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Design of Supramolecular Systems Capable of Recognizing Anions Uniquely by Aliphatic C–H···Anion Hydrogen Bonds: Theoretical Insights

Renato Pereira Orenha,*[a] Claudia Haber Cintra,[a] Maria Laura Lucas Natal,[a] Matheus Cachoeira Colaço,[b] Giovanni Finoto Caramori,[b] Maurício Jeomar Piotrowski[c] and Renato Luis Tame Parreira*[a]

Supplementary Material

[a.] *Núcleo de Pesquisas em Ciências Exatas e Tecnológicas, Universidade de Franca, Franca, SP, Brazil. E–mail: rpo9@hotmail.com / renato.parreira@unifran.edu.br.*
[b.] *Departamento de Química, Universidade Federal de Santa Catarina, Campus Universitário Trindade, CP 476, Florianópolis, SC, 88040–900, Brazil.*
[c.] *Department of Physics, Federal University of Pelotas, PO Box 354, 96010-900, Pelotas, RS, Brazil.*

Table S1. Optimized Cartesian coordinates for the compounds investigated in this study.

Complex	**1**···Cl^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.519791	0.091022	–2.535164
O	–1.622414	–0.511755	–1.856519
O	0.704181	–0.182887	–1.852130
C	–1.684879	0.004850	–0.526201
C	0.616459	0.329305	–0.521750
O	–0.473746	–0.270785	0.179148
H	–0.674356	1.183387	–2.592983
H	–0.452803	–0.368823	–3.524430
H	–2.491958	–0.519978	–0.008735
H	–1.851670	1.096258	–0.561402
H	0.475567	1.424581	–0.555900
H	1.535263	0.047591	–0.001164
Cl	–1.127427	3.943198	–1.298249
Complex	**1**···Cl^- – ZORA–BLYP–D3(BJ)/TZ2P		
Atom	X	Y	Z
C	–0.527608	0.133667	–2.538080
O	–1.631958	–0.495656	–1.861043
O	0.707820	–0.158530	–1.856947
C	–1.693315	0.041010	–0.525195
C	0.610819	0.370833	–0.520695
O	–0.476237	–0.255364	0.186714
H	–0.684972	1.223984	–2.569356
H	–0.460085	–0.320866	–3.529531
H	–2.500908	–0.482797	–0.008011
H	–1.840294	1.132579	–0.570264
H	0.445869	1.459665	–0.564071
H	1.531443	0.094349	–0.000905
Cl	–1.048148	3.523092	–1.298096
Complex	**1**···Br^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.525350	0.106312	–2.533300
O	–1.624243	–0.507295	–1.855532
O	0.701196	–0.168395	–1.852498
C	–1.687869	0.009838	–0.524389
C	0.611230	0.344663	–0.521308
O	–0.474818	–0.265514	0.179941
H	–0.684488	1.197918	–2.578707
H	–0.458051	–0.346069	–3.526170
H	–2.494557	–0.515423	–0.006402
H	–1.852537	1.100896	–0.561256
H	0.458080	1.437386	–0.557819
H	1.532845	0.071050	–0.001000
Br	–1.062289	3.847760	–1.328639
Complex	**1**···Br^- – ZORA–BLYP–D3(BJ)/TZ2P		
Atom	X	Y	Z
C	–0.527201	0.121485	–2.536537
O	–1.631017	–0.506643	–1.859441
O	0.707788	–0.167581	–1.856192
C	–1.691879	0.025382	–0.523526
C	0.611469	0.359264	–0.520472
O	–0.474841	–0.265622	0.187465
H	–0.685179	1.211935	–2.572740
H	–0.460228	–0.330538	–3.528825
H	–2.498990	–0.498294	–0.006024
H	–1.846705	1.116156	–0.564460
H	0.450062	1.449107	–0.561409
H	1.532704	0.086008	–0.000706
Br	–1.046835	3.712469	–1.324211

Complex		**1**···NO_2^- – B97D3/6–31+G(d) + PCM(acetonitrile)	
Atom	X	Y	Z
C	–0.206286	–0.177618	–2.456176
O	–1.505836	–0.576674	–2.019198
O	0.785051	–0.556704	–1.499446
C	–1.784627	0.047285	–0.765770
C	0.484576	0.067191	–0.251548
O	–0.809097	–0.321001	0.210648
H	–0.181080	0.917568	–2.598937
H	0.008547	–0.718337	–3.381466
H	–2.750621	–0.329474	–0.419800
H	–1.790899	1.144699	–0.892374
H	0.524227	1.164659	–0.369531
H	1.214367	–0.290915	0.479068
O	0.444279	3.464623	–2.072314
N	–0.444375	3.860846	–1.252651
O	–1.652548	3.671866	–1.605134
Complex		**1**···NO_2^- – ZORA–BLYP–D3(BJ)/TZ2P	
Atom	X	Y	Z
C	–0.204275	–0.128748	–2.475468
O	–1.511862	–0.531446	–2.034405
O	0.791945	–0.540119	–1.515133
C	–1.777337	0.142020	–0.789737
C	0.498444	0.127615	–0.276085
O	–0.804005	–0.245585	0.205302
H	–0.163452	0.967366	–2.590916
H	0.004818	–0.668401	–3.401947
H	–2.748072	–0.211160	–0.434441
H	–1.753259	1.232942	–0.948564
H	0.546174	1.216137	–0.434150
H	1.225640	–0.224078	0.459526
O	0.439126	3.108428	–1.849426
N	–0.514978	3.807419	–1.341453
O	–1.693231	3.315624	–1.467731
Complex		**2**···Cl^- – B97D3/6–31+G(d) + PCM(acetonitrile)	
Atom	X	Y	Z
C	–0.340346	–0.039049	–2.699516
O	–1.118977	–0.880408	–1.853916
O	0.539329	0.790826	–1.905184
C	–1.579738	–0.143006	–0.717000
C	0.772831	0.340900	–0.572398
O	–0.469816	0.157466	0.144682
C	1.640375	–0.914027	–0.463476
C	0.405604	–0.896711	–3.707388
C	–2.580616	–0.981142	0.050164
H	–1.001473	0.684206	–3.207622
H	–2.023230	0.803619	–1.072415
H	1.278708	1.188119	–0.090668
H	1.125020	–1.794119	–0.863633
H	2.585753	–0.762755	–1.004238
H	1.870210	–1.096092	0.596309
H	–0.315431	–1.438524	–4.336150
H	1.014691	–0.249914	–4.352962
H	1.060052	–1.620237	–3.206647
H	–3.471610	–1.156468	–0.567947
H	–2.133846	–1.945464	0.328953
H	–2.884213	–0.450373	0.962433
Cl	–3.225865	3.371902	–2.034952
Complex		**2**···Cl^- – ZORA–BLYP–D3(BJ)/TZ2P	
Atom	X	Y	Z
C	–0.328485	0.101780	–2.630217
O	–1.082732	–0.768097	–1.788378

O	0.737510	0.747845	–1.844593
C	–1.516684	–0.018317	–0.644939
C	0.882066	0.268725	–0.510598
O	–0.361504	0.219448	0.219351
C	1.609458	–1.087185	–0.424053
C	0.255459	–0.706000	–3.774357
C	–2.543954	–0.821261	0.119737
H	–0.982134	0.918021	–2.976333
H	–1.928503	0.939399	–0.997660
H	1.490068	1.035443	–0.010964
H	1.009763	–1.874227	–0.885988
H	2.580305	–1.017480	–0.930945
H	1.775282	–1.340465	0.630294
H	–0.560810	–1.085100	–4.399290
H	0.894034	–0.058113	–4.384094
H	0.849902	–1.547534	–3.400732
H	–3.453084	–0.890928	–0.485569
H	–2.158960	–1.823983	0.341516
H	–2.781049	–0.310380	1.059017
Cl	–3.238536	2.087159	–2.854778

Complex	**2**···Br^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.368992	–0.029272	–2.698276
O	–1.123908	–0.888994	–1.849836
O	0.529597	0.790142	–1.912955
C	–1.605895	–0.158580	–0.717861
C	0.742458	0.365263	–0.569133
O	–0.503283	0.190182	0.140202
C	1.615683	–0.883825	–0.435418
C	0.364105	–0.870252	–3.728354
C	–2.573161	–1.026449	0.058481
H	–1.045760	0.697765	–3.177376
H	–2.075533	0.772060	–1.077395
H	1.239758	1.221911	–0.094564
H	1.112222	–1.767638	–0.843047
H	2.569705	–0.729654	–0.960189
H	1.827658	–1.060883	0.629012
H	–0.363024	–1.411713	–4.350433
H	0.958000	–0.212988	–4.377608
H	1.032956	–1.593079	–3.244500
H	–3.458503	–1.239540	–0.556319
H	–2.091934	–1.971867	0.345363
H	–2.894526	–0.499035	0.966761
Br	–2.740210	3.275195	–2.120127

Complex	**2**···NO_2^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.184969	–0.163366	–2.622123
O	–1.320380	–0.818513	–2.042730
O	0.969116	–0.375254	–1.796951
C	–1.564198	–0.315282	–0.722838
C	0.733586	0.128386	–0.476389
O	–0.405923	–0.524672	0.096849
C	1.947081	–0.152514	0.382470
C	0.075784	–0.748807	–3.992564
C	–2.734675	–1.060449	–0.119860
H	–0.389156	0.922281	–2.661335
H	–1.751102	0.771803	–0.792794
H	0.515321	1.209380	–0.550492
H	2.134431	–1.233758	0.433342
H	2.827120	0.345997	–0.044940
H	1.780416	0.232477	1.397193
H	–0.799839	–0.590367	–4.635921

H	0.943359	–0.253526	–4.448336
H	0.275539	–1.826292	–3.914890
H	–3.629423	–0.906711	–0.737516
H	–2.514830	–2.135454	–0.065190
H	–2.934048	–0.681511	0.891258
O	–0.338611	3.597413	–2.288783
N	–0.805549	3.740951	–1.114114
O	–2.016591	3.388127	–0.947591

Complex	**3**···Cl^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.277779	–0.396024	–2.770982
O	–1.358270	–1.050842	–2.104233
O	0.889438	–0.413285	–1.946738
C	–1.631323	–0.384300	–0.869581
C	0.611966	0.235481	–0.702211
O	–0.471297	–0.408968	–0.038585
C	1.844939	0.214805	0.175906
C	0.077923	–1.172315	–4.027925
C	–2.744846	–1.170658	–0.198535
Cl	–1.246076	–1.046436	–5.263809
Cl	–3.342771	–0.309769	1.283854
Cl	2.411250	–1.465818	0.590794
H	–0.562301	0.648685	–2.982038
H	–1.913802	0.662771	–1.072254
H	0.339466	1.289065	–0.903307
H	2.671523	0.713533	–0.339111
H	1.629582	0.722722	1.120919
H	0.983036	–0.752305	–4.476238
H	0.219683	–2.233713	–3.801649
H	–3.592202	–1.266328	–0.883662
H	–2.390074	–2.158053	0.113020
Cl	–1.183883	3.287039	–1.998738

Complex	**3**···Br^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.274014	–0.383674	–2.769641
O	–1.352654	–1.046996	–2.107498
O	0.892691	–0.398359	–1.942762
C	–1.630500	–0.386664	–0.869685
C	0.611482	0.237615	–0.692246
O	–0.472344	–0.414069	–0.035448
C	1.842470	0.211292	0.186528
C	0.089022	–1.150629	–4.029151
C	–2.746076	–1.175781	–0.207380
Cl	–1.233465	–1.018942	–5.267474
Cl	–3.341417	–0.323602	1.282077
Cl	2.414283	–1.471712	0.587618
H	–0.563124	0.659117	–2.978809
H	–1.914562	0.660058	–1.066972
H	0.339311	1.292557	–0.882197
H	2.668649	0.716633	–0.322704
H	1.625065	0.709682	1.136161
H	0.993035	–0.722333	–4.471985
H	0.234303	–2.213749	–3.813129
H	–3.593347	–1.260789	–0.894090
H	–2.397816	–2.167689	0.097379
Br	–1.226809	3.193320	–2.033697

Complex	**3**···NO_2^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.365113	–0.101290	–2.599514
O	–1.386704	–0.831055	–1.927192
O	0.873074	–0.220522	–1.902441
C	–1.530029	–0.339710	–0.595340

C	0.731772	0.241346	–0.560872
O	–0.297229	–0.485741	0.113296
C	2.043680	0.083136	0.178240
C	–0.209054	–0.611092	–4.017537
C	–2.549109	–1.189971	0.144512
Cl	0.262804	–2.366719	–4.105799
Cl	–4.218456	–0.922082	–0.517781
Cl	2.617503	–1.642697	0.275904
H	–0.656971	0.964299	–2.645213
H	–1.810817	0.726852	–0.629220
H	0.466901	1.316446	–0.566763
H	2.824451	0.651926	–0.335828
H	1.931764	0.443072	1.205489
H	–1.158508	–0.505965	–4.551308
H	0.574170	–0.042029	–4.527510
H	–2.317885	–2.254357	0.037668
H	–2.568767	–0.906087	1.200718
O	–1.732157	3.042289	–1.720609
N	–0.659913	3.727408	–1.695491
O	0.058885	3.594784	–0.653046

Complex	**4**···Cl^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.310480	0.199480	–2.566497
O	–1.323294	–0.606228	–1.981829
O	0.904096	0.084821	–1.832023
C	–1.544483	–0.191141	–0.639346
C	0.679851	0.479906	–0.486661
O	–0.337085	–0.321348	0.108577
C	1.952395	0.287263	0.340152
C	–0.024646	–0.263776	–3.995492
C	–2.566634	–1.157350	–0.026234
Cl	0.476595	–1.993566	–4.068501
Cl	–2.845634	–0.734544	1.701642
Cl	2.541337	–1.415598	0.306189
Cl	3.219810	1.434984	–0.232397
Cl	–1.468884	0.049683	–5.028230
Cl	–4.102271	–1.092679	–0.963246
H	–0.634501	1.255007	–2.581163
H	–1.895066	0.853851	–0.615000
H	0.378270	1.541590	–0.453478
H	1.745239	0.532000	1.384389
H	0.799010	0.323797	–4.407245
H	–2.202931	–2.187254	–0.059421
Cl	–1.299521	3.500317	–1.291093

Complex	**4**···Br^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.309773	0.201142	–2.572547
O	–1.323890	–0.601030	–1.985484
O	0.904385	0.092110	–1.836016
C	–1.545953	–0.182022	–0.643872
C	0.681610	0.485330	–0.489481
O	–0.339034	–0.312132	0.105633
C	1.951639	0.286708	0.336482
C	–0.020878	–0.269544	–3.996983
C	–2.570705	–1.141668	–0.028455
Cl	0.491545	–1.997048	–4.061786
Cl	–2.853616	–0.701974	1.695093
Cl	2.533798	–1.419611	0.309024
Cl	3.225942	1.425861	–0.240422
Cl	–1.468297	0.027924	–5.031194
Cl	–4.103523	–1.075853	–0.971212
H	–0.634239	1.255812	–2.597004

H	–1.896492	0.862324	–0.621453
H	0.386177	1.548152	–0.453157
H	1.746622	0.536192	1.380030
H	0.798564	0.320818	–4.413161
H	–2.213044	–2.174026	–0.051375
Br	–1.308152	3.443884	–1.222329
Complex	**4**···NO_2^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.273307	0.206336	–2.566315
O	–1.277930	–0.633984	–2.014515
O	0.926380	0.115652	–1.802040
C	–1.541048	–0.234223	–0.676087
C	0.659824	0.482415	–0.457660
O	–0.349790	–0.352720	0.101641
C	1.917746	0.312682	0.396663
C	0.062123	–0.236675	–3.990268
C	–2.563249	–1.220029	–0.095986
Cl	0.614647	–1.952258	–4.066255
Cl	–2.895264	–0.811998	1.626164
Cl	2.555403	–1.371463	0.350630
Cl	3.164137	1.505610	–0.128688
Cl	–1.363103	0.044270	–5.058073
Cl	–4.074401	–1.174644	–1.073535
H	–0.626147	1.254589	–2.588017
H	–1.904056	0.806286	–0.649923
H	0.327985	1.532817	–0.407841
H	1.679371	0.535370	1.439142
H	0.879113	0.376963	–4.376367
H	–2.182611	–2.243938	–0.124784
O	–1.309125	3.218081	–0.502692
N	–0.853822	3.912466	–1.468684
O	–1.019781	3.419641	–2.629913
Complex	**5**···Cl^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.359187	0.181636	–2.566419
O	–1.346613	–0.652630	–1.982580
O	0.853718	0.090838	–1.836665
C	–1.563411	–0.256435	–0.637883
C	0.626857	0.483294	–0.492957
O	–0.356382	–0.347730	0.101827
C	1.949812	0.311092	0.293713
C	–0.095576	–0.312223	–4.009930
C	–2.594229	–1.223470	–0.005925
Cl	0.478479	–2.015380	–4.015549
Cl	–2.875206	–0.702940	1.694892
Cl	2.505020	–1.397766	0.257441
Cl	3.188692	1.379148	–0.459399
Cl	1.658235	0.829987	1.993137
Cl	–1.634374	–0.175655	–4.934722
Cl	1.148836	0.761091	–4.746340
Cl	–4.128265	–1.090694	–0.939077
Cl	–1.996109	–2.918046	–0.041170
H	–0.710619	1.227025	–2.595289
H	–1.956912	0.773587	–0.601877
H	0.311495	1.539513	–0.450770
Cl	–1.540796	3.305408	–1.203045
Complex	**5**···Cl^- – ZORA–BLYP–D3(BJ)/TZ2P		
Atom	X	Y	Z
C	–0.363443	0.194433	–2.573225
O	–1.352317	–0.656178	–1.987265
O	0.860925	0.093612	–1.841167
C	–1.573085	–0.246274	–0.635154

C	0.626992	0.498014	–0.489859
O	–0.356689	–0.349166	0.109566
C	1.943405	0.332355	0.294429
C	–0.103122	–0.293887	–4.011669
C	–2.602789	–1.204950	–0.005784
Cl	0.481207	–2.011738	–4.043397
Cl	–2.898620	–0.689026	1.702963
Cl	2.527920	–1.385233	0.271321
Cl	3.195458	1.404229	–0.451947
Cl	1.660930	0.849097	2.005118
Cl	–1.644741	–0.165811	–4.949622
Cl	1.142811	0.779208	–4.766342
Cl	–4.147472	–1.082806	–0.939319
Cl	–2.021384	–2.924141	–0.024790
H	–0.718397	1.242989	–2.579823
H	–1.948979	0.794656	–0.609266
H	0.291140	1.552035	–0.460117
Cl	–1.436284	3.058231	–1.193239

Complex	**5**···Br^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.331927	0.203172	–2.589150
O	–1.292760	–0.483296	–1.804010
O	0.965521	0.033306	–2.042198
C	–1.259537	0.000688	–0.471503
C	0.992379	0.515101	–0.708577
O	0.034572	–0.167749	0.083686
C	2.394752	0.232309	–0.120446
C	–0.341965	–0.408737	–4.009665
C	–2.257876	–0.829094	0.369356
Cl	0.064788	–2.159769	–3.968456
Cl	–3.900616	–0.598443	–0.332139
Cl	2.760363	–1.528065	–0.123835
Cl	3.604319	1.116134	–1.120297
Cl	2.426834	0.866268	1.565339
Cl	–1.987567	–0.173951	–4.703485
Cl	0.865810	0.482252	–5.005366
Cl	–2.226598	–0.192635	2.054038
Cl	–1.824153	–2.574263	0.361622
H	–0.583675	1.274923	–2.653501
H	–1.554350	1.062799	–0.441788
H	0.803120	1.601317	–0.689024
Br	–0.942453	3.468840	–1.269190

Complex	**5**···NO_2^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.291203	0.154233	–2.628567
O	–1.302996	–0.626004	–2.015205
O	0.919599	0.054922	–1.899330
C	–1.500811	–0.161344	–0.686478
C	0.706296	0.498737	–0.566584
O	–0.298248	–0.288562	0.054869
C	2.025275	0.318239	0.220696
C	–0.045814	–0.396728	–4.055776
C	–2.583788	–1.039318	–0.018178
Cl	0.476656	–2.114465	–4.002021
Cl	–2.833688	–0.433093	1.659251
Cl	2.542756	–1.405021	0.237699
Cl	3.287650	1.332736	–0.567457
Cl	1.752461	0.895757	1.904206
Cl	–1.581614	–0.246345	–4.983615
Cl	1.228490	0.613239	–4.830079
Cl	–4.108760	–0.857476	–0.958327
Cl	–2.086400	–2.767858	0.019745

H	–0.617391	1.204125	–2.699311
H	–1.834759	0.891044	–0.706401
H	0.416436	1.565800	–0.551867
O	–2.000958	2.874320	–1.748699
N	–1.185513	3.816179	–1.481528
O	–0.330123	3.566109	–0.574555

Complex	**1** – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.524931	0.104735	–2.534321
O	–1.625596	–0.496259	–1.855801
O	0.699365	–0.158492	–1.852616
C	–1.688751	0.008185	–0.523640
C	0.612442	0.343251	–0.520834
O	–0.476344	–0.254792	0.179205
H	–0.683580	1.198048	–2.603798
H	–0.456713	–0.355750	–3.522607
H	–2.490295	–0.525447	–0.007716
H	–1.875086	1.099036	–0.547991
H	0.479420	1.441930	–0.546153
H	1.531509	0.060924	–0.002168

Complex	**2** – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.339756	–0.037836	–2.699538
O	–1.121251	–0.877340	–1.854137
O	0.536017	0.794647	–1.904531
C	–1.577719	–0.144561	–0.715327
C	0.773259	0.341480	–0.572809
O	–0.470701	0.158361	0.144413
C	1.638352	–0.914636	–0.466895
C	0.407696	–0.897403	–3.704247
C	–2.580752	–0.981397	0.050486
H	–1.001202	0.683378	–3.211669
H	–2.022176	0.804339	–1.069953
H	1.278987	1.187731	–0.089944
H	1.120970	–1.793855	–0.866137
H	2.582476	–0.763902	–1.009650
H	1.870161	–1.097189	0.592204
H	–0.312323	–1.441062	–4.332331
H	1.016699	–0.251139	–4.350228
H	1.062250	–1.618968	–3.201234
H	–3.471047	–1.156632	–0.568380
H	–2.133184	–1.945444	0.327816
H	–2.883479	–0.451724	0.963472

Complex	**3** – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.273337	–0.379172	–2.770691
O	–1.355818	–1.030567	–2.110709
O	0.888980	–0.386835	–1.944069
C	–1.632369	–0.382071	–0.871161
C	0.611159	0.242235	–0.693997
O	–0.475746	–0.398351	–0.040077
C	1.843576	0.205361	0.188223
C	0.087991	–1.153396	–4.028175
C	–2.741612	–1.179949	–0.204899
Cl	–1.230864	–1.026033	–5.266507
Cl	–3.344679	–0.331432	1.280220
Cl	2.394475	–1.481569	0.577890
H	–0.559494	0.664736	–2.994390
H	–1.932558	0.664711	–1.061862
H	0.351208	1.304030	–0.876996
H	2.672311	0.708221	–0.319237
H	1.626589	0.703339	1.138113

H	0.995387	–0.732587	–4.470843
H	0.229411	–2.214080	–3.799580
H	–3.586650	–1.278941	–0.892263
H	–2.376967	–2.165685	0.099602
Complex	**4** – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.311788	0.207190	–2.572617
O	–1.326611	–0.586449	–1.984360
O	0.898120	0.111862	–1.834789
C	–1.546598	–0.177406	–0.643327
C	0.678894	0.492645	–0.487706
O	–0.342542	–0.297799	0.105076
C	1.955115	0.282587	0.334813
C	–0.018686	–0.278133	–3.996356
C	–2.570083	–1.143807	–0.029088
Cl	0.480498	–2.005053	–4.030987
Cl	–2.848617	–0.718713	1.696395
Cl	2.522413	–1.422357	0.277662
Cl	3.227320	1.426333	–0.231636
Cl	–1.457992	0.020399	–5.038434
Cl	–4.101814	–1.082050	–0.969423
H	–0.639630	1.261467	–2.617661
H	–1.910206	0.864689	–0.615031
H	0.396303	1.559699	–0.437463
H	1.750777	0.519662	1.381459
H	0.807064	0.304417	–4.411289
H	–2.201102	–2.171717	–0.062576
Complex	**5** – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
C	–0.242604	0.190662	–2.664503
O	–1.292289	–0.530432	–2.048735
O	0.941107	0.106787	–1.894120
C	–1.517165	–0.038297	–0.741874
C	0.711128	0.585629	–0.582947
O	–0.338988	–0.132592	0.035165
C	2.004558	0.368870	0.248486
C	0.036262	–0.445549	–4.053411
C	–2.613797	–0.910407	–0.073010
Cl	0.515961	–2.163710	–3.878367
Cl	–2.899918	–0.267666	1.583566
Cl	2.434143	–1.370099	0.311173
Cl	3.326929	1.310750	–0.528348
Cl	1.707698	0.997878	1.908507
Cl	–1.466604	–0.314965	–5.035150
Cl	1.356002	0.493364	–4.838291
Cl	–4.117330	–0.756573	–1.050239
Cl	–2.097932	–2.625111	0.007334
H	–0.535233	1.244146	–2.813028
H	–1.872488	1.005472	–0.779690
H	0.483600	1.664845	–0.599488
Complex	NO_2^- – B97D3/6–31+G(d) + PCM(acetonitrile)		
Atom	X	Y	Z
O	–1.308738	3.219039	–0.501186
N	–0.854915	3.910420	–1.468751
O	–1.019074	3.420729	–2.631351
Complex	**1**···Cl^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile)		
Atom	X	Y	Z
C	–0.523228	0.110419	–2.543076
O	–1.629069	–0.501728	–1.859528
O	0.707460	–0.171364	–1.855081
C	–1.695145	0.023607	–0.523099
C	0.621304	0.348004	–0.517555

O	–0.475712	–0.258770	0.185171
H	–0.677533	1.201177	–2.588898
H	–0.456432	–0.345726	–3.532775
H	–2.501578	–0.499564	–0.005345
H	–1.853012	1.113883	–0.564791
H	0.475785	1.439936	–0.556040
H	1.539204	0.065412	0.002666
Cl	–1.100044	3.739714	–1.296648

Complex	**1**···Br^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile)		
Atom	X	Y	Z
C	–0.524324	0.096931	–2.541054
O	–1.627214	–0.518952	–1.857626
O	0.707637	–0.178136	–1.854576
C	–1.693709	0.001186	–0.520517
C	0.620741	0.335441	–0.515937
O	–0.473494	–0.275471	0.186157
H	–0.684043	1.187151	–2.589831
H	–0.456193	–0.357056	–3.531524
H	–2.498446	–0.524532	–0.003011
H	–1.859836	1.090926	–0.557535
H	0.473899	1.427756	–0.549066
H	1.540294	0.056203	0.002899
Br	–1.086312	3.972553	–1.334379

Complex	**1**···NO_2^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile)		
Atom	X	Y	Z
C	–0.253310	–0.111848	–2.475052
O	–1.541419	–0.538640	–2.001970
O	0.773500	–0.502543	–1.547131
C	–1.792529	0.068595	–0.724792
C	0.504809	0.103650	–0.273528
O	–0.778964	–0.310064	0.219853
H	–0.246859	0.984410	–2.594490
H	–0.060085	–0.635019	–3.413739
H	–2.743248	–0.323137	–0.357595
H	–1.809441	1.164981	–0.837383
H	0.531384	1.200626	–0.378568
H	1.257140	–0.261099	0.429152
O	0.593876	3.366250	–1.669118
N	–0.549606	3.807882	–1.309278
O	–1.550247	3.354956	–1.960360

Complex	**1**···Cl^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.570940	0.202542	–2.524973
O	–1.616476	–0.531409	–1.863552
O	0.685216	–0.012426	–1.861232
C	–1.707834	–0.090673	–0.501553
C	0.570648	0.438245	–0.502156
O	–0.462382	–0.294046	0.180848
H	–0.806437	1.280060	–2.517538
H	–0.480639	–0.199152	–3.536365
H	–2.459488	–0.708131	–0.005426
H	–1.973329	0.979831	–0.475987
H	0.333522	1.515353	–0.494724
H	1.514705	0.213747	–0.000712
Cl	–0.481802	3.913873	–1.666261

Complex	**1**···Cl^- – ZORA–BLYP–D3BJ/TZ2P – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.569080	0.232682	–2.514495
O	–1.624256	–0.521483	–1.867097
O	0.679872	–0.014153	–1.855374
C	–1.712672	–0.105416	–0.499082
C	0.556401	0.469173	–0.510888

O	–0.467353	–0.280651	0.188646
H	–0.788829	1.314194	–2.488943
H	–0.485893	–0.160371	–3.529890
H	–2.440663	–0.760547	–0.012704
H	–2.020536	0.950044	–0.448368
H	0.308383	1.544704	–0.530943
H	1.498647	0.258989	–0.000576
Cl	–0.389258	3.780648	–1.699918
Complex	**1**···Br^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.938398	0.452268	–2.795916
O	–1.936139	–0.398508	–2.206646
O	0.335391	–0.211691	–2.818645
C	–1.536894	–0.724643	–0.867793
C	0.713394	–0.539462	–1.472169
O	–0.269225	–1.397448	–0.869854
H	–0.856381	1.384889	–2.212841
H	–1.232259	0.634420	–3.831465
H	–2.277166	–1.417178	–0.461574
H	–1.462729	0.199292	–0.270026
H	0.808661	0.387431	–0.882064
H	1.650490	–1.097902	–1.520874
Br	0.201002	3.275766	–0.138454
Complex	**1**···Br^- – ZORA–BLYP–D3BJ/TZ2P – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.934019	0.480295	–2.763958
O	–1.940587	–0.395307	–2.206812
O	0.334195	–0.190165	–2.802434
C	–1.546495	–0.750240	–0.874894
C	0.703460	–0.497629	–1.450857
O	–0.265780	–1.394918	–0.863308
H	–0.846136	1.399231	–2.159916
H	–1.227699	0.680167	–3.796352
H	–2.274893	–1.477895	–0.508275
H	–1.514227	0.151211	–0.244198
H	0.767370	0.435147	–0.865703
H	1.651118	–1.038590	–1.487166
Br	0.293442	3.145927	–0.324448
Complex	**1**···NO_2^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.329320	0.210073	–2.502119
O	–1.575753	–0.324072	–2.023210
O	0.759008	–0.246176	–1.682318
C	–1.777915	0.083475	–0.663253
C	0.533563	0.178024	–0.330205
O	–0.699294	–0.367939	0.167303
H	–0.362189	1.312668	–2.496113
H	–0.170900	–0.189327	–3.506060
H	–2.690989	–0.398650	–0.308676
H	–1.850220	1.182649	–0.608588
H	0.494050	1.279558	–0.292807
H	1.341459	–0.228473	0.281591
O	0.477836	3.553319	–1.252382
N	–0.652016	4.042285	–1.595168
O	–1.025217	3.792111	–2.790348
Complex	**1**···NO_2^- – ZORA–BLYP–D3BJ/TZ2P – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.418064	0.189609	–2.557172
O	–1.634027	–0.312519	–1.963458
O	0.724222	–0.257405	–1.805677
C	–1.719865	0.177357	–0.613519
C	0.600971	0.275722	–0.477182

O	–0.585274	–0.249074	0.157889
H	–0.421700	1.290692	–2.592677
H	–0.345537	–0.258666	–3.550579
H	–2.603869	–0.282848	–0.165054
H	–1.768078	1.276460	–0.612358
H	0.537927	1.375548	–0.518460
H	1.455384	–0.087681	0.098220
O	–0.703575	3.354511	–0.607770
N	–0.724707	3.933263	–1.758879
O	0.078295	3.454556	–2.635674
Complex	**2**···Cl^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.400269	0.179492	–2.571127
O	–1.174136	–0.742321	–1.789198
O	0.541873	0.888766	–1.708947
C	–1.563553	–0.129373	–0.552893
C	0.822083	0.266767	–0.452421
O	–0.405008	0.019070	0.295767
C	1.656832	–1.012275	–0.537388
C	0.283976	–0.576040	–3.695237
C	–2.573873	–1.009615	0.151646
H	–1.062720	0.970945	–2.956117
H	–1.974860	0.869752	–0.775213
H	1.369738	1.031850	0.111810
H	1.105394	–1.818070	–1.030039
H	2.586769	–0.813412	–1.084971
H	1.915368	–1.334264	0.479044
H	–0.475311	–1.009060	–4.359290
H	0.895120	0.122823	–4.278953
H	0.923406	–1.377148	–3.310000
H	–3.494433	–1.065053	–0.440633
H	–2.164305	–2.017878	0.286502
H	–2.811559	–0.585674	1.133895
Cl	–3.055437	2.543859	–3.652664
Complex	**2**···Cl^- – ZORA–BLYP–D3BJ/TZ2P – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.398276	0.234945	–2.540605
O	–1.127916	–0.724155	–1.756096
O	0.619992	0.876188	–1.688815
C	–1.539799	–0.107894	–0.543073
C	0.841785	0.259663	–0.431607
O	–0.384062	0.069995	0.324924
C	1.625314	–1.063061	–0.505175
C	0.220577	–0.474200	–3.727906
C	–2.540479	–0.999095	0.164210
H	–1.081943	1.035816	–2.871900
H	–1.964123	0.880188	–0.771740
H	1.426433	0.995157	0.137477
H	1.045229	–1.826599	–1.027626
H	2.574563	–0.898902	–1.030100
H	1.836902	–1.413802	0.512476
H	–0.586100	–0.822352	–4.381685
H	0.829696	0.242775	–4.287531
H	0.844047	–1.320444	–3.417254
H	–3.451412	–1.066734	–0.438888
H	–2.114784	–1.999182	0.302965
H	–2.786036	–0.574539	1.143365
Cl	–2.944511	2.099374	–3.901842
Complex	**2**···Br^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.268909	0.122130	–2.701020
O	–1.073569	–0.799458	–1.946163

O	0.953775	0.396397	–1.978195
C	–1.591064	–0.156087	–0.776828
C	0.791401	0.337028	–0.534452
O	–0.552963	0.652265	–0.151539
C	1.315550	–0.994167	0.008350
C	0.083375	–0.497486	–4.035926
C	–2.161485	–1.206452	0.159189
H	–0.834831	1.060699	–2.819805
H	–2.358027	0.576651	–1.071196
H	1.386268	1.164322	–0.128411
H	0.785738	–1.842547	–0.433579
H	2.382059	–1.080096	–0.236738
H	1.205497	–1.019257	1.100258
H	–0.826265	–0.637159	–4.631945
H	0.763084	0.167983	–4.581442
H	0.574667	–1.466596	–3.885710
H	–3.000830	–1.717141	–0.329637
H	–1.401515	–1.945419	0.433574
H	–2.533141	–0.718359	1.067447
Br	–2.660274	3.204767	–3.362845

Complex	**2**···NO_2^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.269569	0.047518	–2.606893
O	–1.392545	–0.618211	–1.993408
O	0.928006	–0.246906	–1.859566
C	–1.548655	–0.193066	–0.625195
C	0.782890	0.196708	–0.495835
O	–0.340441	–0.476562	0.108910
C	2.036272	–0.155974	0.272853
C	–0.107156	–0.466568	–4.019391
C	–2.693367	–0.959150	–0.001612
H	–0.440788	1.136463	–2.571226
H	–1.712026	0.897102	–0.610787
H	0.576615	1.280456	–0.503031
H	2.196125	–1.241050	0.257444
H	2.900779	0.342646	–0.179702
H	1.940439	0.179474	1.311803
H	–1.014632	–0.254890	–4.597344
H	0.741109	0.034280	–4.499818
H	0.069961	–1.549007	–4.010211
H	–3.619164	–0.751135	–0.550376
H	–2.489747	–2.036838	–0.032759
H	–2.823476	–0.646391	1.040766
O	–1.077442	3.360625	–0.496585
N	–1.476187	3.689002	–1.664776
O	–0.618343	3.559507	–2.602133

Complex	**3**···Cl^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.248254	–0.325520	–2.768138
O	–1.341111	–0.979391	–2.108660
O	0.925200	–0.382522	–1.935546
C	–1.610256	–0.307704	–0.866599
C	0.666711	0.236924	–0.666780
O	–0.449233	–0.380741	–0.023485
C	1.892612	0.133286	0.213707
C	0.099026	–1.081263	–4.036005
C	–2.750611	–1.058373	–0.208417
Cl	–1.230866	–0.910408	–5.272126
Cl	–3.321111	–0.175706	1.283911
Cl	2.366691	–1.597206	0.565481
H	–0.523616	0.725156	–2.957600
H	–1.857239	0.746956	–1.076012

H	0.449989	1.308405	–0.826989
H	2.747060	0.600832	–0.279174
H	1.699140	0.609711	1.176954
H	1.004350	–0.665053	–4.481086
H	0.219500	–2.148555	–3.835193
H	–3.601437	–1.115285	–0.889667
H	–2.436500	–2.055628	0.106965
Cl	–2.156816	2.922400	–2.515061
Complex	**3**···Br^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.248224	–0.343053	–2.770369
O	–1.340750	–1.001811	–2.114446
O	0.921017	–0.388824	–1.934312
C	–1.618038	–0.338000	–0.870540
C	0.650118	0.237715	–0.671324
O	–0.458220	–0.393981	–0.027033
C	1.874466	0.161529	0.213315
C	0.104709	–1.096099	–4.038184
C	–2.749931	–1.103662	–0.214448
Cl	–1.223713	–0.926091	–5.275658
Cl	–3.336391	–0.226388	1.274122
Cl	2.375965	–1.558084	0.579583
H	–0.525815	0.706540	–2.963350
H	–1.879426	0.714128	–1.073254
H	0.413510	1.303414	–0.842909
H	2.722346	0.639433	–0.280924
H	1.670193	0.642258	1.172174
H	1.009713	–0.676266	–4.480424
H	0.227782	–2.163221	–3.838303
H	–3.597521	–1.173824	–0.898329
H	–2.421522	–2.095578	0.102902
Br	–2.057557	3.170199	–2.473536
Complex	**3**···NO_2^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.843659	0.195663	–2.477723
O	–1.586013	–0.876556	–1.883240
O	0.430874	0.319712	–1.849149
C	–1.747221	–0.645153	–0.479408
C	0.256964	0.575183	–0.455960
O	–0.468139	–0.506926	0.154800
C	1.596457	0.767316	0.211473
C	–0.672380	–0.047938	–3.960008
C	–2.415317	–1.852314	0.151867
Cl	0.243167	–1.587923	–4.322966
Cl	–4.146280	–1.993934	–0.404215
Cl	2.692817	–0.689323	0.039322
H	–1.403740	1.140894	–2.345749
H	–2.330427	0.279063	–0.327133
H	–0.316232	1.511777	–0.333429
H	2.102920	1.618320	–0.253326
H	1.459535	0.932688	1.282364
H	–1.648668	–0.139393	–4.439589
H	–0.103094	0.770301	–4.405464
H	–1.906000	–2.773770	–0.138285
H	–2.435816	–1.742272	1.237578
O	0.154796	3.665278	–1.450579
N	1.113939	3.576943	–2.288266
O	2.271435	3.363918	–1.790672
Complex	**4**···Cl^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.303804	0.192611	–2.625864
O	–1.333192	–0.579518	–2.015632

O	0.904823	0.122033	–1.868598
C	–1.557905	–0.132593	–0.673760
C	0.664454	0.547231	–0.525683
O	–0.347007	–0.266247	0.079428
C	1.932679	0.396185	0.306201
C	0.002198	–0.352542	–4.020882
C	–2.594939	–1.073323	–0.056778
Cl	0.491130	–2.091477	–3.977911
Cl	–2.867558	–0.640747	1.675138
Cl	2.560389	–1.300199	0.300269
Cl	3.188201	1.554567	–0.290927
Cl	–1.431868	–0.105461	–5.094002
Cl	–4.138272	–0.972013	–0.990269
H	–0.625519	1.242141	–2.722303
H	–1.887326	0.919635	–0.657167
H	0.332979	1.602061	–0.505136
H	1.728458	0.654407	1.344656
H	0.831687	0.200845	–4.460127
H	–2.262457	–2.111019	–0.085779
Cl	–1.352809	3.466712	–0.119931

Complex	**4**···Br^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.302942	0.191531	–2.611408
O	–1.327689	–0.592378	–2.007771
O	0.908245	0.108600	–1.858206
C	–1.556042	–0.147314	–0.667455
C	0.672906	0.528143	–0.514303
O	–0.347212	–0.274838	0.090185
C	1.940047	0.361245	0.317524
C	–0.002314	–0.328349	–4.016493
C	–2.593073	–1.086521	–0.048082
Cl	0.488936	–2.067121	–4.005294
Cl	–2.871631	–0.640902	1.679575
Cl	2.551715	–1.339927	0.299194
Cl	3.204043	1.513438	–0.272172
Cl	–1.441286	–0.064267	–5.078407
Cl	–4.132616	–0.995095	–0.987483
H	–0.626598	1.242679	–2.683887
H	–1.891841	0.902882	–0.658918
H	0.357430	1.587014	–0.493345
H	1.736460	0.614212	1.357471
H	0.824611	0.233804	–4.449391
H	–2.257149	–2.123296	–0.068500
Br	–1.409310	3.665953	–0.282823

Complex	**4**···NO_2^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.304805	0.271790	–2.650087
O	–1.287277	–0.538137	–2.008645
O	0.908261	0.287667	–1.892364
C	–1.542656	–0.030531	–0.694706
C	0.656321	0.744759	–0.564115
O	–0.332143	–0.073527	0.072466
C	1.930828	0.650745	0.269752
C	0.030054	–0.295660	–4.027196
C	–2.543410	–0.976998	–0.029886
Cl	0.607988	–2.006868	–3.940155
Cl	–2.852631	–0.449539	1.670297
Cl	2.600337	–1.028119	0.312497
Cl	3.155152	1.822267	–0.364870
Cl	–1.413880	–0.149914	–5.106323
Cl	–4.079850	–1.003349	–0.978863
H	–0.690324	1.297714	–2.767597

H	–1.917414	1.004610	–0.755111
H	0.307574	1.792363	–0.569284
H	1.721409	0.934778	1.300455
H	0.830716	0.287253	–4.481262
H	–2.165264	–1.998573	0.008941
O	–1.918042	3.069625	–1.927111
N	–1.140175	3.964869	–1.447534
O	–0.705404	3.747224	–0.267663

Complex	**5**···Cl^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.407913	0.233076	–2.552786
O	–1.394270	–0.622454	–1.974343
O	0.810559	0.129660	–1.824711
C	–1.615976	–0.266534	–0.616088
C	0.577281	0.542040	–0.482319
O	–0.403626	–0.298913	0.125415
C	1.893764	0.388774	0.309297
C	–0.153604	–0.236686	–4.001184
C	–2.581756	–1.309313	0.001881
Cl	0.424244	–1.944310	–4.041739
Cl	–2.887180	–0.847816	1.719970
Cl	2.464130	–1.321846	0.301592
Cl	3.137646	1.451985	–0.447144
Cl	1.598295	0.926067	2.008273
Cl	–1.700318	–0.093881	–4.922035
Cl	1.085366	0.846225	–4.737833
Cl	–4.134497	–1.259265	–0.916582
Cl	–1.879128	–2.963327	–0.073263
H	–0.748516	1.283537	–2.562181
H	–2.089933	0.724110	–0.546608
H	0.260350	1.600729	–0.468860
Cl	–0.554236	3.659733	–1.675216

Complex	**5**···Cl^- – ZORA–BLYP–D3BJ/TZ2P – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.399450	0.262852	–2.550496
O	–1.430112	–0.561504	–1.974659
O	0.806642	0.088710	–1.816355
C	–1.635302	–0.242614	–0.607651
C	0.577232	0.565555	–0.495392
O	–0.427864	–0.249215	0.136485
C	1.877235	0.414281	0.314065
C	–0.170267	–0.216987	–3.994925
C	–2.556363	–1.344360	–0.006694
Cl	0.322142	–1.968599	–4.049411
Cl	–2.874542	–0.937151	1.730866
Cl	2.428370	–1.319632	0.380487
Cl	3.152633	1.424262	–0.456732
Cl	1.575697	1.006255	1.999629
Cl	–1.712958	–0.004090	–4.921017
Cl	1.118504	0.796271	–4.738399
Cl	–4.127826	–1.331297	–0.909987
Cl	–1.798496	–2.971492	–0.123705
H	–0.681709	1.338754	–2.547065
H	–2.162036	0.715710	–0.499798
H	0.275707	1.635822	–0.536350
Cl	–0.456555	3.520058	–1.709361

Complex	**5**···Br^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.357725	0.234809	–2.573933
O	–1.319737	–0.472540	–1.794008
O	0.945308	0.051735	–2.029839
C	–1.287552	–0.015543	–0.447953

C	0.964727	0.544750	–0.694699
O	0.015445	–0.159531	0.103227
C	2.369378	0.297661	–0.102617
C	–0.375649	–0.344088	–4.004965
C	–2.261639	–0.887780	0.381811
Cl	0.019734	–2.101867	–4.001045
Cl	–3.920303	–0.688858	–0.301055
Cl	2.766157	–1.459376	–0.082238
Cl	3.572796	1.186844	–1.109026
Cl	2.394106	0.952130	1.579955
Cl	–2.024275	–0.088728	–4.695553
Cl	0.834628	0.555496	–4.993581
Cl	–2.239572	–0.294440	2.085644
Cl	–1.780116	–2.619886	0.329115
H	–0.599972	1.311126	–2.614098
H	–1.620081	1.031805	–0.385326
H	0.753135	1.628400	–0.691931
Br	–0.234219	3.890013	–1.855032
Complex	**5**···NO_2^- – BLYP–D3BJ/Def2–TZVP + CPCM(acetonitrile) – r(C–H···Anion) = 3.5 Å		
Atom	X	Y	Z
C	–0.324666	0.281591	–2.664265
O	–1.318772	–0.507302	–2.019546
O	0.881677	0.283971	–1.908622
C	–1.550024	–0.002630	–0.704255
C	0.641305	0.750757	–0.582006
O	–0.346392	–0.053621	0.055124
C	1.959565	0.619780	0.213213
C	–0.024308	–0.350287	–4.044115
C	–2.597626	–0.904545	–0.018454
Cl	0.578740	–2.037315	–3.869005
Cl	–2.896535	–0.261593	1.641174
Cl	2.527704	–1.089879	0.256572
Cl	3.204032	1.658732	–0.581760
Cl	–1.546941	–0.340163	–5.013467
Cl	–4.126183	–0.827395	–0.975301
H	–0.694449	1.307556	–2.815023
H	–1.926639	1.033557	–0.758769
H	0.323296	1.808068	–0.579824
Cl	1.670786	1.211280	1.893169
Cl	1.219327	0.663617	–4.870872
Cl	–2.025176	–2.611494	0.081453
O	–1.920406	3.016129	–1.887976
N	–1.197486	3.957033	–1.407590
O	–0.655464	3.718598	–0.278221

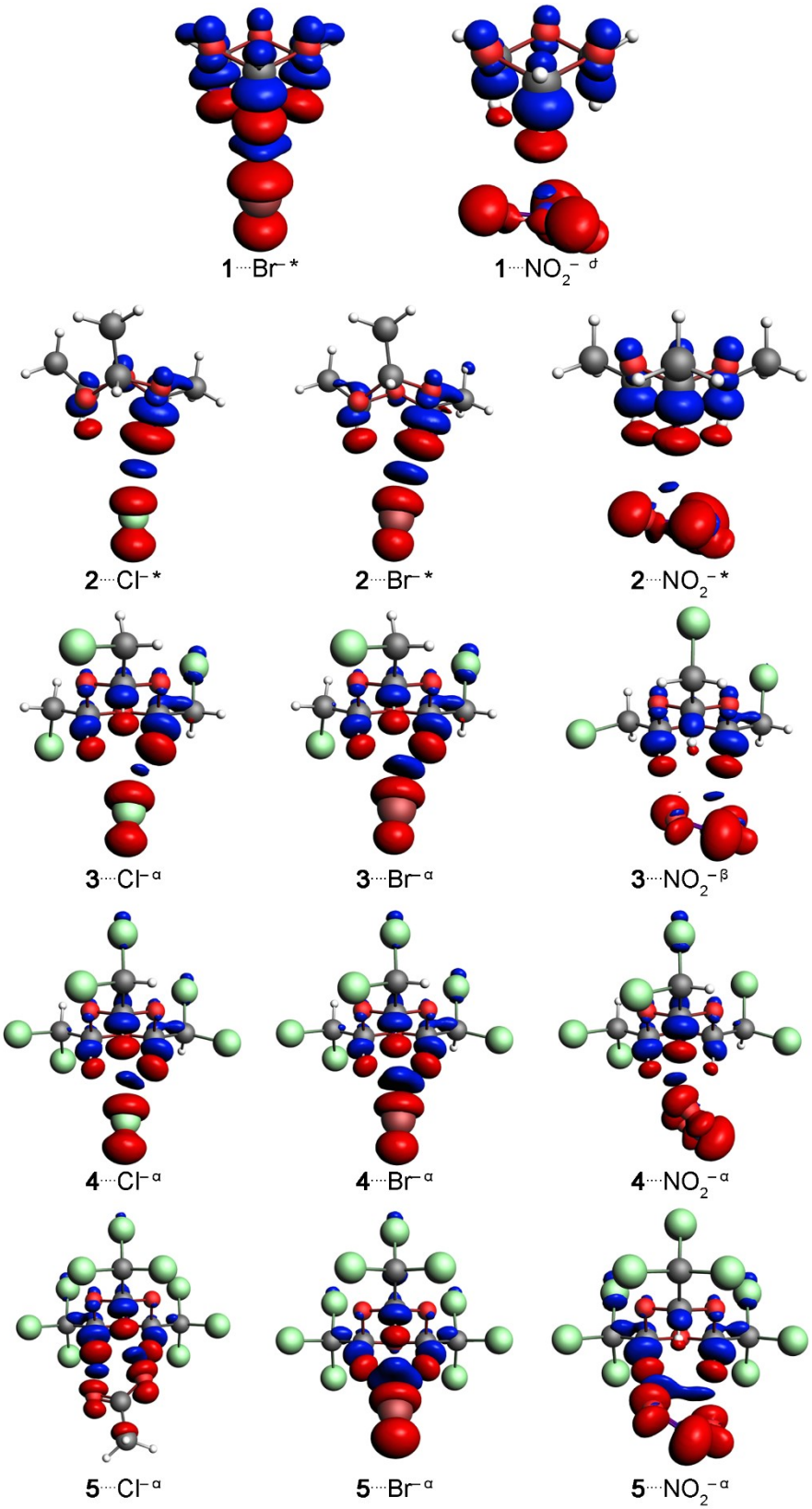

Figure S1. The first density deformation channel surface plots, $\Delta\rho_1$, with isovalue: $^{\alpha}$ = 0.0010; $^{\beta}$ = 0.0008; ^{d} = 0.0006; and * = 0.0005 a.u., to complexes **1**···(Br^- and NO_2^-) and (**2**–**5**)···(Cl^-, Br^- and NO_2^-), where the red and blue regions indicate the electronic density outflow and inflow, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = green; and Br = brown.

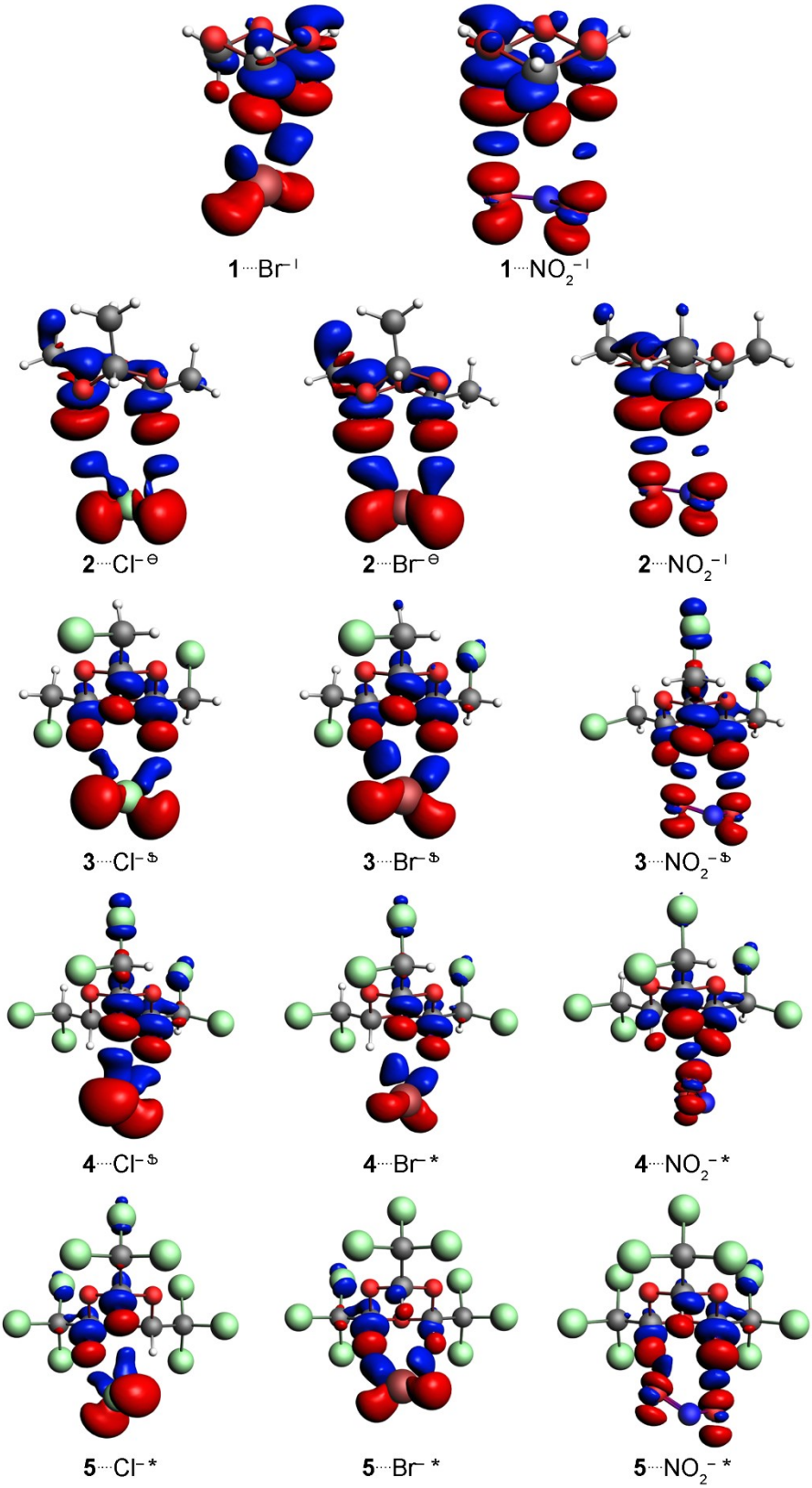

Figure S2. The second density deformation channel surface plots, $\Delta\rho_2$, with isovalue: * = 0.0005; $^{\text{b}}$ = 0.0003; $^{\text{I}}$ = 0.0002; and $^{\text{Θ}}$ = 0.0001 a.u., to complexes **1**···(Br^- and NO_2^-) and (**2**–**5**)···(Cl^-, Br^- and NO_2^-), where the red and blue regions indicate the electronic density outflow and inflow, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = green; and Br = brown.

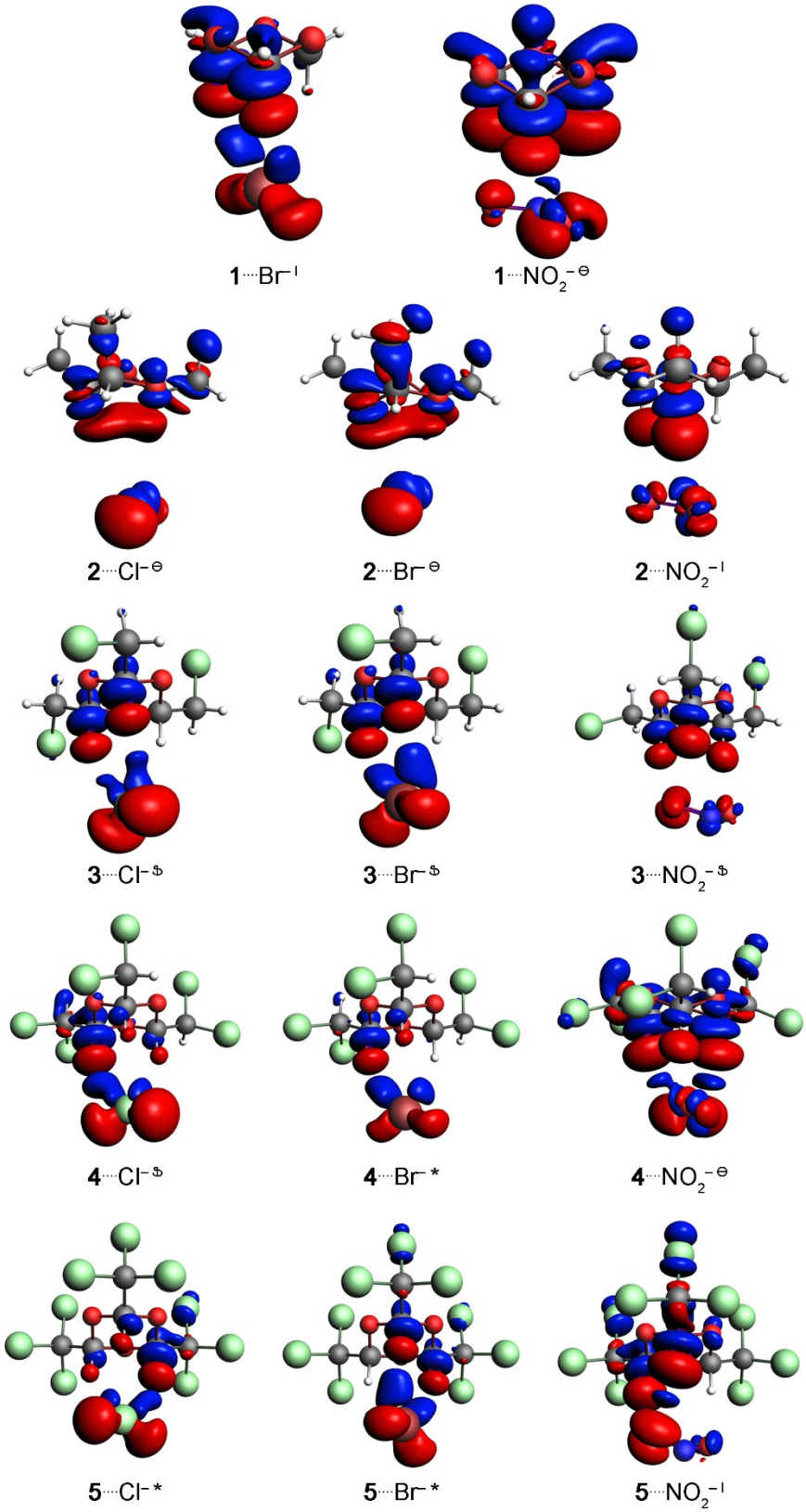

Figure S3. The third density deformation channel surface plots, $\Delta\rho_3$, with isovalue: * = 0.0005; $^{\delta}$ = 0.0003; ^{I} = 0.0002; and $^{\theta}$ = 0.0001 a.u., to complexes **1**···(Cl^-, Br^- and NO_2^-) and (**2**–**5**)···(AcO^-, Cl^-, Br^- and NO_2^-), where the red and blue regions indicate the electronic density outflow and inflow, respectively. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = green; and Br = brown.

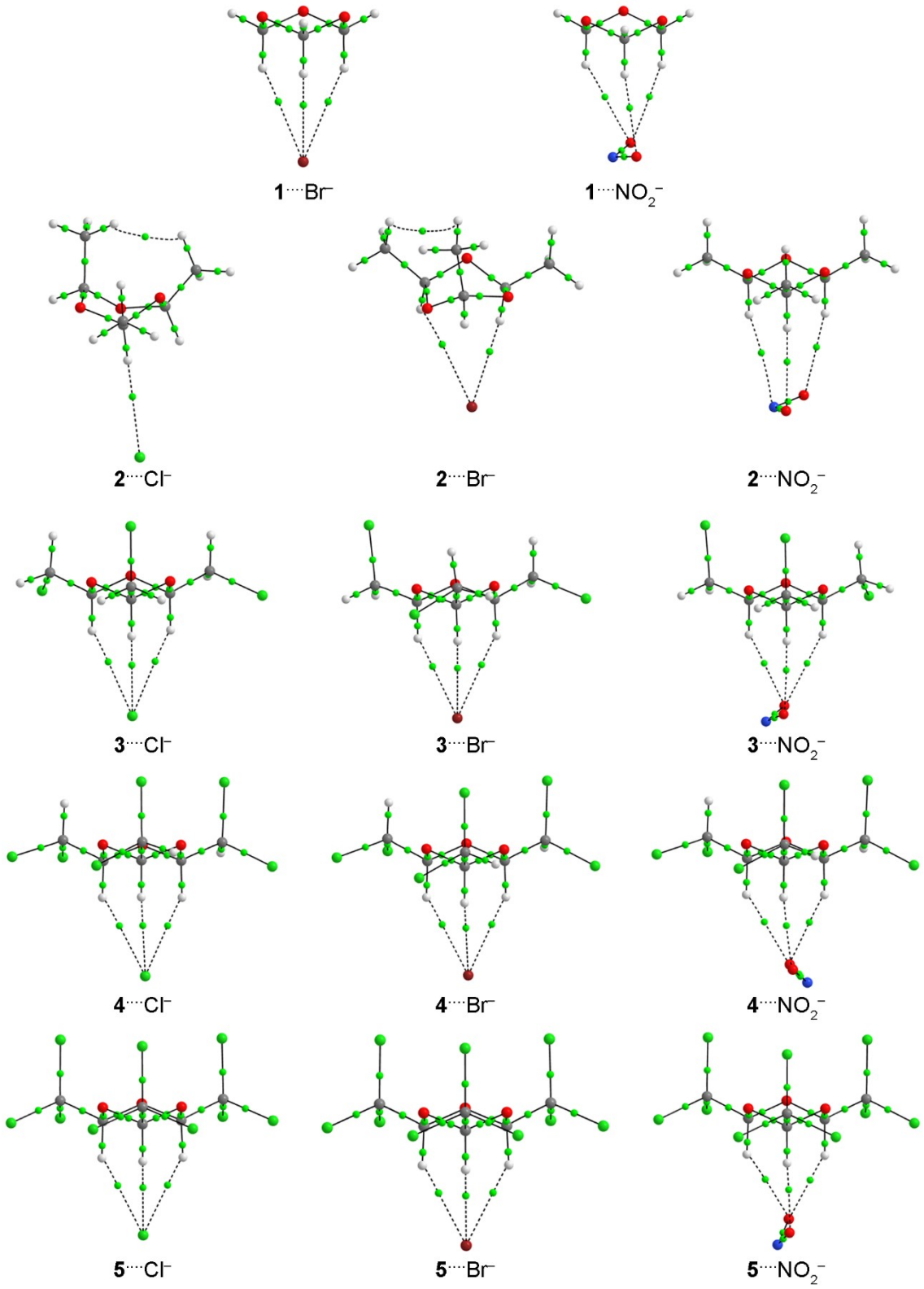

Figure S4. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the complexes **1**···(Br^- and NO_2^-) and (**2**–**5**)···(Cl^-, Br^- and NO_2^-). Atoms color code: H = white; C = gray; N = blue; O = red; Cl = green; and Br = brown.

Table S2. Ratio between the kinetic electron energy density, G_b, and potential electron energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions between the receptors (**1**–**5**) and anions (Cl^-, Br^- and NO_2^-). The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
		1.425	0.005
1···Cl^-	C–H···Cl^-	1.412	0.006
		1.424	0.005
		1.278	0.008
1···Br^-	C–H···Br^-	1.279	0.008
		1.277	0.008
		1.208	0.007
1···NO_2^-	C–H···O^-	1.366	0.005
		1.206	0.007
2···Cl^-	C–H···Cl^-	1.389	0.006
		1.314	0.005
2···Br^-	C–H···Br^-	1.215	0.011
		1.230	0.006
	C–H···O^-		
2···NO_2^-		1.199	0.007
	C–H···N–O^-	1.434	0.004
		1.353	0.008
3···Cl^-	C–H···Cl^-	1.351	0.008
		1.277	0.010
		1.219	0.011
3···Br^-	C–H···Br^-	1.225	0.011
		1.189	0.012
		1.145	0.009
3···NO_2^-	C–H···O^-	1.136	0.009
		1.036	0.013
		1.239	0.011
4···Cl^-	C–H···Cl^-	1.313	0.009
		1.264	0.010
		1.170	0.014
4···Br^-	C–H···Br^-	1.192	0.012
		1.162	0.014
		1.098	0.010
4···NO_2^-	C–H···O^-	1.074	0.012
		0.992	0.017
		1.219	0.012
5···Cl^-	C–H···Cl^-	1.219	0.012
		1.240	0.011
		1.147	0.015
5···Br^-	C–H···Br^-	1.146	0.015
		1.149	0.015
		1.079	0.012
5···NO_2^-	C–H···O^-	0.995	0.017
		0.981	0.020

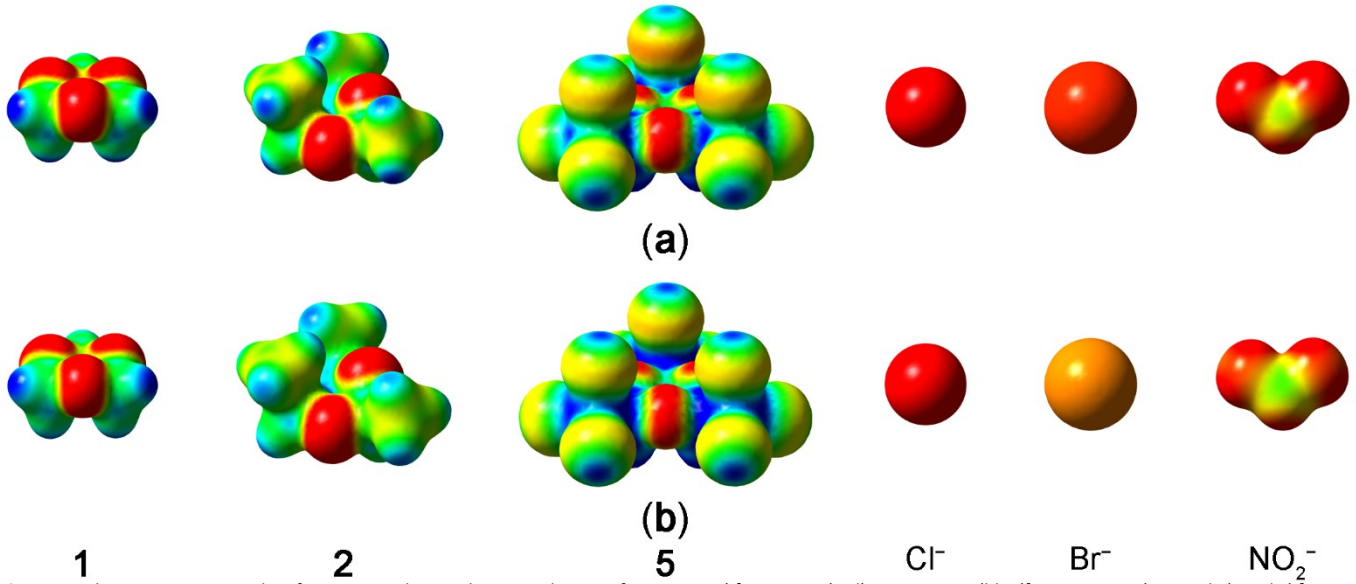

Figure S5. Electrostatic potential surfaces mapped in an electronic density of 0.020 a.u.: i) [0.000 a.u. (red) to 0.150 a.u. (blue)] to receptors (**1**, **2** and **5**); and ii) [–0.250 a.u. (red) to 0.000 a.u. (blue)] to anions (Cl^-, Br^- and NO_2^-) using the: (**a**) B97D3/Def2–TZVP + PCM (acetonitrile); and (**b**) B97D3/6–31+G(d), theory level.

Table S3. Difference between the sum of the atomic charges of the three main hydrogen atoms (highlighted in the blue color in the Scheme 1) and the anion charge, q_D / a.u., through of the: (**a**) B97D3/Def2–TZVP + PCM (acetonitrile); and (**b**) B97D3/6–31+G(d), theory level.

Complex	q_D from B97D3/Def2–TZVP + PCM (acetonitrile)	q_D from B97D3/6–31+G(d)
1···Cl^-	0.913	1.003
1···Br^-	0.964	1.021
1···NO_2^-	0.928	0.964
2···Cl^-	0.752	0.875
5···Cl^-	1.217	1.189

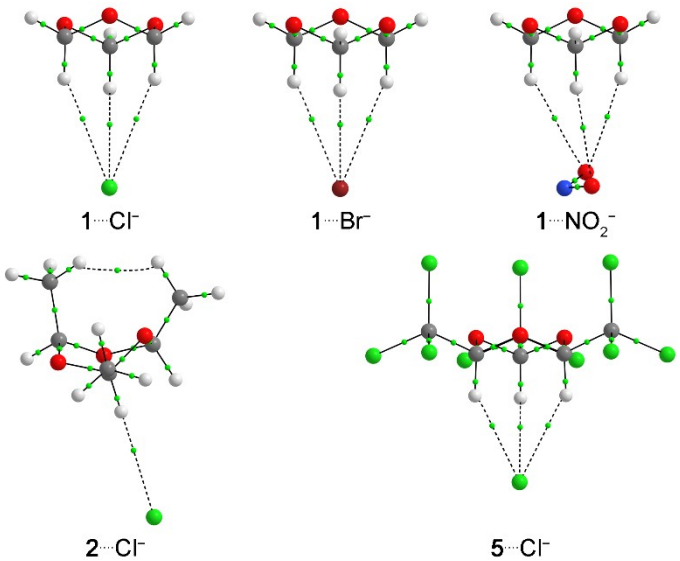

Figure S6. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the complexes **1**···(Cl^-, Br^- and NO_2^-) and (**2** and **5**)···Cl^- using the B97D3/Def2–TZVP + PCM (acetonitrile) computational model. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = green; and Br = brown.

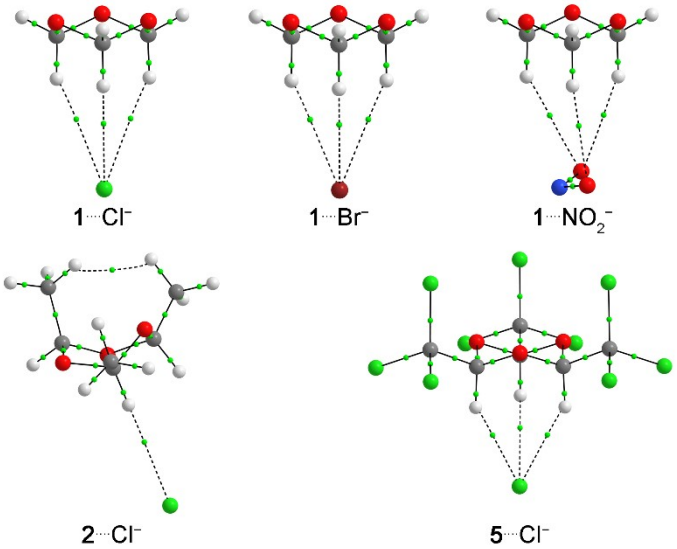

Figure S7. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the complexes **1**···(Cl^-, Br^- and NO_2^-) and (**2** and **5**)···Cl^- using the B97D3/6–31+G(d) theory level. Atoms color code: H = white; C = gray; N = blue; O = red; Cl = green; and Br = brown.

Table S4. Ratio between the kinetic electron energy density, G_b, and potential electron energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions present in the complexes **1**···(Cl^-, Br^- and NO_2^-), **2**···Cl^- and **5**···Cl^- through of the: (**a**) B97D3/Def2–TZVP + PCM (acetonitrile); and (**b**) B97D3/6–31+G(d), theory level. The values of all the parameters are in a.u.

Computational Model		B97D3/Def2–TZVP + PCM (acetonitrile)		B97D3/6–31+G(d)	
Complex	BCP	$-G_b/V_b$	ρ_b	$-G_b/V_b$	ρ_b
		1.225	0.006	1.432	0.005
1···Cl^-	C-H···Cl^-	1.223	0.006	1.419	0.006
		1.225	0.006	1.431	0.005
		1.182	0.008	1.272	0.008
1···Br^-	C-H···Br^-	1.182	0.008	1.274	0.008
		1.181	0.008	1.272	0.008
		1.286	0.007	1.219	0.007
1···NO_2^-	C-H···O^-	1.384	0.005	1.380	0.005
		1.326	0.007	1.212	0.007
2···Cl^-	C-H···Cl^-	1.215	0.007	1.414	0.006
		1.247	0.012	1.209	0.012
5···Cl^-	C-H···Cl^-	1.247	0.012	1.209	0.012
		1.252	0.012	1.230	0.012