733240	-3.637694	-4.359975
H	-5.557381	0.303745	-2.161829
H	-5.671370	2.521800	-1.159609
H	-4.551054	4.593910	-0.380992
H	-2.074015	4.844107	-0.648343
H	-0.741685	3.092903	-1.666174
H	0.209792	0.220851	-3.595832
H	0.190901	1.784114	-2.795272
H	0.107203	-0.772649	-1.207760
H	0.533140	-1.241966	0.944971
H	0.384298	-2.763326	2.659084
H	2.710613	0.864187	3.226794
N	-1.632144	-2.048406	0.057883
O	-1.993321	-0.978695	0.622457
O	-2.428277	-2.932765	-0.320252
O	-0.324027	-2.231178	-0.152609
N	3.529080	0.302066	5.720542
O	4.051191	1.303088	5.204370
O	3.698075	-0.054747	6.904054
N	0.838415	-3.814461	5.084723
O	1.134522	-4.125970	6.255211
O	0.143071	-4.510896	4.325124
H	2.419327	-2.060013	6.400784
Complex 6-Cl ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.618188	-2.835453	-4.007767
C	-4.404002	-1.732443	-3.780865
C	-3.841397	-0.516561	-3.280989
C	-2.412889	-0.443918	-3.032459

ARTICLE			Journal Name
C	-1.641356	-1.627876	-3.267991
C	-2.222528	-2.781363	-3.736724
C	-4.640916	0.601389	-3.018501
C	-4.102638	1.785842	-2.504258
C	-2.672680	1.875110	-2.256562
C	-1.844950	0.762401	-2.550383
C	-4.934672	2.913360	-2.216534
C	-4.407585	4.070540	-1.699138
C	-3.010329	4.158541	-1.439554
C	-2.171827	3.102597	-1.709569
C	-0.337729	0.848829	-2.358874
N	0.120160	0.242263	-1.097814
C	0.691933	0.933884	-0.115467
C	1.202328	0.553572	1.150657
C	1.514036	1.955774	1.541142
C	1.029449	2.375933	0.126995
N	1.239992	-0.657372	1.740692
O	1.903267	2.509609	2.560294
O	0.917628	3.410497	-0.525251
C	1.839102	-1.001663	2.943583
C	1.198805	-2.028569	3.680583
C	1.642989	-2.403912	4.938020
C	2.749360	-1.760973	5.521791
C	3.430414	-0.792513	4.797562
C	3.019666	-0.439384	3.502310
H	-4.060432	-3.758579	-4.376556
H	-5.476545	-1.766066	-3.965571
H	-0.584600	-1.643892	-3.029027
H	-1.612499	-3.670724	-3.872316
H	-5.712249	0.544235	-3.208884
H	-6.002434	2.827648	-2.412349
H	-5.053032	4.918527	-1.478933
H	-2.597681	5.069867	-1.012841
H	-1.117752	3.210741	-1.476153
H	0.162918	0.337111	-3.189651
H	0.003611	1.882980	-2.373618
H	-0.082573	-0.766031	-0.910797
H	0.697443	-1.424779	1.248762
H	0.325297	-2.494270	3.230387
H	1.116399	-3.187305	5.478897
H	4.317466	-0.308886	5.190293
Cl	-0.306744	-2.661604	0.019696
H	3.087154	-2.033252	6.518302
N	3.963443	0.386402	2.728450
O	3.909491	0.322258	1.481928
O	4.832226	1.030422	3.354562
Complex			7-Cl ⁻ [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	-3.962199	-2.821732	-3.666431
C	-4.659446	-1.648376	-3.514592
C	-3.999838	-0.445895	-3.109665
C	-2.565295	-0.463454	-2.883707
C	-1.887507	-1.716655	-3.038658
C	-2.562566	-2.854372	-3.411469
C	-4.709936	0.744924	-2.919822

Journal Name			ARTICLE
C	-4.077063	1.919218	-2.498382
C	-2.639913	1.918902	-2.276402
C	-1.901357	0.729398	-2.500223
C	-4.818841	3.123154	-2.282048
C	-4.199079	4.271557	-1.856114
C	-2.794755	4.273177	-1.620759
C	-2.040595	3.141468	-1.825097
C	-0.386264	0.723157	-2.348524
N	0.070372	0.173634	-1.060186
C	0.751492	0.879692	-0.160781
C	1.359917	0.521390	1.073753
C	1.835802	1.918312	1.322261
C	1.187873	2.300180	-0.027107
N	1.422809	-0.705392	1.640963
O	2.467466	2.503881	2.195321
O	1.084059	3.311470	-0.719483
C	1.988247	-1.099766	2.852521
C	1.957138	-2.483716	3.144936
C	2.493380	-2.965767	4.335935
C	3.071706	-2.097713	5.265553
C	3.088434	-0.734205	4.957393
C	2.564332	-0.207081	3.776904
H	-4.478053	-3.732567	-3.963464
H	-5.733952	-1.613350	-3.687376
H	-0.832575	-1.803680	-2.804870
H	-2.021266	-3.794225	-3.483396
H	-5.785466	0.755029	-3.094119
H	-5.893308	3.103637	-2.457895
H	-4.776478	5.178735	-1.689562
H	-2.308924	5.178993	-1.265439
H	-0.977568	3.187360	-1.611613
H	0.055066	0.120621	-3.151276
H	0.019897	1.728880	-2.445736
H	-0.018463	-0.853635	-0.895120
H	1.024911	-1.487566	1.057775
H	1.508429	-3.156976	2.417453
H	2.460680	-4.032776	4.543127
Cl	0.271869	-2.859048	-0.273044
H	3.495798	-2.446654	6.198801
H	2.615970	0.860581	3.575472
N	3.693105	0.201344	5.945518
O	4.220766	-0.291258	6.966446
C	-3.962199	-2.821732	-3.666431
Complex 8-Cl⁻ [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.978416	-2.804071	-3.662913
C	-4.657764	-1.615843	-3.550757
C	-3.986430	-0.417778	-3.152173
C	-2.558877	-0.456721	-2.888391
C	-1.900108	-1.724134	-3.004501
C	-2.586307	-2.856466	-3.373223
C	-4.679043	0.789117	-3.004192
C	-4.035885	1.959940	-2.589042
C	-2.605737	1.937663	-2.326646
C	-1.883832	0.730776	-2.507178

ARTICLE			Journal Name
C	−4.760550	3.181499	−2.417874
C	−4.131543	4.326994	−1.997757
C	−2.734565	4.307440	−1.722273
C	−1.996721	3.157946	−1.881923
C	−0.374097	0.699209	−2.310988
N	0.034394	0.152190	−1.005136
C	0.693376	0.853100	−0.088442
C	1.253441	0.495533	1.172275
C	1.733201	1.892766	1.423253
C	1.144463	2.267777	0.050865
N	1.273812	−0.728114	1.751862
O	2.334653	2.491729	2.312552
O	1.081237	3.276577	−0.650899
C	1.805829	−1.108176	2.983558
C	1.723308	−2.473654	3.328453
C	2.239803	−2.887006	4.553372
C	2.839622	−2.005566	5.459367
C	2.912277	−0.658710	5.098986
C	2.406773	−0.200314	3.881496
H	−4.503348	−3.711414	−3.954602
H	−5.726897	−1.565088	−3.750780
H	−0.853260	−1.826456	−2.742652
H	−2.060472	−3.806822	−3.413581
H	−5.749249	0.815115	−3.207326
H	−5.829807	3.177980	−2.623976
H	−4.696187	5.247893	−1.866242
H	−2.241832	5.211254	−1.371267
H	−0.939934	3.188010	−1.637060
H	0.079356	0.079712	−3.093779
H	0.053410	1.696176	−2.405898
H	−0.073857	−0.875344	−0.834776
H	0.878944	−1.510340	1.162956
H	1.268041	−3.186479	2.647466
Cl	0.156368	−2.850043	−0.197401
H	3.227141	−2.376442	6.400138
H	2.480486	0.851837	3.614681
H	3.373533	0.053359	5.779485
N	2.151267	−4.325996	4.915583
O	1.605561	−5.103126	4.113371
O	2.631915	−4.681047	6.013128
Complex			9-Cl [−] [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	−3.112457	−2.907884	−4.593096
C	−3.723544	−1.687177	−4.443341
C	−2.978567	−0.534851	−4.040660
C	−1.549373	−0.656078	−3.812976
C	−0.964244	−1.955303	−3.964276
C	−1.719282	−3.041379	−4.337121
C	−3.600456	0.704651	−3.853609
C	−2.884403	1.831006	−3.434784
C	−1.451368	1.726836	−3.211212
C	−0.801208	0.486251	−3.430426
C	−3.536934	3.086257	−3.222389
C	−2.835962	4.188182	−2.799386
C	−1.435119	4.088709	−2.563461

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C	−0.765314	2.904353	−2.763262
C	0.708407	0.369236	−3.271893
N	1.113060	−0.209499	−1.979618
C	1.844348	0.435886	−1.081501
C	2.421836	0.040728	0.159224
C	3.005857	1.395858	0.399069
C	2.391443	1.822836	−0.950409
N	2.465580	−1.185774	0.734418
O	3.682213	1.931887	1.272225
O	2.375673	2.832089	−1.652532
C	2.809061	−1.465137	2.049352
C	3.145650	−2.780249	2.473154
C	3.319496	−3.084312	3.829276
C	3.232226	−2.087215	4.792636
C	2.962527	−0.770082	4.386252
C	2.744579	−0.466612	3.050050
N	3.451958	−3.869420	1.520047
O	3.306677	−5.044787	1.920332
O	3.902903	−3.561618	0.403430
H	−3.692568	−3.779969	−4.887734
H	−4.792811	−1.575217	−4.615743
H	0.080285	−2.117260	−3.725585
H	−1.248395	−4.018659	−4.404711
H	−4.672458	0.792078	−4.028114
H	−4.609894	3.144030	−3.399199
H	−3.346175	5.135400	−2.636262
H	−0.884870	4.958478	−2.211874
H	0.298232	2.873009	−2.550368
H	1.106960	−0.268909	−4.069727
H	1.189681	1.341071	−3.371789
H	0.879579	−1.214409	−1.770428
H	2.059167	−1.970786	0.155978
H	3.552558	−4.110383	4.091233
H	3.386443	−2.325954	5.841579
H	2.906500	0.027903	5.123434
H	2.529810	0.553176	2.754187
Cl	0.805719	−3.106662	−1.023265
Compound			1 [ZORA-BLYP-D3(BJ)/TZ2P]
Atom	X	Y	Z
C	−3.697783	−2.918109	−3.595404
C	−4.420221	−1.836834	−3.156506
C	−3.779777	−0.602194	−2.822522
C	−2.338650	−0.487227	−2.958626
C	−1.630490	−1.644601	−3.425602
C	−2.284365	−2.816216	−3.730856
C	−4.513417	0.495745	−2.358605
C	−3.895844	1.702549	−2.011229
C	−2.452927	1.830604	−2.132594
C	−1.698787	0.731929	−2.616193
C	−4.659299	2.811553	−1.528405
C	−4.049927	3.988238	−1.171941
C	−2.636180	4.116124	−1.278858
C	−1.863782	3.077894	−1.742510
C	−0.185997	0.813708	−2.697281
N	0.442062	0.185202	−1.501927

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C	1.010340	0.895604	−0.510295
C	1.430559	0.561156	0.793714
C	1.956863	1.954513	1.051893
C	1.484900	2.305061	−0.389565
N	1.313032	−0.627874	1.439952
O	2.502159	2.543616	1.967933
O	1.475084	3.287526	−1.116858
C	1.714075	−1.013648	2.743620
C	1.395715	−2.319893	3.156096
C	1.764536	−2.762078	4.425993
C	2.451832	−1.908973	5.295888
C	2.764452	−0.610961	4.877677
C	2.403139	−0.151501	3.609031
H	−4.198086	−3.851250	−3.843280
H	−5.501692	−1.900351	−3.051040
H	−0.552765	−1.603929	−3.555644
H	−1.717562	−3.673771	−4.086507
H	−5.594125	0.405797	−2.258673
H	−5.738713	2.698223	−1.448185
H	−4.640677	4.824214	−0.804815
H	−2.157221	5.047870	−0.987609
H	−0.790305	3.220539	−1.796188
H	0.186442	0.301936	−3.589480
H	0.176864	1.838898	−2.742161
H	0.105713	−0.752147	−1.293593
H	0.842584	−1.369194	0.926400
H	0.858017	−2.986879	2.482647
H	1.511739	−3.774013	4.734179
H	3.298205	0.060837	5.545858
H	2.644940	0.860825	3.297408
H	2.739459	−2.252214	6.286333
Compound 2 [ZORA–BLYP–D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	−3.670974	−2.941487	−3.513997
C	−4.397458	−1.857386	−3.089018
C	−3.762935	−0.612832	−2.782102
C	−2.324036	−0.490157	−2.932693
C	−1.611485	−1.650553	−3.385277
C	−2.259595	−2.832137	−3.663468
C	−4.500213	0.487661	−2.329847
C	−3.888050	1.703519	−2.005181
C	−2.447096	1.839357	−2.140450
C	−1.690387	0.738988	−2.615656
C	−4.654889	2.813776	−1.530695
C	−4.050362	3.998466	−1.193163
C	−2.638402	4.133912	−1.312844
C	−1.863256	3.095172	−1.770636
C	−0.179129	0.828841	−2.710414
N	0.458960	0.209220	−1.514889
C	1.011271	0.922996	−0.519706
C	1.416743	0.593906	0.788383
C	1.935726	1.985003	1.057322
C	1.480524	2.338124	−0.391818
N	1.288583	−0.598446	1.434731
O	2.467504	2.572151	1.981955

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O	1.475345	3.319600	-1.116421
C	1.678247	-0.980999	2.734772
C	1.354520	-2.286424	3.149936
C	1.712247	-2.728579	4.417955
C	2.394585	-1.870990	5.290450
C	2.716625	-0.572623	4.874381
C	2.363082	-0.118857	3.605576
H	-4.166521	-3.882468	-3.740722
H	-5.477495	-1.926476	-2.973554
H	-0.535433	-1.604568	-3.527943
H	-1.689809	-3.691933	-4.008765
H	-5.579337	0.392004	-2.219381
H	-5.732834	2.694672	-1.440649
H	-4.643407	4.835113	-0.831538
H	-2.163202	5.072172	-1.036709
H	-0.791447	3.244466	-1.835301
H	0.190502	0.312019	-3.600650
H	0.178787	1.855205	-2.763818
H	0.138028	-0.734882	-1.311872
H	0.815936	-1.336244	0.918133
H	0.817764	-2.954734	2.478183
H	1.454845	-3.735491	4.732269
H	3.243435	0.096149	5.548410
H	2.606837	0.894371	3.297477
C	2.830167	-2.368371	6.642361
F	2.915546	-1.364430	7.570717
F	1.975264	-3.315861	7.150036
F	4.076603	-2.960589	6.595088
Compound 3 [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.696011	-2.939373	-3.446484
C	-4.413191	-1.846686	-3.027729
C	-3.769849	-0.601560	-2.742513
C	-2.332098	-0.487580	-2.908881
C	-1.629547	-1.656398	-3.355441
C	-2.285834	-2.838312	-3.612255
C	-4.497060	0.507989	-2.295976
C	-3.875519	1.723905	-1.989616
C	-2.434990	1.850477	-2.138462
C	-1.689402	0.741567	-2.610967
C	-4.632173	2.843005	-1.519657
C	-4.018255	4.027149	-1.197582
C	-2.606432	4.153152	-1.328918
C	-1.840956	3.105951	-1.783678
C	-0.178904	0.821472	-2.722001
N	0.465558	0.196651	-1.532144
C	1.037137	0.901988	-0.543803
C	1.450043	0.569689	0.759805
C	1.995895	1.947863	1.025875
C	1.527413	2.313387	-0.418524
N	1.306414	-0.619641	1.413008
O	2.550932	2.518349	1.947066
O	1.523190	3.295537	-1.139652
C	1.688667	-0.993171	2.716207
C	1.324605	-2.280736	3.149761

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C	1.679058	-2.712215	4.424218
C	2.395927	-1.877862	5.289786
C	2.750148	-0.603532	4.845385
C	2.405726	-0.144822	3.569751
H	-4.197938	-3.880905	-3.656119
H	-5.492275	-1.909411	-2.900264
H	-0.555021	-1.616977	-3.511679
H	-1.723623	-3.704815	-3.953100
H	-5.575568	0.419241	-2.174349
H	-5.709999	2.730923	-1.420009
H	-4.603569	4.870529	-0.839108
H	-2.123895	5.090996	-1.064413
H	-0.768753	3.248201	-1.857772
H	0.178408	0.301117	-3.615204
H	0.185970	1.845095	-2.778964
H	0.141793	-0.746617	-1.329444
H	0.809157	-1.349006	0.908152
H	0.768404	-2.943509	2.491821
H	2.683297	0.856802	3.247170
H	2.674671	-2.216329	6.280531
C	3.527781	0.333426	5.748510
F	2.815446	1.471119	6.024272
F	3.846864	-0.241937	6.948365
F	4.703583	0.730746	5.167120
C	1.238481	-4.076587	4.905300
F	0.104318	-3.994523	5.678870
F	0.946296	-4.926413	3.869423
F	2.193607	-4.686059	5.671700
Compound 4 [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.688739	-2.932695	-3.521738
C	-4.418573	-1.840664	-3.123821
C	-3.784435	-0.595991	-2.816789
C	-2.341741	-0.482837	-2.934265
C	-1.625665	-1.651046	-3.360396
C	-2.274034	-2.831621	-3.642500
C	-4.526221	0.514631	-2.397742
C	-3.915722	1.732255	-2.076790
C	-2.470796	1.857881	-2.175467
C	-1.709020	0.745878	-2.613870
C	-4.688758	2.854679	-1.642551
C	-4.086914	4.042201	-1.310563
C	-2.671390	4.167904	-1.394382
C	-1.889991	3.116744	-1.811006
C	-0.195480	0.825050	-2.669012
N	0.407467	0.204473	-1.455242
C	0.976686	0.908141	-0.465681
C	1.398501	0.578012	0.837107
C	1.925890	1.965064	1.103496
C	1.454528	2.324038	-0.340218
N	1.278719	-0.617580	1.485313
O	2.471022	2.547624	2.022502
O	1.446526	3.304470	-1.063900
C	1.702970	-1.009317	2.766374
C	1.406618	-2.328609	3.170324

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C	1.802533	−2.787366	4.418039
C	2.498245	−1.922600	5.268585
C	2.795577	−0.611483	4.883300
C	2.400561	−0.147530	3.632850
N	2.925476	−2.409725	6.595906
O	3.544784	−1.618671	7.334840
O	2.641717	−3.586833	6.901640
H	−4.184127	−3.873336	−3.750027
H	−5.501266	−1.903008	−3.031715
H	−0.546700	−1.611597	−3.482146
H	−1.701757	−3.696982	−3.969273
H	−5.608262	0.426254	−2.312556
H	−5.769422	2.742739	−1.579673
H	−4.684597	4.888664	−0.980877
H	−2.198825	5.108977	−1.123366
H	−0.815839	3.258991	−1.848464
H	0.194260	0.302579	−3.547448
H	0.170975	1.848541	−2.715812
H	0.083945	−0.740306	−1.260128
H	0.799718	−1.354055	0.972388
H	0.863542	−2.993572	2.500521
H	1.583864	−3.797975	4.744511
H	3.335038	0.033719	5.568002
H	2.623874	0.872271	3.330618
Compound 5 [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	−3.672846	−2.922503	−3.537658
C	−4.404122	−1.841700	−3.112561
C	−3.773702	−0.597765	−2.795015
C	−2.333886	−0.472738	−2.932649
C	−1.616396	−1.628917	−3.388012
C	−2.260877	−2.809830	−3.677641
C	−4.516081	0.500450	−2.345435
C	−3.908619	1.716158	−2.011680
C	−2.466226	1.853438	−2.130376
C	−1.704593	0.754879	−2.601610
C	−4.682117	2.824816	−1.544288
C	−4.083050	4.009913	−1.198915
C	−2.669875	4.146846	−1.301902
C	−1.888170	3.109180	−1.751009
C	−0.192827	0.844820	−2.680608
N	0.432586	0.199224	−1.490841
C	1.013930	0.881400	−0.494648
C	1.444734	0.530180	0.797820
C	1.981621	1.905126	1.087411
C	1.498554	2.296030	−0.346991
N	1.316633	−0.671404	1.438611
O	2.536648	2.459570	2.017373
O	1.480566	3.289828	−1.049594
C	1.755970	−1.069922	2.712614
C	1.408394	−2.363673	3.139890
C	1.825060	−2.802698	4.391324
C	2.580987	−2.011947	5.251698
C	2.909797	−0.739102	4.791213
C	2.521816	−0.239264	3.550726

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H	-4.165052	-3.863202	-3.772291
H	-5.484822	-1.913022	-3.005547
H	-0.539788	-1.579977	-3.526396
H	-1.687691	-3.666346	-4.025286
H	-5.596061	0.403353	-2.245405
H	-5.760894	2.704408	-1.467060
H	-4.681135	4.845804	-0.844086
H	-2.199543	5.085902	-1.020264
H	-0.815739	3.259667	-1.803246
H	0.185622	0.344689	-3.576743
H	0.167481	1.871116	-2.709264
H	0.120219	-0.753231	-1.315758
H	0.801917	-1.392402	0.939327
H	0.818626	-3.032086	2.519672
H	2.797576	0.772252	3.257405
H	2.898065	-2.365464	6.223948
N	3.736311	0.142372	5.685034
O	4.025476	-0.302888	6.808754
O	4.074062	1.248332	5.239744
N	1.439675	-4.182703	4.823869
O	0.774955	-4.867518	4.024650
O	1.806910	-4.553368	5.949147
Compound 6 [ZORA-BLYP-D3(BJ)/TZ2P]			
Atom	X	Y	Z
C	-3.404473	-2.845858	-4.267627
C	-4.238187	-1.836727	-3.854383
C	-3.717985	-0.623486	-3.304439
C	-2.280783	-0.452114	-3.191269
C	-1.453313	-1.535524	-3.637740
C	-1.994148	-2.689554	-4.155237
C	-4.565951	0.399743	-2.866293
C	-4.068322	1.583658	-2.310049
C	-2.632284	1.768382	-2.185549
C	-1.761624	0.747374	-2.642539
C	-4.949491	2.613878	-1.854733
C	-4.460178	3.766954	-1.294189
C	-3.054950	3.950192	-1.161347
C	-2.171131	2.988756	-1.591588
C	-0.261422	0.894262	-2.486933
N	0.213178	0.227861	-1.246863
C	0.738011	0.889109	-0.209759
C	1.115303	0.545388	1.097108
C	1.615412	1.913604	1.421746
C	1.193918	2.316678	-0.028945
N	0.991676	-0.597175	1.827252
O	2.110404	2.439581	2.398949
O	1.163728	3.315855	-0.723335
C	1.610256	-0.849790	3.066370
C	0.843262	-1.500154	4.052172
C	1.353019	-1.754682	5.319947
C	2.649895	-1.340929	5.652096
C	3.432760	-0.714494	4.689855
C	2.941018	-0.496684	3.397315
H	-3.813690	-3.763457	-4.682804
H	-5.318039	-1.942862	-3.936201

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H	−0.372261	−1.451127	−3.580275
H	−1.338210	−3.490159	−4.488628
H	−5.643227	0.268243	−2.954147
H	−6.021304	2.459666	−1.961712
H	−5.139813	4.542603	−0.949794
H	−2.673025	4.864331	−0.713601
H	−1.109961	3.173542	−1.468449
H	0.265742	0.457396	−3.339698
H	0.049626	1.935275	−2.423283
H	−0.004968	−0.760071	−1.155170
H	0.250138	−1.244410	1.576091
H	−0.183722	−1.769811	3.813558
H	0.729599	−2.252825	6.057832
H	4.448911	−0.402012	4.901701
H	3.048393	−1.514616	6.647296
N	3.921969	0.000093	2.402274
O	3.689370	−0.225503	1.196212
O	4.950340	0.550265	2.825633
Compound			7 [ZORA–BLYP–D3(BJ)/TZ2P]
Atom	X	Y	Z
C	−3.830269	−2.833148	−3.753734
C	−4.537899	−1.736359	−3.328448
C	−3.874639	−0.530610	−2.939693
C	−2.426222	−0.462021	−3.004753
C	−1.733487	−1.634084	−3.457420
C	−2.409408	−2.776913	−3.817460
C	−4.592831	0.583484	−2.491294
C	−3.953696	1.763276	−2.093774
C	−2.503743	1.846070	−2.147280
C	−1.764871	0.729730	−2.614010
C	−4.703520	2.888392	−1.627440
C	−4.074922	4.039018	−1.222796
C	−2.654679	4.123615	−1.265433
C	−1.894740	3.068401	−1.712071
C	−0.250504	0.763976	−2.636888
N	0.314966	0.113548	−1.421706
C	0.968772	0.794920	−0.469188
C	1.453879	0.470362	0.812759
C	2.031559	1.846837	1.024013
C	1.496549	2.193323	−0.393489
N	1.370229	−0.710438	1.487339
O	2.637039	2.429141	1.902463
O	1.487684	3.159402	−1.136913
C	1.816361	−1.050804	2.781897
C	1.626467	−2.381071	3.203804
C	2.038288	−2.788644	4.471045
C	2.646012	−1.883548	5.343169
C	2.819515	−0.572054	4.902097
C	2.422560	−0.124952	3.643771
H	−4.347623	−3.743510	−4.045695
H	−5.624443	−1.764940	−3.277307
H	−0.650172	−1.627597	−3.533203
H	−1.854013	−3.645909	−4.162152
H	−5.679223	0.528660	−2.444253
H	−5.788290	2.808547	−1.599022

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H	−4.655052	4.887370	−0.868215
H	−2.161536	5.036036	−0.939553
H	−0.816539	3.179771	−1.722600
H	0.139072	0.246308	−3.517935
H	0.144518	1.777656	−2.663317
H	−0.071729	−0.800979	−1.202383
H	0.923039	−1.478271	0.994057
H	1.154765	−3.097546	2.533254
H	1.884415	−3.818677	4.780344
H	2.977697	−2.169222	6.333914
H	2.593561	0.908052	3.351152
N	3.461991	0.412021	5.830553
O	3.855471	−0.014996	6.930910
O	3.559335	1.586442	5.447788
Compound			8 [ZORA–BLYP–D3(BJ)/TZ2P]
Atom	X	Y	Z
C	−3.788752	−2.853405	−3.745540
C	−4.505146	−1.753518	−3.343750
C	−3.850443	−0.541258	−2.960884
C	−2.401492	−0.469620	−3.006407
C	−1.699495	−1.644683	−3.436248
C	−2.367453	−2.793659	−3.791453
C	−4.577560	0.576116	−2.535647
C	−3.947054	1.761788	−2.141865
C	−2.496598	1.847195	−2.173969
C	−1.748814	0.727731	−2.618264
C	−4.706315	2.890094	−1.699168
C	−4.086522	4.046210	−1.296596
C	−2.665953	4.133225	−1.317495
C	−1.896943	3.075077	−1.741181
C	−0.234419	0.763847	−2.616451
N	0.309264	0.121035	−1.387066
C	0.940609	0.806950	−0.424807
C	1.389432	0.490567	0.873829
C	1.965705	1.867126	1.086752
C	1.470981	2.203619	−0.344926
N	1.270701	−0.682969	1.555605
O	2.550080	2.460962	1.974828
O	1.482148	3.166868	−1.092299
C	1.692095	−1.017331	2.860084
C	1.437753	−2.322699	3.305288
C	1.836228	−2.686590	4.588256
C	2.480815	−1.800428	5.451079
C	2.725984	−0.505547	4.988186
C	2.341655	−0.102367	3.708133
H	−4.299356	−3.769323	−4.031766
H	−5.592136	−1.784910	−3.306272
H	−0.615280	−1.636379	−3.497880
H	−1.805143	−3.665383	−4.117367
H	−5.664360	0.518977	−2.503402
H	−5.791239	2.808125	−1.686879
H	−4.673913	4.896942	−0.960158
H	−2.179889	5.050111	−0.993436
H	−0.818866	3.188526	−1.735458
H	0.171126	0.240360	−3.486676

Journal Name			ARTICLE
H	0.160516	1.777529	−2.641958
H	−0.071083	−0.798187	−1.176200
H	0.806152	−1.443056	1.066069
H	0.939630	−3.056760	2.679573
H	2.773467	−2.125624	6.442159
H	2.544380	0.909645	3.367329
H	3.227127	0.208970	5.635523
N	1.557870	−4.077408	5.044496
O	0.985084	−4.843645	4.247971
O	1.914093	−4.389519	6.192473
Compound			9 [ZORA–BLYP–D3(BJ)/TZ2P]
Atom	X	Y	Z
C	−2.673262	−3.079719	−4.678152
C	−3.391889	−1.967930	−4.315372
C	−2.738009	−0.760254	−3.917332
C	−1.287577	−0.705954	−3.907152
C	−0.583576	−1.893350	−4.296567
C	−1.250814	−3.037678	−4.666422
C	−3.467700	0.368531	−3.528403
C	−2.839178	1.549617	−3.118138
C	−1.387841	1.618564	−3.096521
C	−0.637022	0.487665	−3.505014
C	−3.601532	2.689055	−2.710911
C	−2.984456	3.840859	−2.292022
C	−1.563222	3.912172	−2.260824
C	−0.791199	2.842780	−2.649446
C	0.876828	0.513150	−3.454219
N	1.377472	−0.105224	−2.196031
C	2.015487	0.579257	−1.244453
C	2.459495	0.263448	0.057519
C	3.045236	1.631534	0.273644
C	2.558305	1.975912	−1.162259
N	2.315798	−0.921194	0.713551
O	3.631895	2.220350	1.164225
O	2.580146	2.937634	−1.909554
C	2.711143	−1.287832	1.991171
C	2.460122	−2.610380	2.475464
C	2.857455	−2.983488	3.772452
C	3.496755	−2.076345	4.598943
C	3.748151	−0.774137	4.129432
C	3.366317	−0.383791	2.855507
N	1.793257	−3.634559	1.676976
O	1.616764	−4.761369	2.165624
O	1.408566	−3.346964	0.497223
H	−3.182940	−3.993034	−4.974151
H	−4.479816	−1.986495	−4.319388
H	0.502195	−1.901643	−4.308488
H	−0.686537	−3.921019	−4.955079
H	−4.555557	0.323878	−3.537190
H	−4.687021	2.618959	−2.738505
H	−3.574450	4.699909	−1.982293
H	−1.079132	4.825824	−1.924804
H	0.287097	2.944985	−2.605399
H	1.306041	−0.031967	−4.299527
H	1.278112	1.524063	−3.490012

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H	1.020601	−1.034777	−1.986460
H	1.850097	−1.706232	0.233860
H	2.646389	−3.995762	4.095863
H	3.799884	−2.371590	5.599067
H	4.250524	−0.053555	4.770013
H	3.570483	0.625353	2.506500
Anion	NO_3^- [ZORA–BLYP–D3(BJ)/TZ2P]		
Atom	X	Y	Z
N	−1.598069	−2.250987	0.192675
O	−2.056765	−1.174288	0.718997
O	−2.374563	−3.255735	0.006911
O	−0.363017	−2.323175	−0.147938

ARTICLE

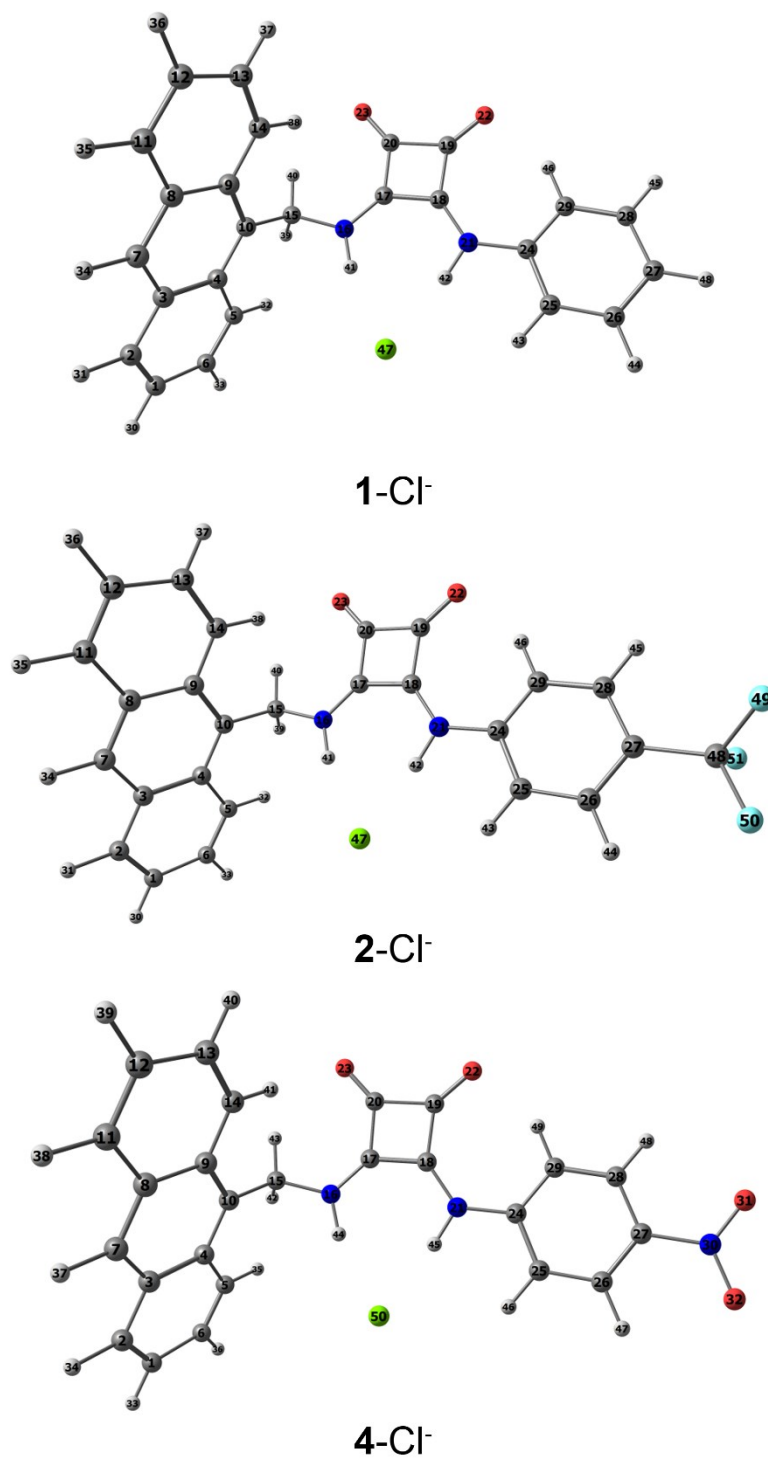


Figure S1. Atoms numeration to structures 1-Cl⁻, 2-Cl⁻ and 4-Cl⁻. Atoms color: Carbon (gray); oxygen (red); hydrogen (white); chlorine (green); nitrogen (blue); fluorine (light blue).

Table S2. Bond lengths (r / Å) and angles (< / °) to 1-Cl⁻, 2-Cl⁻ and 4-Cl⁻ structures.

Geometric Parameter	1-Cl ⁻			
	B97D3/6-31+G(d) PCM(DMSO)	B97D3/6-31+G(d)	B97D3/Def2-TZVP PCM(DMSO)	ZORA-BLYP-D3(BJ)/TZ2P COSMO(DMSO)
r[C(1)–C(2)]	1.379	1.379	1.371	1.374
r[C(1)–C(6)]	1.427	1.426	1.421	1.426
r[C(1)–H(30)]	1.091	1.092	1.087	1.088
r[C(2)–C(3)]	1.434	1.432	1.428	1.432
r[C(2)–H(31)]	1.092	1.093	1.088	1.089
r[C(3)–C(4)]	1.456	1.454	1.450	1.454
r[C(3)–C(7)]	1.404	1.403	1.397	1.401
r[C(4)–C(5)]	1.437	1.435	1.431	1.435
r[C(4)–C(10)]	1.422	1.422	1.415	1.419
r[C(5)–C(6)]	1.381	1.380	1.373	1.376
r[C(5)–H(32)]	1.088	1.087	1.084	1.085
r[C(6)–H(33)]	1.091	1.091	1.087	1.088
r[C(7)–C(8)]	1.405	1.403	1.398	1.401
r[C(7)–H(34)]	1.092	1.094	1.088	1.089
r[C(8)–C(9)]	1.454	1.456	1.448	1.454
r[C(8)–C(11)]	1.433	1.433	1.428	1.432
r[C(9)–C(10)]	1.422	1.422	1.415	1.419
r[C(9)–C(14)]	1.436	1.436	1.430	1.436
r[C(10)–C(15)]	1.517	1.522	1.513	1.519
r[C(11)–C(12)]	1.379	1.379	1.371	1.374
r[C(11)–H(35)]	1.092	1.093	1.088	1.089
r[C(12)–C(13)]	1.427	1.426	1.421	1.426
r[C(12)–H(36)]	1.091	1.092	1.087	1.088
r[C(13)–C(14)]	1.382	1.381	1.374	1.377
r[C(13)–H(37)]	1.091	1.091	1.087	1.088
r[C(14)–H(38)]	1.087	1.089	1.084	1.085
r[C(15)–N(16)]	1.476	1.468	1.471	1.482
r[C(15)–H(39)]	1.096	1.100	1.093	1.093
r[C(15)–H(40)]	1.093	1.093	1.089	1.090
r[N(16)–C(17)]	1.329	1.334	1.323	1.326
r[N(16)–H(41)]	1.034	1.043	1.032	1.034
r[C(17)–C(18)]	1.435	1.429	1.429	1.436
r[C(17)–C(20)]	1.484	1.486	1.481	1.483
r[C(18)–C(19)]	1.493	1.500	1.491	1.491
r[C(18)–N(21)]	1.348	1.350	1.343	1.346
r[C(19)–C(20)]	1.520	1.533	1.521	1.520
r[C(19)–O(22)]	1.239	1.233	1.229	1.241
r[C(20)–O(23)]	1.240	1.237	1.230	1.242
r[N(21)–C(24)]	1.410	1.403	1.403	1.412
r[N(21)–H(42)]	1.037	1.047	1.036	1.037
r[C(24)–C(25)]	1.412	1.414	1.406	1.410
r[C(24)–C(29)]	1.409	1.411	1.403	1.406
r[C(25)–C(26)]	1.400	1.398	1.392	1.396
r[C(25)–H(43)]	1.091	1.091	1.087	1.088
r[C(26)–C(27)]	1.405	1.405	1.398	1.402
r[C(26)–H(44)]	1.091	1.092	1.087	1.088
r[C(27)–C(28)]	1.405	1.404	1.397	1.401
r[C(27)–H(47)]	1.091	1.092	1.086	1.088
r[C(28)–C(29)]	1.402	1.401	1.394	1.399
r[C(28)–H(45)]	1.091	1.093	1.087	1.088
r[C(29)–H(46)]	1.089	1.090	1.085	1.086

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<[C(2)–C(1)–C(6)]	119.7	119.9	119.8	119.8
<[C(2)–C(1)–H(30)]	120.5	120.3	120.5	120.4
<[C(1)–C(2)–C(3)]	121.1	121.0	121.1	121.0
<[C(1)–C(2)–H(31)]	120.7	120.8	120.7	120.7
<[C(6)–C(1)–H(30)]	119.8	119.8	119.8	119.7
<[C(1)–C(6)–C(5)]	120.9	120.8	120.9	120.9
<[C(1)–C(6)–H(33)]	119.5	119.9	119.5	119.4
<[C(3)–C(2)–H(31)]	118.2	118.2	118.2	118.2
<[C(2)–C(3)–C(4)]	119.6	119.4	119.5	119.5
<[C(2)–C(3)–C(7)]	120.9	121.2	121.0	121.1
<[C(4)–C(3)–C(7)]	119.5	119.4	119.5	119.5
<[C(3)–C(4)–C(5)]	117.2	117.5	117.2	117.3
<[C(3)–C(4)–C(10)]	119.4	119.7	119.5	119.5
<[C(3)–C(7)–C(8)]	121.6	121.7	121.6	121.6
<[C(3)–C(7)–H(34)]	119.2	119.2	119.2	119.2
<[C(5)–C(4)–C(10)]	123.4	122.9	123.3	123.3
<[C(4)–C(5)–C(6)]	121.6	121.4	121.6	121.5
<[C(4)–C(5)–H(32)]	120.1	120.5	119.9	119.9
<[C(4)–C(10)–C(9)]	120.4	120.2	120.4	120.4
<[C(4)–C(10)–C(15)]	120.0	119.3	119.9	119.8
<[C(6)–C(5)–H(32)]	118.4	118.0	118.5	118.6
<[C(5)–C(6)–H(33)]	119.6	119.2	119.6	119.7
<[C(8)–C(7)–H(34)]	119.2	119.2	119.2	119.2
<[C(7)–C(8)–C(9)]	119.5	119.5	119.5	119.5
<[C(7)–C(8)–C(11)]	121.0	121.0	121.1	121.1
<[C(9)–C(8)–C(11)]	119.5	119.4	119.5	119.4
<[C(8)–C(9)–C(10)]	119.5	119.4	119.5	119.5
<[C(8)–C(9)–C(14)]	117.4	117.5	117.4	117.4
<[C(8)–C(11)–C(12)]	121.0	121.1	121.1	121.1
<[C(8)–C(11)–H(35)]	118.3	118.2	118.2	118.2
<[C(10)–C(9)–C(14)]	123.1	123.1	123.1	123.1
<[C(9)–C(10)–C(15)]	119.5	120.4	119.7	119.8
<[C(9)–C(14)–C(13)]	121.4	121.3	121.4	121.3
<[C(9)–C(14)–H(38)]	120.1	120.5	120.1	120.1
<[C(10)–C(15)–N(16)]	110.6	113.2	110.9	111.5
<[C(10)–C(15)–H(39)]	111.3	109.5	110.9	110.7
<[C(10)–C(15)–H(40)]	111.8	111.2	111.6	111.5
<[C(12)–C(11)–H(35)]	120.7	120.7	120.7	120.7
<[C(11)–C(12)–C(13)]	119.7	119.8	119.8	119.8
<[C(11)–C(12)–H(36)]	120.4	120.3	120.4	120.5
<[C(13)–C(12)–H(36)]	119.8	119.9	119.8	119.7
<[C(12)–C(13)–C(14)]	120.9	121.0	120.9	120.9
<[C(12)–C(13)–H(37)]	119.5	119.8	119.5	119.4
<[C(14)–C(13)–H(37)]	119.5	119.2	119.6	119.6
<[C(13)–C(14)–H(38)]	118.5	118.2	118.5	118.5
<[N(16)–C(15)–H(39)]	108.8	108.2	108.9	108.5
<[N(16)–C(15)–H(40)]	107.7	107.9	107.8	107.7
<[C(15)–N(16)–C(17)]	123.9	123.5	123.7	124.1
<[C(15)–N(16)–H(41)]	117.4	118.2	117.8	117.6
<[H(39)–C(15)–H(40)]	106.4	106.6	106.5	106.9
<[C(17)–N(16)–H(41)]	118.4	117.5	118.2	118.3
<[N(16)–C(17)–C(18)]	133.1	132.2	133.0	133.0
<[N(16)–C(17)–C(20)]	135.2	135.7	135.2	135.4
<[C(18)–C(17)–C(20)]	91.7	92.1	91.9	91.7
<[C(17)–C(18)–C(19)]	91.6	91.9	91.7	91.6

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<[C(17)–C(18)–N(21)]	128.3	127.8	128.1	128.2
<[C(17)–C(20)–C(19)]	88.6	88.4	88.5	88.7
<[C(17)–C(20)–O(23)]	135.6	135.1	135.6	135.6
<[C(19)–C(18)–N(21)]	140.1	140.3	140.2	140.2
<[C(18)–C(19)–C(20)]	88.1	87.6	87.9	88.1
<[C(18)–C(19)–O(22)]	137.5	137.0	137.6	137.4
<[C(18)–N(21)–C(24)]	130.0	129.7	130.0	130.4
<[C(18)–N(21)–H(42)]	115.3	115.1	115.2	115.2
<[C(20)–C(19)–O(22)]	134.4	135.4	134.5	134.5
<[C(19)–C(20)–O(23)]	135.7	136.5	135.9	135.7
<[C(24)–N(21)–H(42)]	114.7	115.1	114.8	114.5
<[N(21)–C(24)–C(25)]	116.9	116.9	117.1	116.9
<[N(21)–C(24)–C(29)]	123.2	123.4	123.3	123.4
<[C(25)–C(24)–C(29)]	119.8	119.8	119.6	119.8
<[C(24)–C(25)–C(26)]	120.0	120.0	120.1	120.1
<[C(24)–C(25)–H(43)]	119.5	119.0	119.2	119.4
<[C(24)–C(29)–C(28)]	119.4	119.3	119.5	119.4
<[C(24)–C(29)–H(46)]	120.1	120.0	120.0	120.0
<[C(26)–C(25)–H(43)]	120.5	121.0	120.6	120.6
<[C(25)–C(26)–C(27)]	120.5	120.7	120.5	120.4
<[C(25)–C(26)–H(44)]	119.3	119.1	119.3	119.4
<[C(27)–C(26)–H(44)]	120.3	120.2	120.2	120.2
<[C(26)–C(27)–C(28)]	119.2	119.0	119.1	119.2
<[C(26)–C(27)–H(47)]	120.4	120.5	120.4	120.4
<[C(28)–C(27)–H(47)]	120.4	120.5	120.4	120.4
<[C(27)–C(28)–C(29)]	121.1	121.3	121.1	121.1
<[C(27)–C(28)–H(45)]	120.0	120.0	119.9	119.9
<[C(29)–C(28)–H(45)]	118.9	118.7	119.0	119.0
<[C(28)–C(29)–H(46)]	120.5	120.6	120.5	120.6
2–Cl[–]				
Geometric Parameter	B97D3/6–31+G(d) – PCM – DMSO	B97D3/6–31+G(d)	B97D3/Def2–TZVP – PCM – DMSO	ZORA–BLYP–D3(BJ)/TZ2P – COSMO – DMSO
r[C(1)–C(2)]	1.379	–	1.371	–
r[C(1)–C(6)]	1.427	–	1.421	–
r[C(1)–H(30)]	1.091	–	1.087	–
r[C(2)–C(3)]	1.434	–	1.428	–
r[C(2)–H(31)]	1.092	–	1.088	–
r[C(3)–C(4)]	1.456	–	1.449	–
r[C(3)–C(7)]	1.404	–	1.397	–
r[C(4)–C(5)]	1.437	–	1.431	–
r[C(4)–C(10)]	1.422	–	1.415	–
r[C(5)–C(6)]	1.381	–	1.373	–
r[C(5)–H(32)]	1.088	–	1.084	–
r[C(6)–H(33)]	1.091	–	1.087	–
r[C(7)–C(8)]	1.404	–	1.398	–
r[C(7)–H(34)]	1.092	–	1.088	–
r[C(8)–C(9)]	1.454	–	1.448	–
r[C(8)–C(11)]	1.433	–	1.428	–
r[C(9)–C(10)]	1.422	–	1.415	–
r[C(9)–C(14)]	1.436	–	1.430	–
r[C(10)–C(15)]	1.517	–	1.513	–
r[C(11)–C(12)]	1.379	–	1.371	–
r[C(11)–H(35)]	1.092	–	1.088	–
r[C(12)–C(13)]	1.427	–	1.421	–
r[C(12)–H(36)]	1.091	–	1.087	–
r[C(13)–C(14)]	1.382	–	1.374	–

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r[C(13)–H(37)]	1.091	–	1.087	–	–
r[C(14)–H(38)]	1.087	–	1.084	–	–
r[C(15)–N(16)]	1.477	–	1.471	–	–
r[C(15)–H(39)]	1.096	–	1.093	–	–
r[C(15)–H(40)]	1.093	–	1.089	–	–
r[N(16)–C(17)]	1.327	–	1.321	–	–
r[N(16)–H(41)]	1.034	–	1.032	–	–
r[C(17)–C(18)]	1.433	–	1.427	–	–
r[C(17)–C(20)]	1.487	–	1.485	–	–
r[C(18)–C(19)]	1.490	–	1.489	–	–
r[C(18)–N(21)]	1.352	–	1.347	–	–
r[C(19)–C(20)]	1.523	–	1.524	–	–
r[C(19)–O(22)]	1.238	–	1.228	–	–
r[C(20)–O(23)]	1.237	–	1.227	–	–
r[N(21)–C(24)]	1.401	–	1.395	–	–
r[N(21)–H(42)]	1.039	–	1.038	–	–
r[C(24)–C(25)]	1.413	–	1.408	–	–
r[C(24)–C(29)]	1.411	–	1.404	–	–
r[C(25)–C(26)]	1.395	–	1.387	–	–
r[C(25)–H(43)]	1.090	–	1.086	–	–
r[C(26)–C(27)]	1.406	–	1.400	–	–
r[C(26)–H(44)]	1.089	–	1.085	–	–
r[C(27)–C(28)]	1.408	–	1.400	–	–
r[C(27)–H(48)]	1.499	–	1.499	–	–
r[C(28)–C(29)]	1.396	–	1.390	–	–
r[C(28)–H(45)]	1.090	–	1.086	–	–
r[C(29)–H(46)]	1.089	–	1.085	–	–
r[C(48)–F(49)]	1.373	–	1.362	–	–
r[C(48)–F(50)]	1.367	–	1.362	–	–
r[C(48)–F(51)]	1.382	–	1.373	–	–
<[C(2)–C(1)–C(6)]	119.7	–	119.8	–	–
<[C(2)–C(1)–H(30)]	120.5	–	120.5	–	–
<[C(1)–C(2)–C(3)]	121.1	–	121.1	–	–
<[C(1)–C(2)–H(31)]	120.7	–	120.7	–	–
<[C(6)–C(1)–H(30)]	119.8	–	119.7	–	–
<[C(1)–C(6)–C(5)]	120.9	–	120.9	–	–
<[C(1)–C(6)–H(33)]	119.5	–	119.5	–	–
<[C(3)–C(2)–H(31)]	118.2	–	118.2	–	–
<[C(2)–C(3)–C(4)]	119.6	–	119.5	–	–
<[C(2)–C(3)–C(7)]	120.9	–	121.0	–	–
<[C(4)–C(3)–C(7)]	119.5	–	119.5	–	–
<[C(3)–C(4)–C(5)]	117.2	–	117.2	–	–
<[C(3)–C(4)–C(10)]	119.4	–	119.5	–	–
<[C(3)–C(7)–C(8)]	121.6	–	121.6	–	–
<[C(3)–C(7)–H(34)]	119.2	–	119.2	–	–
<[C(5)–C(4)–C(10)]	123.4	–	123.3	–	–
<[C(4)–C(5)–C(6)]	121.6	–	121.6	–	–
<[C(4)–C(5)–H(32)]	120.1	–	119.9	–	–
<[C(4)–C(10)–C(9)]	120.4	–	120.4	–	–
<[C(4)–C(10)–C(15)]	120.0	–	119.8	–	–
<[C(6)–C(5)–H(32)]	118.4	–	118.5	–	–
<[C(5)–C(6)–C(3)]	119.6	–	119.6	–	–
<[C(8)–C(7)–H(34)]	119.2	–	119.2	–	–
<[C(7)–C(8)–C(9)]	119.5	–	119.5	–	–
<[C(7)–C(8)–C(11)]	121.0	–	121.1	–	–

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<[C(9)–C(8)–C(11)]	119.5	–	119.5	–
<[C(8)–C(9)–C(10)]	119.5	–	119.5	–
<[C(8)–C(9)–C(14)]	117.4	–	117.4	–
<[C(8)–C(11)–C(12)]	121.0	–	121.1	–
<[C(8)–C(11)–H(35)]	118.3	–	118.2	–
<[C(10)–C(9)–C(14)]	123.1	–	123.1	–
<[C(9)–C(10)–C(15)]	119.5	–	119.7	–
<[C(9)–C(14)–C(13)]	121.4	–	121.4	–
<[C(9)–C(14)–H(38)]	120.2	–	120.1	–
<[C(10)–C(15)–N(16)]	110.6	–	110.9	–
<[C(10)–C(15)–H(39)]	111.4	–	110.9	–
<[C(10)–C(15)–H(40)]	111.9	–	111.7	–
<[C(12)–C(11)–H(35)]	120.7	–	120.7	–
<[C(11)–C(12)–C(13)]	119.7	–	119.8	–
<[C(11)–C(12)–H(36)]	120.4	–	120.4	–
<[C(13)–C(12)–H(36)]	119.8	–	119.8	–
<[C(12)–C(13)–C(14)]	120.9	–	120.9	–
<[C(12)–C(13)–H(37)]	119.5	–	119.5	–
<[C(14)–C(13)–H(37)]	119.5	–	119.6	–
<[C(13)–C(14)–H(38)]	118.5	–	118.5	–
<[N(16)–C(15)–H(39)]	108.7	–	108.9	–
<[N(16)–C(15)–H(40)]	107.7	–	107.8	–
<[C(15)–N(16)–C(17)]	124.0	–	123.8	–
<[C(15)–N(16)–H(41)]	117.4	–	117.7	–
<[H(39)–C(15)–H(40)]	106.4	–	106.6	–
<[C(17)–N(16)–H(41)]	118.3	–	118.2	–
<[N(16)–C(17)–C(18)]	133.3	–	133.1	–
<[N(16)–C(17)–C(20)]	135.1	–	135.2	–
<[C(18)–C(17)–C(20)]	91.6	–	91.7	–
<[C(17)–C(18)–C(19)]	91.9	–	92.0	–
<[C(17)–C(18)–N(21)]	128.1	–	127.9	–
<[C(17)–C(20)–C(19)]	88.5	–	88.4	–
<[C(17)–C(20)–O(23)]	135.6	–	135.6	–
<[C(19)–C(18)–N(21)]	140.0	–	140.0	–
<[C(18)–C(19)–C(20)]	88.0	–	87.8	–
<[C(18)–C(19)–O(22)]	137.5	–	137.6	–
<[C(18)–N(21)–C(24)]	129.8	–	129.8	–
<[C(18)–N(21)–H(42)]	115.3	–	115.2	–
<[C(20)–C(19)–O(22)]	134.5	–	134.6	–
<[C(19)–C(20)–O(23)]	135.8	–	135.9	–
<[C(24)–N(21)–H(42)]	114.9	–	115.0	–
<[N(21)–C(24)–C(25)]	117.1	–	117.2	–
<[N(21)–C(24)–C(29)]	123.3	–	123.4	–
<[C(25)–C(24)–C(29)]	119.6	–	119.4	–
<[C(24)–C(25)–C(26)]	120.3	–	120.4	–
<[C(24)–C(25)–H(43)]	119.5	–	119.3	–
<[C(24)–C(29)–C(28)]	119.6	–	119.7	–
<[C(24)–C(29)–H(46)]	120.3	–	120.1	–
<[C(26)–C(25)–H(43)]	120.1	–	120.3	–
<[C(25)–C(26)–C(27)]	120.1	–	120.2	–
<[C(25)–C(26)–H(44)]	119.4	–	119.5	–
<[C(27)–C(26)–H(44)]	120.5	–	120.3	–
<[C(26)–C(27)–C(28)]	119.5	–	119.4	–
<[C(26)–C(27)–C(48)]	121.0	–	120.2	–
<[C(28)–C(27)–C(48)]	119.4	–	120.3	–

<[C(27)–C(28)–C(29)]	120.8	–	120.9	–
<[C(27)–C(28)–H(45)]	120.1	–	120.0	–
<[C(27)–C(48)–F(49)]	112.6	–	112.8	–
<[C(27)–C(48)–F(50)]	113.2	–	112.7	–
<[C(27)–C(48)–F(51)]	112.3	–	112.2	–
<[C(29)–C(28)–H(45)]	119.0	–	119.1	–
<[C(28)–C(29)–H(46)]	120.1	–	120.2	–
<[F(49)–C(48)–F(50)]	106.6	–	106.8	–
<[F(49)–C(48)–F(51)]	105.4	–	105.9	–
<[F(50)–C(48)–F(51)]	106.0	–	105.9	–
4–Cl[–]				
Geometric Parameter	B97D3/6–31+G(d) – PCM – DMSO	B97D3/6–31+G(d)	B97D3/Def2–TZVP – PCM – DMSO	ZORA–BLYP–D3(BJ)/TZ2P – COSMO – DMSO
r[C(1)–C(2)]	1.379	–	1.371	–
r[C(1)–C(6)]	1.427	–	1.421	–
r[C(1)–H(33)]	1.091	–	1.087	–
r[C(2)–C(3)]	1.434	–	1.428	–
r[C(2)–H(34)]	1.092	–	1.088	–
r[C(3)–C(4)]	1.456	–	1.449	–
r[C(3)–C(7)]	1.404	–	1.397	–
r[C(4)–C(5)]	1.437	–	1.431	–
r[C(4)–C(10)]	1.422	–	1.415	–
r[C(5)–C(6)]	1.381	–	1.373	–
r[C(5)–H(35)]	1.088	–	1.084	–
r[C(6)–H(36)]	1.091	–	1.087	–
r[C(7)–C(8)]	1.404	–	1.398	–
r[C(7)–H(37)]	1.092	–	1.088	–
r[C(8)–C(9)]	1.454	–	1.448	–
r[C(8)–C(11)]	1.433	–	1.428	–
r[C(9)–C(10)]	1.422	–	1.415	–
r[C(9)–C(14)]	1.436	–	1.430	–
r[C(10)–C(15)]	1.517	–	1.512	–
r[C(11)–C(12)]	1.379	–	1.371	–
r[C(11)–H(38)]	1.092	–	1.088	–
r[C(12)–C(13)]	1.427	–	1.421	–
r[C(12)–H(39)]	1.091	–	1.087	–
r[C(13)–C(14)]	1.382	–	1.374	–
r[C(13)–H(40)]	1.091	–	1.087	–
r[C(14)–H(41)]	1.087	–	1.084	–
r[C(15)–N(16)]	1.477	–	1.472	–
r[C(15)–H(42)]	1.096	–	1.092	–
r[C(15)–H(43)]	1.093	–	1.089	–
r[N(16)–C(17)]	1.325	–	1.319	–
r[N(16)–H(44)]	1.035	–	1.033	–
r[C(17)–C(18)]	1.432	–	1.426	–
r[C(17)–C(20)]	1.492	–	1.489	–
r[C(18)–C(19)]	1.488	–	1.487	–
r[C(18)–N(21)]	1.356	–	1.351	–
r[C(19)–C(20)]	1.527	–	1.527	–
r[C(19)–O(22)]	1.236	–	1.226	–
r[C(20)–O(23)]	1.233	–	1.224	–
r[N(21)–C(24)]	1.390	–	1.384	–
r[N(21)–H(45)]	1.042	–	1.041	–
r[C(24)–C(25)]	1.419	–	1.413	–
r[C(24)–C(29)]	1.416	–	1.410	–
r[C(25)–C(26)]	1.388	–	1.382	–

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r[C(25)–H(46)]	1.090	–	1.086	–	–
r[C(26)–C(27)]	1.409	–	1.401	–	–
r[C(26)–H(47)]	1.087	–	1.083	–	–
r[C(27)–C(28)]	1.408	–	1.400	–	–
r[C(27)–N(30)]	1.449	–	1.452	–	–
r[C(28)–C(29)]	1.391	–	1.384	–	–
r[C(28)–H(48)]	1.087	–	1.083	–	–
r[C(29)–H(49)]	1.089	–	1.085	–	–
r[N(30)–O(31)]	1.250	–	1.239	–	–
r[N(30)–O(32)]	1.250	–	1.239	–	–
<[C(2)–C(1)–C(6)]	119.7	–	119.8	–	–
<[C(2)–C(1)–H(33)]	120.5	–	120.5	–	–
<[C(1)–C(2)–C(3)]	121.1	–	121.1	–	–
<[C(1)–C(2)–H(34)]	120.7	–	120.7	–	–
<[C(6)–C(1)–H(33)]	119.8	–	119.7	–	–
<[C(1)–C(6)–C(5)]	120.9	–	120.9	–	–
<[C(1)–C(6)–H(36)]	119.5	–	119.5	–	–
<[C(3)–C(2)–H(34)]	118.2	–	118.2	–	–
<[C(2)–C(3)–C(4)]	119.6	–	119.5	–	–
<[C(2)–C(3)–C(7)]	120.9	–	121.0	–	–
<[C(4)–C(3)–C(7)]	119.5	–	119.5	–	–
<[C(3)–C(4)–C(5)]	117.2	–	117.2	–	–
<[C(3)–C(4)–C(10)]	119.4	–	119.5	–	–
<[C(3)–C(7)–C(8)]	121.7	–	121.6	–	–
<[C(3)–C(7)–H(37)]	119.2	–	119.2	–	–
<[C(5)–C(4)–C(10)]	123.5	–	123.3	–	–
<[C(4)–C(5)–C(6)]	121.5	–	121.5	–	–
<[C(4)–C(5)–H(35)]	120.1	–	120.0	–	–
<[C(4)–C(10)–C(9)]	120.5	–	120.4	–	–
<[C(4)–C(10)–C(15)]	119.9	–	119.8	–	–
<[C(6)–C(5)–H(35)]	118.4	–	118.5	–	–
<[C(5)–C(6)–H(36)]	119.6	–	119.6	–	–
<[C(8)–C(7)–H(37)]	119.2	–	119.2	–	–
<[C(7)–C(8)–C(9)]	119.5	–	119.5	–	–
<[C(7)–C(8)–C(11)]	121.0	–	121.1	–	–
<[C(9)–C(8)–C(11)]	119.6	–	119.5	–	–
<[C(8)–C(9)–C(10)]	119.5	–	119.5	–	–
<[C(8)–C(9)–C(14)]	117.4	–	117.4	–	–
<[C(8)–C(11)–C(12)]	121.0	–	121.1	–	–
<[C(8)–C(11)–H(38)]	118.3	–	118.2	–	–
<[C(10)–C(9)–C(14)]	123.2	–	123.1	–	–
<[C(9)–C(10)–C(15)]	119.5	–	119.7	–	–
<[C(9)–C(14)–C(13)]	121.4	–	121.4	–	–
<[C(9)–C(14)–H(41)]	120.2	–	120.1	–	–
<[C(10)–C(15)–N(16)]	110.5	–	110.8	–	–
<[C(10)–C(15)–H(42)]	111.4	–	110.9	–	–
<[C(10)–C(15)–H(43)]	112.0	–	111.8	–	–
<[C(12)–C(11)–H(38)]	120.7	–	120.7	–	–
<[C(11)–C(12)–C(13)]	119.7	–	119.8	–	–
<[C(11)–C(12)–H(39)]	120.4	–	120.4	–	–
<[C(13)–C(12)–H(39)]	119.8	–	119.8	–	–
<[C(12)–C(13)–C(14)]	120.9	–	120.9	–	–
<[C(12)–C(13)–H(40)]	119.5	–	119.5	–	–
<[C(14)–C(13)–H(40)]	119.5	–	119.6	–	–
<[C(13)–C(14)–H(41)]	118.4	–	118.5	–	–

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<[N(16)–N(15)–H(42)]	108.5	–	108.7	–	–
<[N(16)–C(15)–H(43)]	107.8	–	107.8	–	–
<[C(15)–N(16)–C(17)]	124.1	–	123.9	–	–
<[C(15)–N(16)–H(44)]	117.4	–	117.7	–	–
<[H(42)–C(15)–H(43)]	106.4	–	106.6	–	–
<[C(17)–N(16)–H(44)]	118.2	–	118.1	–	–
<[N(16)–C(17)–C(18)]	133.6	–	133.4	–	–
<[N(16)–C(17)–C(20)]	135.0	–	135.1	–	–
<[C(18)–C(17)–C(20)]	91.4	–	91.5	–	–
<[C(17)–C(18)–C(19)]	92.3	–	92.4	–	–
<[C(17)–C(18)–N(21)]	127.9	–	127.8	–	–
<[C(17)–C(20)–C(19)]	88.5	–	88.3	–	–
<[C(17)–C(20)–O(23)]	135.6	–	135.6	–	–
<[C(19)–C(18)–N(21)]	139.8	–	139.9	–	–
<[C(18)–C(19)–C(20)]	87.9	–	87.7	–	–
<[C(18)–C(19)–O(22)]	137.6	–	137.7	–	–
<[C(18)–N(21)–C(24)]	129.9	–	129.9	–	–
<[C(18)–N(21)–H(45)]	115.1	–	115.0	–	–
<[C(20)–C(19)–O(22)]	134.5	–	134.5	–	–
<[C(19)–C(20)–O(23)]	136.0	–	136.0	–	–
<[C(24)–N(21)–H(45)]	115.1	–	115.1	–	–
<[N(21)–C(24)–C(25)]	117.0	–	117.1	–	–
<[N(21)–C(24)–C(29)]	123.3	–	123.3	–	–
<[C(25)–C(24)–C(29)]	119.7	–	119.6	–	–
<[C(24)–C(25)–C(26)]	120.4	–	120.4	–	–
<[C(24)–C(25)–H(46)]	119.4	–	119.2	–	–
<[C(24)–C(29)–C(28)]	119.8	–	119.8	–	–
<[C(24)–C(29)–H(49)]	120.2	–	120.0	–	–
<[C(26)–C(25)–H(46)]	120.2	–	120.4	–	–
<[C(25)–C(26)–C(27)]	119.3	–	119.4	–	–
<[C(25)–C(26)–H(47)]	120.5	–	120.7	–	–
<[C(27)–C(26)–H(47)]	120.1	–	119.9	–	–
<[C(26)–C(27)–C(28)]	120.8	–	120.8	–	–
<[C(26)–C(27)–N(30)]	119.6	–	119.6	–	–
<[C(28)–C(27)–N(30)]	119.6	–	119.6	–	–
<[C(27)–C(28)–C(29)]	120.0	–	120.0	–	–
<[C(27)–C(28)–H(48)]	119.8	–	119.6	–	–
<[C(27)–N(30)–O(31)]	118.6	–	118.5	–	–
<[C(27)–N(30)–O(32)]	118.6	–	118.5	–	–
<[C(29)–C(28)–H(48)]	120.2	–	120.4	–	–
<[C(28)–C(29)–H(49)]	120.1	–	120.2	–	–
<[O(31)–N(30)–O(32)]	122.8	–	123.0	–	–

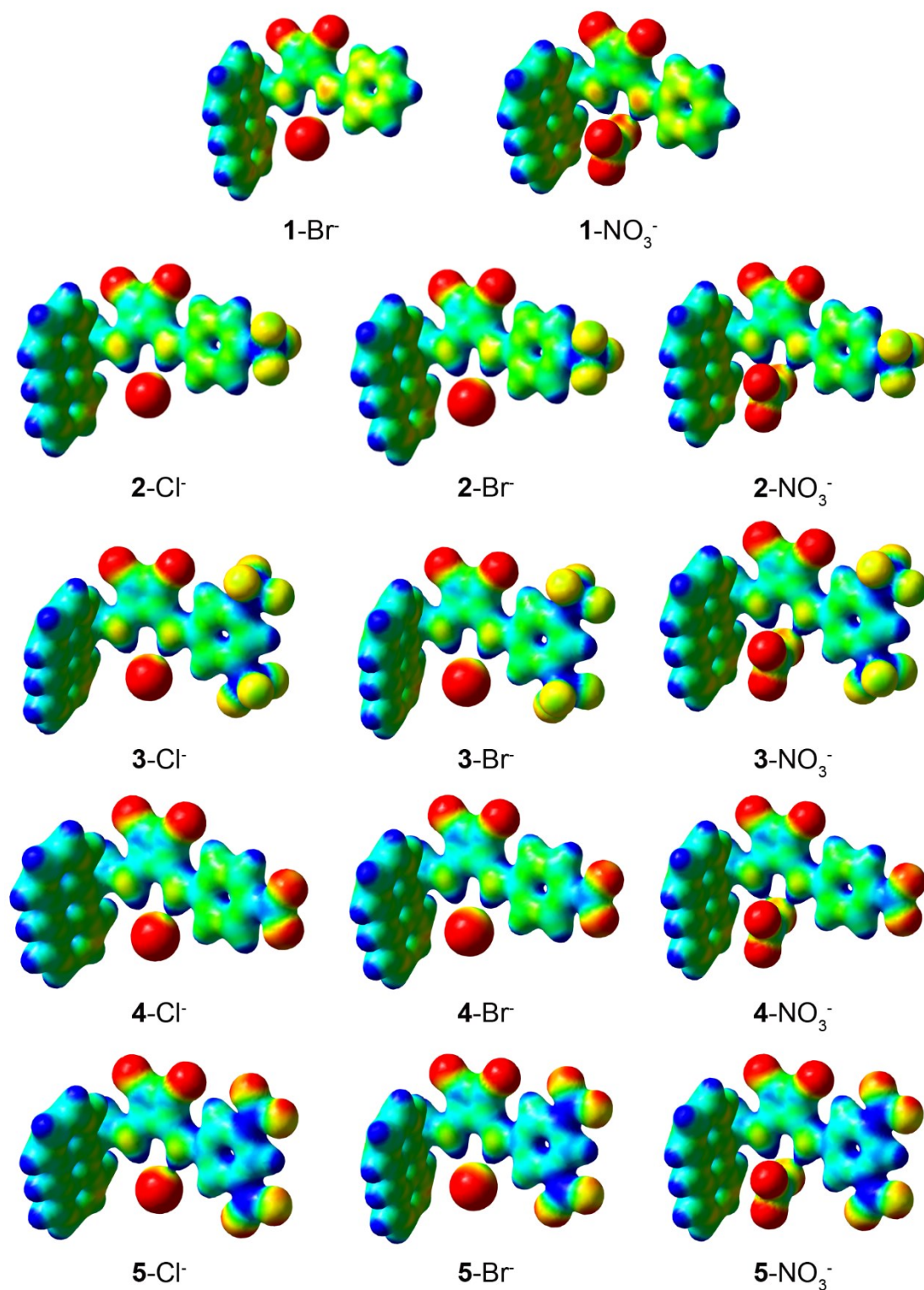


Figure S2. Electrostatic potential map for the compounds analyzed in this study. The isovalues and scales [isovalue (scale red – blue) a.u.] used to represent the surfaces are 0.030 (–0.100 – 0.100) a.u.

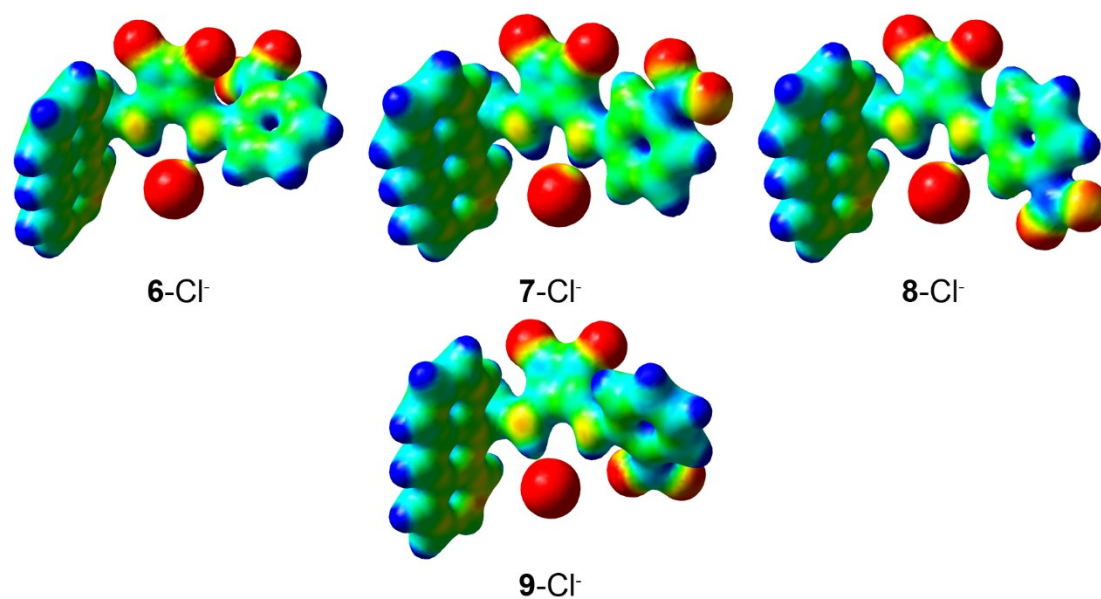


Figure S3. Electrostatic potential map for the compounds analyzed in this study. The isovalues and scales [isovalue (scale red – blue) a.u.] used to represent the surfaces are 0.030 (–0.100 – 0.100) a.u.

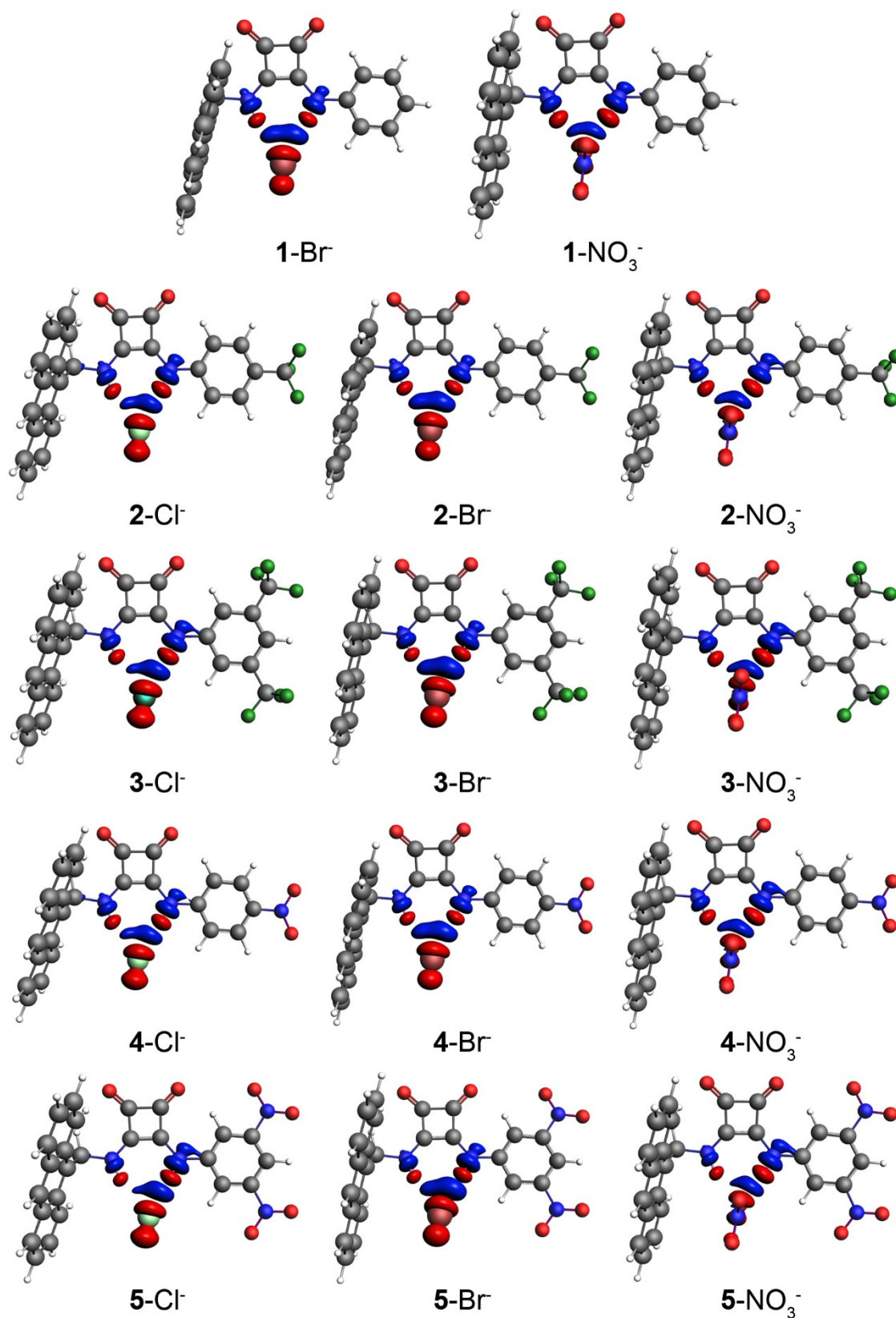


Figure S4. Selected density deformation channels surface plots, $\Delta\rho_1$. Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is 0.002 a.u. Surfaces generated from geometry optimized with the B97D3/6-31+G(d), PCM – DMSO, theory level.

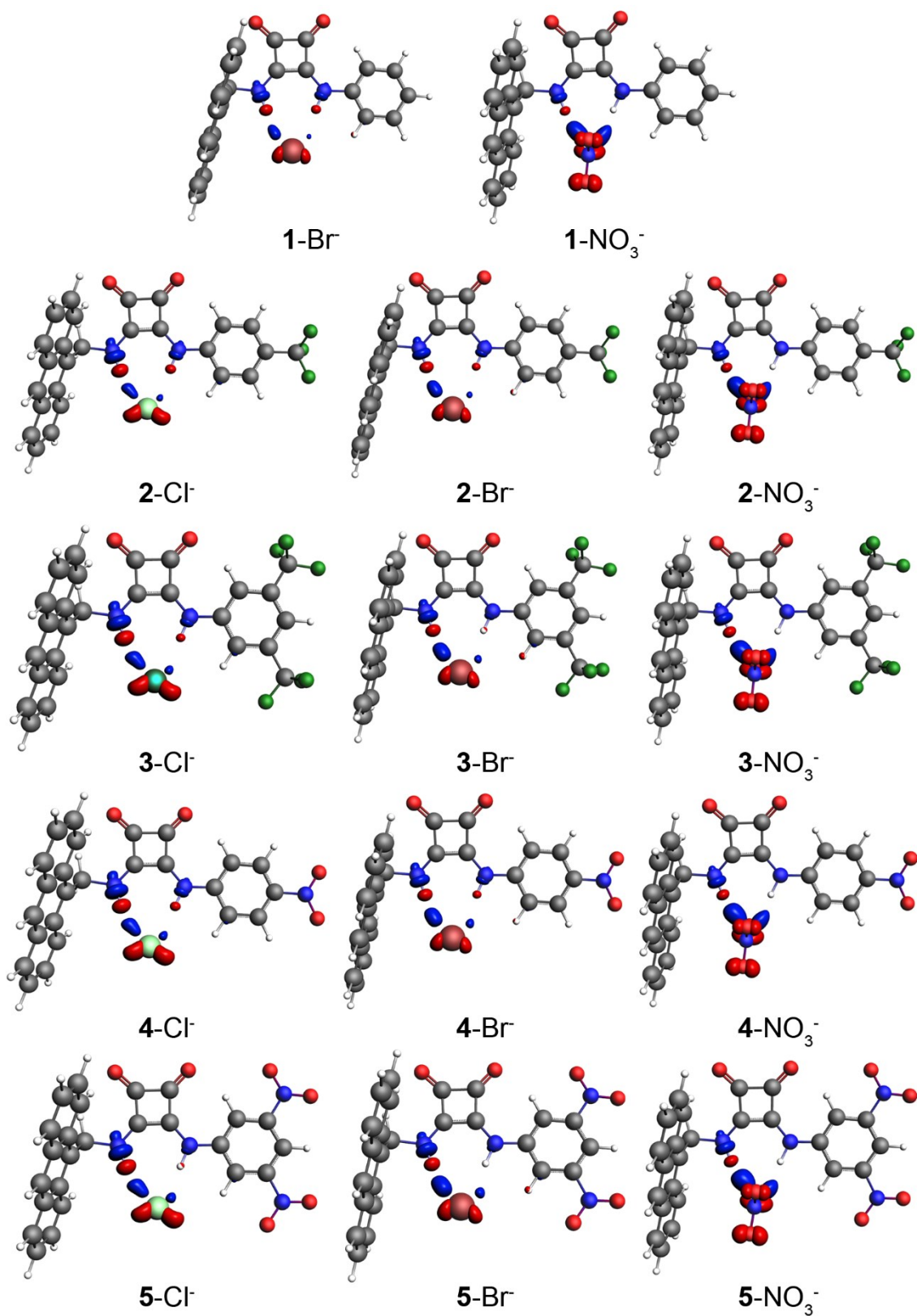


Figure S5. Selected density deformation channels surface plots, $\Delta\rho_2$. Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is 0.002 a.u. Surfaces generated from geometry optimized with the B97D3/6-31+G(d), PCM – DMSO, theory level.

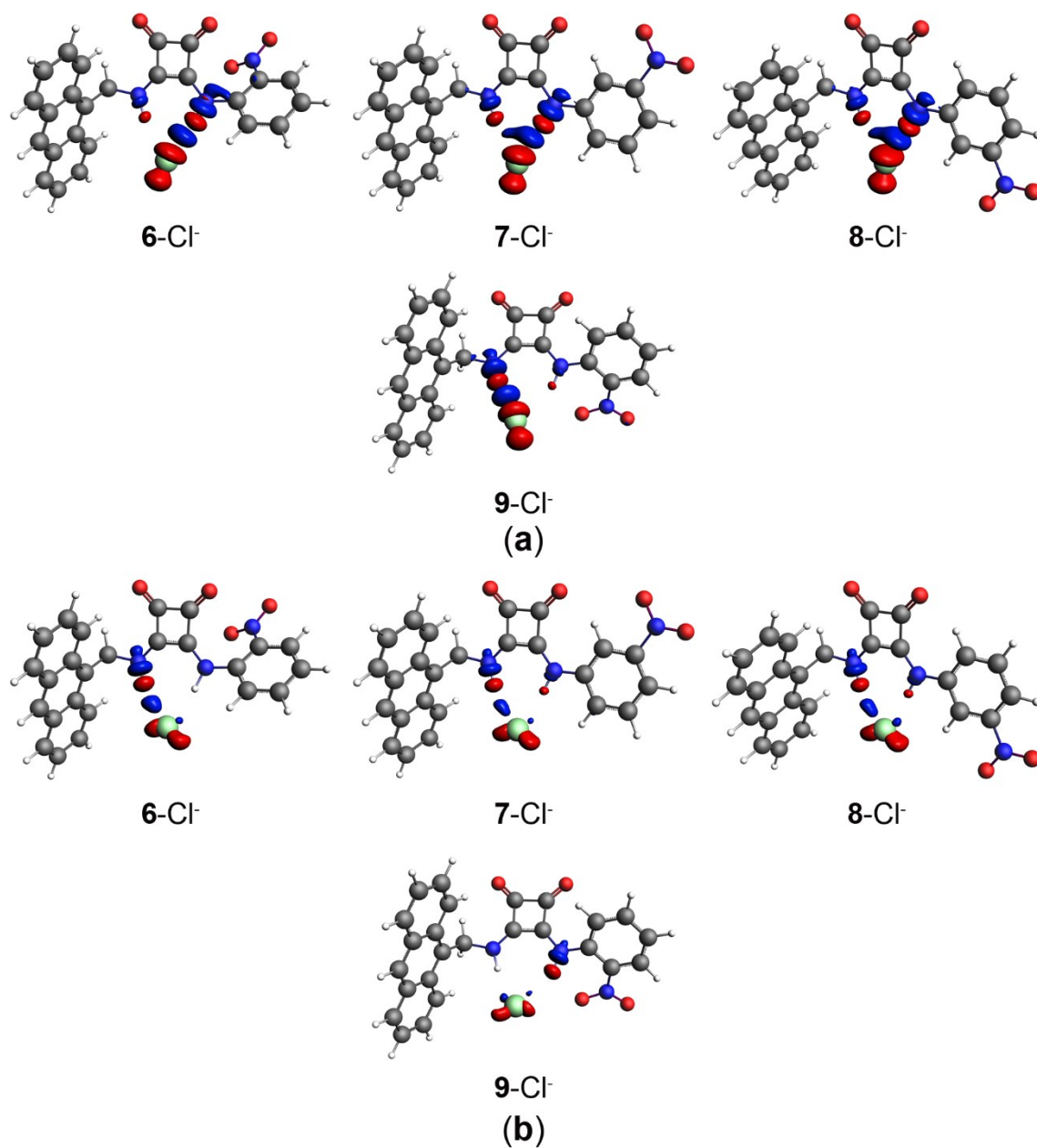


Figure S6. Selected density deformation channels surface plots, (a) $\Delta\rho_1$ and (b) $\Delta\rho_2$. Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is 0.002 a.u. Surfaces generated from geometry optimized with the B97D3/6-31+G(d), PCM – DMSO, theory level.

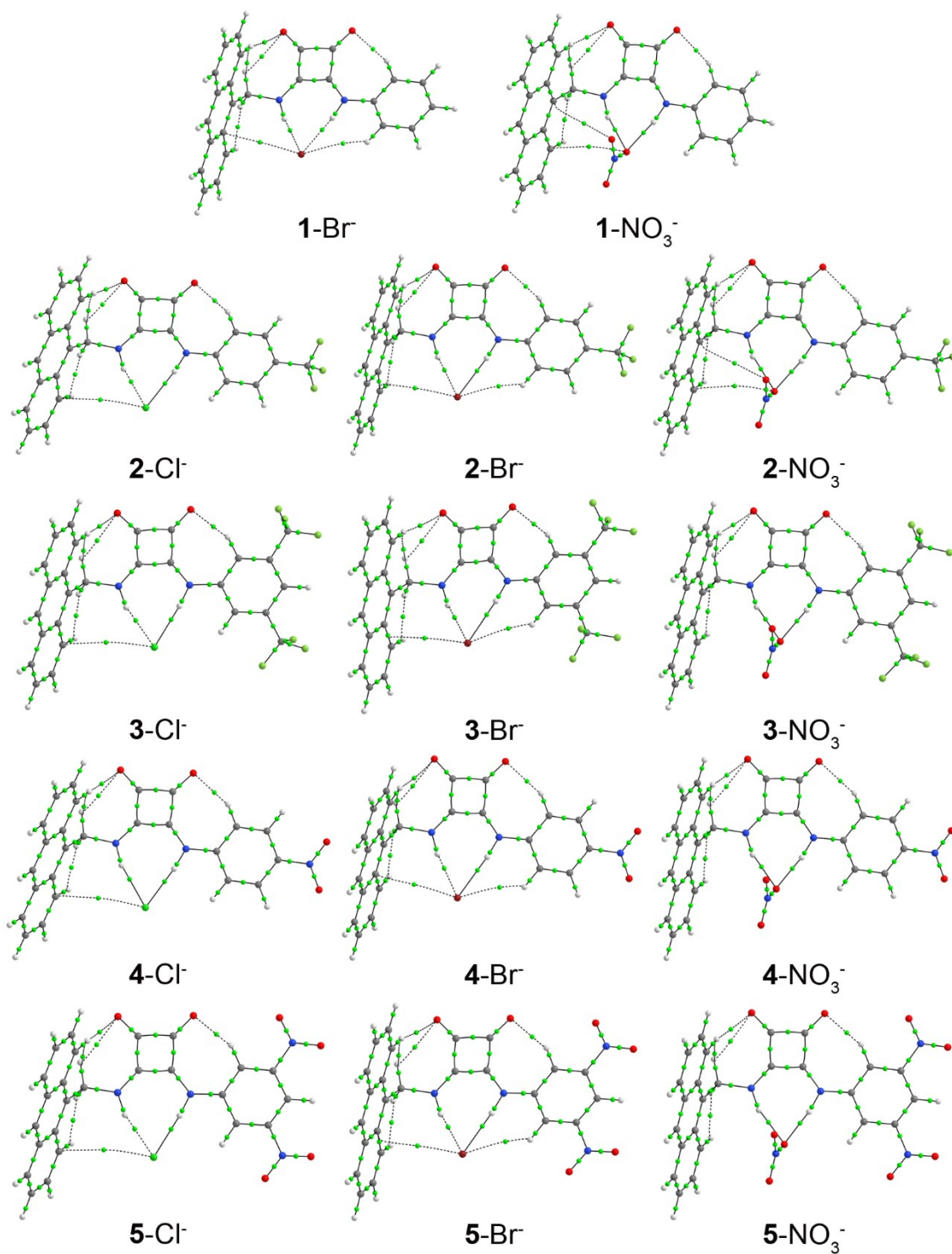


Figure S7 Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points) for the structures studied in this paper. Atoms color: H = white; C = gray; O = light red; Cl = light green; F = green; Br = red.

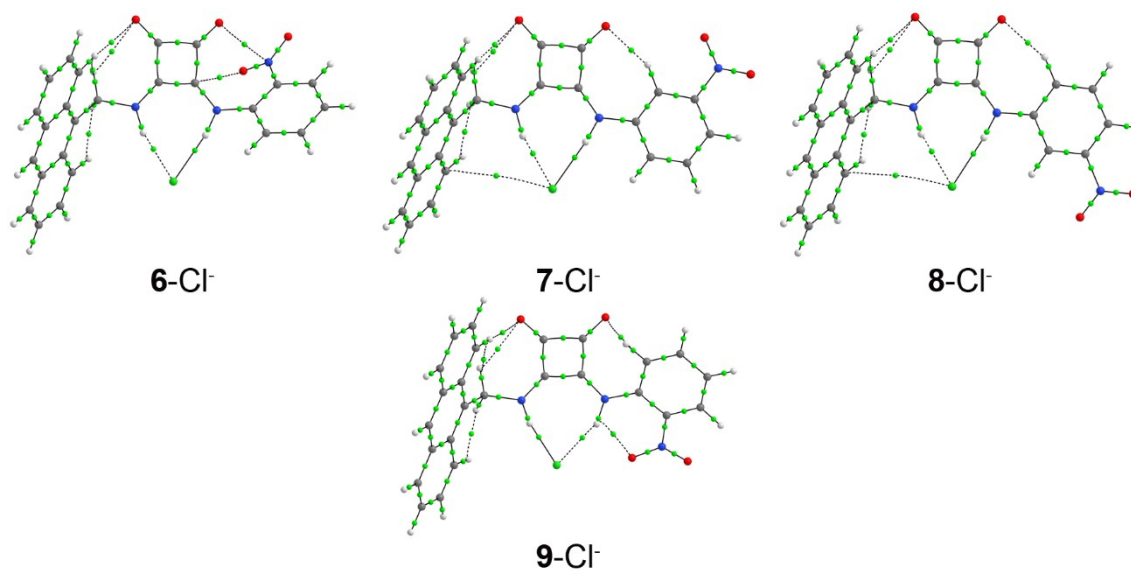


Figure S8 Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points) for the structures studied in this paper. Atoms color: H = white; C = gray; O = light red; Cl = light green; F = green; Br = red.

Table S3. Electron density, ρ_b , Laplacian of ρ_b , $\nabla^2\rho_b$, and $-G_b/V_b$, at BCPs, and Delocalization Index, DI, between the atoms present between the BCPs of the compounds investigated. The values of all the parameters are in a.u.

Complex	BCP	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$	DI
1-Cl⁻	C...Cl ⁻	0.002	0.006	1.304	0.019
	N(1)-H(1)...Cl ^{-[a]}	0.024	0.067	0.965	0.120
	N(2)-H(2)...Cl ^{-[b]}	0.027	0.070	0.941	0.127
1-Br⁻	C...Br ⁻	0.005	0.012	1.229	0.030
	N(1)-H(1)...Br ^{-[a]}	0.024	0.059	0.978	0.127
	N(2)-H(2)...Br ^{-[b]}	0.025	0.060	0.960	0.134
	C-H...Br ⁻	0.006	0.017	1.323	0.046
1-NO₃⁻	C...O ⁻	0.002	0.008	1.389	0.007
	C...O ⁻	0.003	0.009	1.392	0.011
	N(1)-H(1)...O ^{-[a]}	0.029	0.089	0.957	0.087
	N(2)-H(2)...O ^{-[b]}	0.032	0.095	0.949	0.097
2-Cl⁻	C...Cl ⁻	0.002	0.006	1.305	0.019
	N(1)-H(1)...Cl ^{-[a]}	0.024	0.067	0.966	0.120
	N(2)-H(2)...Cl ^{-[b]}	0.028	0.073	0.929	0.133
2-Br⁻	C...Br ⁻	0.005	0.011	1.226	0.033
	N(1)-H(1)...Br ^{-[a]}	0.024	0.059	0.976	0.128
	N(2)-H(2)...Br ^{-[b]}	0.026	0.062	0.946	0.139
	C-H...Br ⁻	0.006	0.018	1.324	0.047
2-NO₃⁻	C...O ⁻	0.002	0.008	1.394	0.007
	C...O ⁻	0.003	0.009	1.401	0.010
	N(1)-H(1)...O ^{-[a]}	0.029	0.088	0.957	0.087
	N(2)-H(2)...O ^{-[b]}	0.034	0.100	0.949	0.101
3-Cl⁻	C...Cl ⁻	0.002	0.006	1.306	0.019
	N(1)-H(1)...Cl ^{-[a]}	0.024	0.066	0.972	0.117
	N(2)-H(2)...Cl ^{-[b]}	0.030	0.075	0.915	0.139
3-Br⁻	C...Br ⁻	0.005	0.011	1.227	0.032
	N(1)-H(1)...Br ^{-[a]}	0.023	0.058	0.984	0.125
	N(2)-H(2)...Br ^{-[b]}	0.028	0.064	0.930	0.146
	C-H...Br ⁻	0.007	0.020	1.317	0.049
3-NO₃⁻	N(1)-H(1)...O ^{-[a]}	0.029	0.086	0.956	0.085
	N(2)-H(2)...O ^{-[b]}	0.036	0.105	0.949	0.106
4-Cl⁻	C...Cl ⁻	0.002	0.006	1.304	0.019
	N(1)-H(1)...Cl ^{-[a]}	0.025	0.068	0.959	0.122
	N(2)-H(2)...Cl ^{-[b]}	0.030	0.075	0.915	0.139
4-Br⁻	C...Br ⁻	0.005	0.012	1.226	0.028
	N(1)-H(1)...Br ^{-[a]}	0.024	0.060	0.969	0.130
	N(2)-H(2)...Br ^{-[b]}	0.027	0.063	0.933	0.145
	C-H...Br ⁻	0.007	0.019	1.322	0.048
4-NO₃⁻	N(1)-H(1)...O ^{-[a]}	0.030	0.089	0.956	0.088
	N(2)-H(2)...O ^{-[b]}	0.036	0.105	0.948	0.106
5-Cl⁻	C...Cl ⁻	0.002	0.006	1.309	0.018
	N(1)-H(1)...Cl ^{-[a]}	0.023	0.065	0.977	0.116
	N(2)-H(2)...Cl ^{-[b]}	0.032	0.078	0.902	0.145
5-Br⁻	C...Br ⁻	0.005	0.011	1.228	0.027
	N(1)-H(1)...Br ^{-[a]}	0.023	0.058	0.984	0.125
	N(2)-H(2)...Br ^{-[b]}	0.029	0.066	0.920	0.151
	C-H...Br ⁻	0.007	0.020	1.322	0.048
5-NO₃⁻	N(1)-H(1)...O ^{-[a]}	0.028	0.085	0.957	0.084
	N(2)-H(2)...O ^{-[b]}	0.038	0.110	0.950	0.110
6-Cl⁻	N(1)-H(1)...Cl ^{-[a]}	0.023	0.064	0.985	0.113
	N(2)-H(2)...Cl ^{-[b]}	0.031	0.076	0.912	0.144
7-Cl⁻	N(1)-H(1)...Cl ^{-[a]}	0.024	0.067	0.969	0.119
	N(2)-H(2)...Cl ^{-[b]}	0.029	0.074	0.923	0.135
	C...Cl ⁻	0.002	0.006	1.304	0.019
8-Cl⁻	N(1)-H(1)...Cl ^{-[a]}	0.024	0.066	0.972	0.118
	N(2)-H(2)...Cl ^{-[b]}	0.029	0.075	0.919	0.137
	C...Cl ⁻	0.002	0.006	1.306	0.019
9-Cl⁻	N(1)-H(1)...Cl ^{-[a]}	0.029	0.075	0.924	0.137
	N(2)-H(2)...Cl ^{-[b]}	0.015	0.047	1.122	0.071
	N(2)-H(2)...ONO ^[b]	0.022	0.085	1.095	0.038

[a] BCP related to -NH group closer to anthracene ring. [b] BCP related to -NH group closer to benzene ring.