

ARTICLE

Designing Boron and Metal Complexes to Fluoride Recognition: Computational Perspective

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Supplementary Material

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Table S1. Optimized Cartesian coordinates of the complexes investigated in this study using the BP86–D3(BJ)/def2–TZVP computational model.

Complex		**1**···F⁻	
Atom	X	Y	Z
P	3.304240	0.118159	–0.025745
F	–3.036773	0.023046	2.356327
B	–2.890388	0.006965	0.874207
C	1.533326	0.105353	0.190644
C	0.984831	0.559516	1.406223
C	–0.394705	0.523812	1.591673
C	–1.279672	0.057828	0.596282
C	–0.692368	–0.419617	–0.593184
C	0.682508	–0.393821	–0.811446
C	3.937988	1.676409	0.621616
C	5.140577	1.723097	1.342403
C	5.624062	2.951504	1.796914
C	4.913899	4.126806	1.532917
C	3.712136	4.078881	0.817562
C	3.217527	2.856547	0.362702
C	3.723442	–0.036548	–1.771331
C	3.663566	–1.305945	–2.373670
C	3.929406	–1.434189	–3.737002
C	4.259526	–0.305974	–4.496184
C	4.326037	0.954150	–3.893633
C	4.057545	1.094648	–2.530722
C	4.078509	–1.261177	0.837690
C	3.376672	–1.948523	1.839199
C	4.000102	–2.994462	2.522462
C	5.315015	–3.352431	2.209038
C	6.012387	–2.669489	1.206015
C	5.398251	–1.625099	0.514954
C	–3.798814	1.302447	0.392511
C	–3.327347	2.478216	–0.249145
C	–4.206828	3.529884	–0.568534
C	–5.570254	3.482729	–0.271953
C	–6.040117	2.329480	0.365029
C	–5.192354	1.261417	0.693802
C	–1.885849	2.681402	–0.666603
C	–6.490101	4.634545	–0.594115
C	–5.846925	0.055450	1.335544
C	–3.391479	–1.439364	0.250419
C	–3.929206	–1.570965	–1.058812
C	–4.323688	–2.825833	–1.555555
C	–4.199341	–3.998067	–0.805675
C	–3.611994	–3.881667	0.458288
C	–3.199528	–2.645431	0.980829
C	–4.103868	–0.398654	–2.003535
C	–4.672151	–5.329102	–1.336072
C	–2.509492	–2.676888	2.328712
H	1.635905	0.949877	2.191713
H	–0.810896	0.879138	2.536386
H	–1.335178	–0.824912	–1.377799
H	1.096124	–0.751237	–1.755875
H	5.690484	0.806787	1.558150
H	6.555454	2.988085	2.363240
H	5.294376	5.084160	1.892177
H	3.154141	4.994515	0.618152
H	2.272130	2.816365	–0.180357
H	3.417580	–2.187464	–1.779704
H	3.882950	–2.417881	–4.205671
H	4.471659	–0.411130	–5.561195
H	4.591865	1.831841	–4.484008

H	4.116976	2.076508	–2.060373
H	2.347637	–1.674073	2.074159
H	3.454073	–3.533603	3.297553
H	5.797442	–4.172179	2.743477
H	7.035349	–2.953904	0.956647
H	5.937793	–1.103164	–0.276925
H	–3.804889	4.417334	–1.069101
H	–7.105117	2.252833	0.610489
H	–1.760886	3.671799	–1.127837
H	–1.557115	1.926226	–1.396200
H	–1.190269	2.608489	0.180239
H	–6.071528	5.271033	–1.387084
H	–6.653998	5.275094	0.288786
H	–7.479019	4.280219	–0.921787
H	–6.849496	0.314268	1.707270
H	–5.246143	–0.339491	2.163132
H	–5.957528	–0.764755	0.608260
H	–4.733971	–2.885382	–2.569552
H	–3.448591	–4.786677	1.053892
H	–4.239873	–0.761465	–3.033269
H	–3.242973	0.282523	–1.989593
H	–4.980464	0.212675	–1.740270
H	–4.044291	–6.154599	–0.968992
H	–4.661642	–5.349482	–2.435694
H	–5.706144	–5.542374	–1.016229
H	–2.252098	–3.711969	2.599013
H	–3.139574	–2.256976	3.125253
H	–1.588354	–2.076925	2.320177

Complex		**2**···F^-	
Atom	X	Y	Z
F	–0.372592	–0.112805	1.643807
N	2.664869	–0.376252	2.409091
B	–0.690568	–0.078653	0.173056
C	0.159426	–1.321211	–0.538608
C	–0.623644	–2.296819	–1.156615
C	–0.125162	–3.338050	–1.968301
C	1.219311	–3.385370	–2.245282
C	4.138119	–0.534859	2.631797
C	3.463362	–2.466614	–2.048009
C	4.363136	–1.545096	–1.565407
C	3.923459	–0.628934	–0.591597
C	2.611039	–0.596018	–0.130259
C	1.597299	–1.439903	–0.726561
C	2.097038	–2.435372	–1.658300
C	–0.205287	1.426033	–0.321107
C	–0.470800	2.528308	0.545474
C	0.061211	3.799921	0.288333
C	0.862284	4.058953	–0.829149
C	1.047564	3.007211	–1.727719
C	0.517118	1.723629	–1.507894
C	–1.369841	2.414468	1.760803
C	1.479907	5.415598	–1.059262
C	0.712255	0.753376	–2.658203
C	–2.326584	–0.327174	0.102577
C	–2.937322	–1.234317	1.019707
C	–4.331179	–1.400121	1.059773
C	–5.190175	–0.704894	0.204369
C	–4.595237	0.138671	–0.736590
C	–3.203602	0.327026	–0.806052
C	–2.142654	–2.105959	1.972550
C	–6.688120	–0.860266	0.291798
C	–2.718848	1.236174	–1.915162

C	2.373830	0.306378	1.040980
C	2.010436	–1.726640	2.495816
C	2.095573	0.521221	3.470602
H	–1.706272	–2.224579	–1.038817
H	–0.812141	–4.066461	–2.405706
H	1.637322	–4.132000	–2.924765
H	4.291908	–0.990098	3.616265
H	4.611466	0.452133	2.592829
H	4.546137	–1.183897	1.851107
H	3.775369	–3.227979	–2.767249
H	5.401496	–1.538212	–1.899669
H	4.642887	0.074703	–0.167449
H	–0.171115	4.618593	0.978365
H	1.605945	3.192081	–2.652149
H	–1.816646	3.394274	1.988387
H	–0.816878	2.083785	2.652672
H	–2.173949	1.684884	1.601261
H	1.686741	5.586778	–2.125673
H	2.437619	5.513387	–0.520686
H	0.824350	6.222691	–0.699634
H	0.534135	1.276392	–3.610852
H	0.040750	–0.108788	–2.609045
H	1.740682	0.360944	–2.692569
H	–4.756148	–2.111875	1.776070
H	–5.233019	0.664747	–1.455058
H	–2.753692	–2.961903	2.296756
H	–1.828546	–1.551364	2.868268
H	–1.226572	–2.487991	1.503625
H	–7.168339	–0.677775	–0.680715
H	–7.122167	–0.143065	1.008776
H	–6.968427	–1.867871	0.632819
H	–3.542156	1.452654	–2.611873
H	–1.899960	0.782172	–2.487372
H	–2.336078	2.191572	–1.529184
H	1.346335	0.650605	1.120735
H	3.048822	1.170787	1.017495
H	2.180265	–2.118603	3.504758
H	2.470015	–2.384341	1.752057
H	0.943933	–1.597744	2.289474
H	2.324241	0.094366	4.453267
H	1.014862	0.582352	3.311060
H	2.555423	1.510817	3.372227

Complex		**3**···F^-	
Atom	X	Y	Z
Fe	–2.482635	–0.834023	–0.630888
C	–1.621050	–1.388325	–2.392652
C	–4.493828	–0.842544	–1.000777
C	–1.551580	–2.440801	–1.428967
C	–0.944466	–0.252228	–1.837309
C	–4.018116	0.506042	–0.867079
C	–4.209088	–1.536269	0.223513
C	–0.814433	–1.940318	–0.287275
C	–0.386927	–0.571013	–0.549451
C	–3.441199	0.646588	0.436942
C	–3.554571	–0.615293	1.109352
B	0.612903	0.364310	0.341724
C	2.227515	0.291310	–0.073484
C	3.132512	1.007892	0.768573
C	2.820308	–0.440272	–1.139891
C	4.518808	0.963739	0.560655
C	4.217799	–0.466189	–1.314969
C	5.093745	0.222576	–0.476585

C	0.043339	1.914032	0.336874
C	0.295285	2.787168	–0.756875
C	–0.761774	2.440326	1.387211
C	–0.271302	4.073024	–0.810534
C	–1.299758	3.735614	1.308179
C	–1.083572	4.572357	0.209258
C	2.038472	–1.200971	–2.192030
C	2.659888	1.881086	1.912103
C	6.589217	0.156599	–0.664089
C	–1.080689	1.674508	2.655160
C	–1.719013	5.937928	0.120126
C	–0.698295	–2.699336	0.988604
N	0.505716	–3.674904	1.087306
C	1.799688	–2.918300	1.063773
C	0.477325	–4.656273	–0.043663
C	0.388188	–4.409151	2.389540
F	0.589287	–0.206057	1.719138
C	1.225347	2.433658	–1.899552
H	–2.141503	–1.427906	–3.346909
H	–4.958305	–1.272093	–1.885093
H	–2.010392	–3.424027	–1.513890
H	–0.875115	0.719639	–2.318247
H	–4.060431	1.277272	–1.632251
H	–4.425611	–2.581305	0.431494
H	–2.958360	1.540205	0.819080
H	–3.190847	–0.842356	2.108397
H	5.170447	1.530019	1.235172
H	4.630504	–1.049415	–2.145060
H	–0.060397	4.705370	–1.679953
H	–1.918961	4.097435	2.136478
H	1.274381	–1.869375	–1.777712
H	1.493661	–0.520302	–2.865249
H	2.722484	–1.799601	–2.810403
H	2.137331	2.774127	1.536622
H	1.945392	1.353610	2.555558
H	3.514105	2.213513	2.520034
H	7.058621	–0.501012	0.086515
H	6.849773	–0.237029	–1.657017
H	7.053169	1.148808	–0.554744
H	–1.858753	2.200862	3.228432
H	–1.418592	0.653680	2.446441
H	–0.192848	1.576054	3.297823
H	–1.148070	6.603017	–0.544115
H	–2.744618	5.876823	–0.281591
H	–1.788549	6.414840	1.109221
H	–1.575453	–3.342736	1.137628
H	–0.578132	–2.017631	1.835140
H	2.620842	–3.632597	1.188613
H	1.887292	–2.397320	0.108383
H	1.784314	–2.175964	1.866244
H	0.563367	–4.106991	–0.985948
H	1.319278	–5.347166	0.072786
H	–0.470498	–5.204419	–0.011810
H	1.233550	–5.099610	2.482788
H	0.406011	–3.677541	3.204252
H	–0.555968	–4.964276	2.400024
H	1.044758	3.096816	–2.758851
H	2.278745	2.549596	–1.599104
H	1.117137	1.397900	–2.236196

Complex		**4**···F⁻	
Atom	X	Y	Z
Te	–1.537311	–0.197204	–0.979709

F	0.928083	0.096573	–1.404658
C	1.231147	1.443145	0.677361
C	2.259543	2.031740	1.408954
C	2.172447	3.298228	2.021879
C	1.022220	4.037267	1.876551
C	–1.243059	4.314136	1.022782
C	–2.356379	3.853715	0.360876
C	–2.336992	2.551580	–0.179031
C	–1.211936	1.749016	–0.089535
C	–0.000192	2.186488	0.552788
C	–0.076599	3.514488	1.144794
C	3.165052	–0.190033	–0.210074
C	3.975464	–0.971131	0.656964
C	5.353711	–1.112291	0.424730
C	5.995261	–0.489111	–0.649145
C	5.212874	0.332241	–1.466521
C	3.834372	0.499838	–1.259760
C	3.128270	1.476042	–2.177957
C	7.467290	–0.688555	–0.911264
C	3.425798	–1.665040	1.884746
C	0.751391	–1.296831	0.650281
C	0.683828	–2.491616	–0.125145
C	–0.231360	–3.505416	0.188407
C	–1.107991	–3.404415	1.274098
C	–0.961519	–2.290675	2.105071
C	–0.045522	–1.260023	1.829312
C	0.018398	–0.152659	2.860054
C	–2.163058	–4.446679	1.538693
C	1.528951	–2.703154	–1.361115
C	–3.645222	–0.220942	–0.553998
C	–4.637895	0.064125	–1.497605
C	–5.985414	–0.049550	–1.135814
C	–6.335524	–0.444932	0.158667
C	–5.338446	–0.737963	1.096256
C	–3.991782	–0.634199	0.739737
C	–1.724990	0.586647	–2.968411
B	1.550966	–0.008888	0.000836
H	3.196401	1.479141	1.503759
H	3.019616	3.692040	2.587778
H	0.926707	5.034205	2.312903
H	–1.236561	5.306952	1.478824
H	–3.253524	4.466523	0.263386
H	–3.243207	2.183844	–0.661027
H	5.945081	–1.720995	1.116852
H	5.693303	0.880759	–2.283920
H	2.419585	2.107213	–1.624579
H	2.545570	0.961471	–2.955501
H	3.863692	2.125167	–2.675896
H	7.916755	0.201137	–1.376317
H	7.637992	–1.534840	–1.597789
H	8.014318	–0.908304	0.017165
H	4.249351	–1.983561	2.540550
H	2.833500	–2.554655	1.625013
H	2.761968	–1.009064	2.464155
H	–0.272983	–4.395409	–0.447822
H	–1.576809	–2.217977	3.007744
H	1.036656	0.227082	3.002236
H	–0.353035	–0.525421	3.825457
H	–0.601905	0.712468	2.581184
H	–2.331594	–4.585604	2.616474
H	–1.889684	–5.416536	1.099468
H	–3.127046	–4.144701	1.096170

H	1.604980	–3.775298	–1.592908
H	2.537714	–2.288590	–1.240547
H	1.085951	–2.198860	–2.234067
H	–4.381147	0.378030	–2.510050
H	–6.761244	0.173866	–1.870193
H	–7.387319	–0.529416	0.436748
H	–5.608784	–1.052290	2.105810
H	–3.214372	–0.878218	1.468467
H	–2.349845	1.485220	–2.939446
H	–2.157788	–0.191356	–3.606313
H	–0.702499	0.824985	–3.276949

Complex		**5**···F^-	
Atom	X	Y	Z
C	2.000115	–1.325205	4.383994
C	3.063533	–1.106875	3.533408
C	0.664550	–1.200921	3.911178
C	2.826547	–0.700147	2.199468
C	1.546052	–0.520135	1.688624
C	0.426618	–0.844234	2.532122
B	1.386285	0.174819	0.253896
C	–0.921846	–0.789790	2.048895
C	–0.435815	–1.398742	4.786921
C	–1.728875	–1.254101	4.326128
C	–1.958520	–0.968971	2.961191
B	–1.302629	–0.701886	0.502817
C	2.561821	–0.258619	–0.766224
C	0.838229	1.702827	0.175328
C	–1.960568	–2.070058	–0.075941
C	–2.205728	0.559358	0.054520
C	3.624817	0.633075	–1.072193
C	2.633937	–1.565640	–1.322006
C	4.643459	0.255303	–1.960853
C	3.745193	2.005734	–0.443934
C	3.660509	–1.903331	–2.218197
C	1.654586	–2.665822	–0.969202
C	4.667335	–1.000929	–2.574113
C	5.739644	–1.370764	–3.568205
C	0.387500	2.193359	–1.086585
C	0.718244	2.584724	1.281336
C	–0.231864	3.443062	–1.193994
C	0.593265	1.447560	–2.388356
C	0.108890	3.842250	1.128767
C	1.238019	2.279199	2.669413
C	–0.402314	4.284313	–0.091079
C	–1.124121	5.599715	–0.219066
C	–2.445047	–2.132815	–1.392228
C	–2.961896	–3.288808	–1.984449
C	–3.031739	–4.451447	–1.213856
S	–2.235043	–0.648000	–2.394808
C	–2.576757	–4.437219	0.107840
C	–2.053185	–3.264871	0.658560
C	–2.718274	0.655668	–1.248375
C	–2.539060	1.617561	0.915307
C	–3.472224	1.734229	–1.717940
C	–3.306288	2.702629	0.490911
C	–3.772556	2.764725	–0.825140
C	–3.598243	–0.719839	–3.574791
H	2.163824	–1.598280	5.429905
H	4.088912	–1.220208	3.893594
H	3.683544	–0.481038	1.556993
H	–0.238239	–1.659284	5.830130
H	–2.574896	–1.389222	5.003862

H	–2.992587	–0.926652	2.605668
H	5.450301	0.965351	–2.170111
H	3.041274	2.725017	–0.888483
H	3.529840	1.986608	0.633317
H	4.763740	2.396456	–0.583269
H	3.684298	–2.916633	–2.632905
H	0.715869	–2.584137	–1.537182
H	2.095846	–3.648183	–1.191838
H	1.379668	–2.636887	0.093601
H	6.679058	–0.837062	–3.363034
H	5.944125	–2.451297	–3.555058
H	5.435014	–1.109902	–4.595685
H	–0.596687	3.767585	–2.173727
H	0.503360	0.362829	–2.289730
H	–0.128036	1.793674	–3.143470
H	1.604190	1.641801	–2.783578
H	0.021250	4.491807	2.005756
H	1.271992	3.202288	3.265788
H	0.596902	1.560543	3.200311
H	2.243986	1.840893	2.653203
H	–2.206273	5.437159	–0.356322
H	–0.990502	6.220572	0.678029
H	–0.773458	6.171557	–1.091834
H	–3.312696	–3.305281	–3.015157
H	–3.443122	–5.361546	–1.652377
H	–2.624696	–5.347343	0.708664
H	–1.696606	–3.265450	1.690077
H	–2.159541	1.587869	1.937420
H	–3.830067	1.789702	–2.744700
H	–3.528338	3.515686	1.184235
H	–4.367268	3.613124	–1.166325
H	–4.553287	–0.833938	–3.051991
H	–3.558556	0.205157	–4.159531
H	–3.393592	–1.560719	–4.245569
F	0.002916	–0.615034	–0.347602

Complex		**6**···F^-	
Atom	X	Y	Z
Sb	1.700975	0.013223	–0.281481
F	–0.641014	–0.457776	–0.851740
C	0.681785	–0.135887	1.573910
C	–0.719951	–0.078673	1.583699
C	–1.332293	–0.281215	2.833671
C	–0.587963	–0.494211	3.996978
C	0.811043	–0.523029	3.947577
C	1.457715	–0.347628	2.720478
C	1.393446	1.592496	–1.676208
C	1.894127	–1.871862	–1.224821
C	1.929441	–3.016801	–0.419704
C	2.033742	–4.276318	–1.016893
C	2.100159	–4.387499	–2.409800
C	2.066223	–3.240036	–3.208961
C	1.963876	–1.975948	–2.618407
C	3.712407	0.384205	0.366168
C	4.727761	–0.547752	0.115864
C	6.035104	–0.289162	0.543339
C	6.328550	0.898780	1.220173
C	5.315607	1.831360	1.471049
C	4.008581	1.575634	1.045640
C	–1.627264	1.726316	–0.321058
C	–1.230739	2.881211	0.403384
C	–1.190503	4.140750	–0.221614
C	–1.549879	4.327001	–1.558076

C	–1.987070	3.199948	–2.260602
C	–2.026108	1.927409	–1.674482
C	–0.860044	2.868974	1.871893
C	–1.461927	5.680193	–2.218005
C	–2.503687	0.793110	–2.555754
C	–2.948042	–0.675727	0.279872
C	–4.196441	–0.075761	0.593193
C	–5.367843	–0.848381	0.667495
C	–5.364365	–2.228815	0.450206
C	–4.127270	–2.830326	0.197110
C	–2.936554	–2.090755	0.123920
C	–4.342223	1.403007	0.882935
C	–6.638155	–3.036076	0.488531
C	–1.659552	–2.876583	–0.085283
B	–1.556072	0.174630	0.211365
H	–2.424289	–0.271256	2.887350
H	–1.098911	–0.644046	4.950849
H	1.396412	–0.692851	4.852950
H	2.547883	–0.378016	2.666158
H	2.346986	1.754537	–2.191016
H	0.595294	1.292785	–2.359344
H	1.086456	2.479935	–1.111516
H	1.865570	–2.935350	0.667554
H	2.057951	–5.171070	–0.392652
H	2.177419	–5.371980	–2.874214
H	2.117402	–3.326550	–4.295649
H	1.934455	–1.085923	–3.249580
H	4.504459	–1.478062	–0.410944
H	6.824028	–1.017814	0.347750
H	7.348147	1.098822	1.554247
H	5.542856	2.758619	2.000210
H	3.224829	2.307971	1.253901
H	–0.875772	5.008456	0.367309
H	–2.309046	3.311915	–3.301399
H	–0.788032	3.899194	2.248632
H	–1.601000	2.334706	2.481800
H	0.104632	2.375423	2.058625
H	–2.278497	5.829159	–2.939975
H	–1.502100	6.491296	–1.476858
H	–0.515533	5.789802	–2.773605
H	–3.078005	1.184840	–3.407752
H	–1.656865	0.214013	–2.954661
H	–3.130071	0.082719	–1.999931
H	–6.312020	–0.351305	0.913884
H	–4.080490	–3.917330	0.070933
H	–5.330835	1.608672	1.318735
H	–3.577375	1.762475	1.584902
H	–4.235696	2.011582	–0.026967
H	–7.394443	–2.562110	1.130975
H	–7.078973	–3.132031	–0.517998
H	–6.456982	–4.055339	0.860411
H	–0.873348	–2.558081	0.613367
H	–1.843884	–3.950195	0.065688
H	–1.243036	–2.736838	–1.092273

Complex		**7**···F⁻	
Atom	X	Y	Z
Sb	0.219126	0.021719	1.890872
Pd	–0.007602	0.001944	–0.739627
Cl	–0.071919	–0.178412	–3.217915
P	2.302748	–0.198654	–0.530765
P	–1.057551	2.078698	–0.385162
P	–1.398869	–1.825012	–0.318668

F	0.446585	0.092038	3.942836
C	1.917607	–1.313596	1.954128
C	2.683068	–1.413278	0.784593
C	3.713436	–2.359655	0.717960
C	3.955539	–3.201005	1.809027
C	3.206215	–3.071441	2.981486
C	2.188096	–2.113009	3.063646
C	3.293024	–0.733608	–1.955802
C	4.390161	–0.001724	–2.431414
C	5.102016	–0.456310	–3.546395
C	4.728215	–1.643714	–4.183330
C	3.631443	–2.375409	–3.709825
C	2.907344	–1.915701	–2.610342
C	3.151356	1.295652	0.107262
C	2.750976	2.543967	–0.394748
C	3.311191	3.719808	0.102140
C	4.266091	3.661722	1.122887
C	4.668599	2.422833	1.630252
C	4.118958	1.242521	1.122321
C	0.372686	2.179950	2.017288
C	–0.214530	2.946034	0.998053
C	–0.094157	4.342997	1.048579
C	0.633425	4.951884	2.073490
C	1.227270	4.175961	3.072029
C	1.079807	2.784716	3.057765
C	–1.141755	3.328025	–1.711475
C	–0.185962	3.266121	–2.737175
C	–0.165247	4.240970	–3.738109
C	–1.108158	5.273819	–3.729690
C	–2.077216	5.328311	–2.720482
C	–2.096082	4.359981	–1.714529
C	–2.786754	1.932701	0.187327
C	–3.783370	1.638230	–0.760677
C	–5.078379	1.322182	–0.351961
C	–5.397205	1.291495	1.011159
C	–4.417323	1.601503	1.957372
C	–3.120397	1.925179	1.550149
C	–1.679126	–0.920418	2.303316
C	–2.306459	–1.620344	1.261426
C	–3.587065	–2.151464	1.477212
C	–4.219930	–1.983161	2.711139
C	–3.568345	–1.316655	3.752517
C	–2.288285	–0.790135	3.553244
C	–2.681861	–2.308510	–1.517942
C	–3.208166	–1.318228	–2.358500
C	–4.248873	–1.622832	–3.238658
C	–4.757882	–2.924481	–3.295543
C	–4.221199	–3.922853	–2.473487
C	–3.185850	–3.618380	–1.586741
C	–0.435296	–3.356653	–0.081941
C	0.159939	–3.928486	–1.222353
C	1.037996	–5.003677	–1.095178
C	1.346027	–5.513061	0.173177
C	0.756574	–4.949936	1.307204
C	–0.135613	–3.880448	1.183263
H	4.323938	–2.436512	–0.183093
H	4.741861	–3.954947	1.744212
H	3.400471	–3.728045	3.831322
H	1.594968	–2.004213	3.970957
H	4.690094	0.918812	–1.928573
H	5.955193	0.117221	–3.913253
H	5.288033	–1.998067	–5.050646

H	3.333264	–3.300480	–4.206477
H	2.041502	–2.471585	–2.248430
H	1.974194	2.588825	–1.159395
H	2.981304	4.683450	–0.288230
H	4.685836	4.582517	1.531318
H	5.408991	2.373044	2.430743
H	4.431458	0.280027	1.529040
H	–0.550010	4.955177	0.269479
H	0.744569	6.037503	2.084529
H	1.812724	4.649633	3.861877
H	1.518819	2.170273	3.842295
H	0.511262	2.426904	–2.764211
H	0.580861	4.186056	–4.532839
H	–1.095394	6.032291	–4.514479
H	–2.818434	6.129515	–2.715240
H	–2.852002	4.404313	–0.928705
H	–3.542387	1.660164	–1.824729
H	–5.838961	1.090747	–1.099743
H	–6.406341	1.028734	1.332440
H	–4.657681	1.584434	3.021308
H	–2.365637	2.167414	2.299435
H	–4.092236	–2.692110	0.675876
H	–5.225384	–2.380598	2.859540
H	–4.062237	–1.189119	4.717372
H	–1.769837	–0.261391	4.351917
H	–2.774546	–0.320181	–2.329034
H	–4.655241	–0.845515	–3.888209
H	–5.567511	–3.165111	–3.986933
H	–4.612093	–4.940810	–2.521095
H	–2.768327	–4.397175	–0.946347
H	–0.065180	–3.518934	–2.210001
H	1.493436	–5.438616	–1.986750
H	2.046148	–6.343819	0.274375
H	0.994637	–5.338809	2.298385
H	–0.590860	–3.449219	2.075650

Complex		**8**···F^-	
Atom	X	Y	Z
Sb	–0.000029	–1.210542	1.310819
Pd	–0.000151	0.938256	–0.186098
Cl	–0.000259	2.778776	–1.793733
P	–2.269996	0.722910	–0.041472
P	2.269735	0.723395	–0.041278
F	–0.000047	–2.861121	2.583153
C	–1.930143	–0.838927	2.246532
C	–2.805185	0.012319	1.555791
C	–4.078819	0.277358	2.083734
C	–4.458268	–0.286108	3.304108
C	–3.579911	–1.131461	3.989625
C	–2.319981	–1.423876	3.454098
C	–3.272699	2.226392	–0.229088
C	–2.831228	3.390222	0.421434
C	–3.587795	4.559889	0.347874
C	–4.780578	4.577903	–0.385881
C	–5.216867	3.422908	–1.042054
C	–4.466754	2.245458	–0.963419
C	–2.855909	–0.442907	–1.309153
C	–2.604406	–0.122308	–2.655501
C	–2.911620	–1.040271	–3.658209
C	–3.451877	–2.289202	–3.326042
C	–3.695480	–2.611532	–1.988983
C	–3.401454	–1.690603	–0.979064
C	1.930036	–0.838753	2.246536

C	2.804923	0.012795	1.555980
C	4.078476	0.278031	2.084013
C	4.458023	–0.285580	3.304291
C	3.579842	–1.131278	3.989607
C	2.319977	–1.423842	3.454005
C	3.271988	2.227225	–0.228574
C	2.830182	3.390745	0.422286
C	3.586278	4.560720	0.348861
C	4.778928	4.579365	–0.385102
C	5.215556	3.424682	–1.041590
C	4.465914	2.246919	–0.963088
C	2.856264	–0.442118	–1.308953
C	2.604717	–0.121564	–2.655303
C	2.912479	–1.039303	–3.658047
C	3.453329	–2.287984	–3.325910
C	3.696972	–2.610278	–1.988849
C	3.402398	–1.689564	–0.978894
C	0.000423	–2.653015	–0.294043
C	0.000514	–2.153409	–1.599475
C	0.000943	–3.030189	–2.685054
C	0.001269	–4.410946	–2.464513
C	0.001162	–4.910317	–1.157365
C	0.000737	–4.033551	–0.065872
H	–4.767174	0.928945	1.542920
H	–5.442553	–0.064179	3.719610
H	–3.874258	–1.565346	4.947078
H	–1.637590	–2.099685	3.966988
H	–1.889523	3.374403	0.973853
H	–3.242788	5.462541	0.854866
H	–5.367428	5.495818	–0.449448
H	–6.144916	3.435596	–1.616091
H	–4.808392	1.343085	–1.472466
H	–2.145929	0.837620	–2.905650
H	–2.713026	–0.789420	–4.701541
H	–3.674094	–3.013277	–4.111526
H	–4.110137	–3.586116	–1.726382
H	–3.584231	–1.949203	0.064609
H	4.766695	0.929879	1.543338
H	5.442241	–0.063494	3.719868
H	3.874270	–1.565315	4.946967
H	1.637706	–2.099880	3.966755
H	1.888583	3.374446	0.974873
H	3.241007	5.463122	0.856117
H	5.365401	5.497527	–0.448579
H	6.143506	3.437848	–1.615776
H	4.807835	1.344792	–1.472378
H	2.145799	0.838160	–2.905429
H	2.713845	–0.788484	–4.701378
H	3.675979	–3.011901	–4.111418
H	4.112090	–3.584673	–1.726276
H	3.585195	–1.948151	0.064778
H	0.000227	–1.073106	–1.767221
H	0.001023	–2.632613	–3.700629
H	0.001608	–5.099499	–3.311688
H	0.001404	–5.988522	–0.983888
H	0.000644	–4.411016	0.955780

Complex		**9**···F^-	
Atom	X	Y	Z
Pt	1.669220	0.000042	–0.263783
Sb	–0.764757	–0.000057	–1.670738
Cl	2.132865	0.000090	–2.683287
Cl	–5.744792	–0.000187	–2.548328

Cl	–7.474543	–0.000120	0.115063
Cl	–6.010598	–0.000018	2.910985
Cl	–2.859397	0.000020	3.026867
P	1.511871	–2.318799	–0.126812
F	–0.796850	–0.000070	–3.682713
O	–2.828205	–0.000128	–2.039442
O	–1.579986	–0.000052	0.304815
C	–3.582071	–0.000112	–0.936925
C	–4.980692	–0.000133	–0.987415
C	–5.741269	–0.000105	0.199162
C	–5.088865	–0.000059	1.440038
C	–3.678684	–0.000043	1.496936
C	–2.915835	–0.000068	0.320090
C	–0.657305	–2.162516	–1.897166
C	–1.659793	–2.706945	–2.706228
C	–1.640332	–4.072779	–3.001555
C	–0.616869	–4.885703	–2.504504
C	0.369306	–4.339570	–1.685264
C	0.351308	–2.970445	–1.365376
C	3.098516	–3.176012	–0.331470
C	4.145172	–2.505330	–0.985960
C	5.373208	–3.143074	–1.172905
C	5.564533	–4.448078	–0.708111
C	4.525806	–5.117653	–0.051709
C	3.296382	–4.485743	0.140790
C	0.806689	–2.913820	1.437791
C	1.634032	–3.134390	2.550647
C	1.067850	–3.442425	3.786662
C	–0.322118	–3.525013	3.923260
C	–1.146736	–3.303064	2.816963
C	–0.586990	–2.997126	1.575573
C	1.712195	0.000015	1.767201
C	3.011414	0.000042	2.296752
C	3.194059	0.000020	3.686625
C	2.087653	–0.000041	4.540366
C	0.797446	–0.000083	4.000269
C	0.607904	–0.000054	2.616830
P	1.511690	2.318862	–0.126818
C	–0.657464	2.162409	–1.897179
C	–1.659982	2.706761	–2.706256
C	–1.640604	4.072590	–3.001613
C	–0.617191	4.885586	–2.504578
C	0.369013	4.339530	–1.685319
C	0.351095	2.970413	–1.365399
C	3.098265	3.176212	–0.331477
C	4.144982	2.505627	–0.985965
C	5.372964	3.143475	–1.172901
C	5.564171	4.448498	–0.708112
C	4.525376	5.117988	–0.051731
C	3.296007	4.485969	0.140763
C	0.806454	2.913845	1.437778
C	1.633769	3.134432	2.550653
C	1.067555	3.442446	3.786658
C	–0.322418	3.524989	3.923232
C	–1.147010	3.303013	2.816921
C	–0.587230	2.997100	1.575539
H	–2.444337	–2.067260	–3.107546
H	–2.422031	–4.496084	–3.634439
H	–0.589736	–5.948326	–2.749479
H	1.158940	–4.978044	–1.287270
H	3.990597	–1.490072	–1.354478
H	6.183500	–2.616635	–1.679581

H	6.526222	–4.943301	–0.851978
H	4.673967	–6.133728	0.317036
H	2.498357	–5.004677	0.673113
H	2.715778	–3.041330	2.457695
H	1.715040	–3.603823	4.649886
H	–0.762049	–3.756726	4.894679
H	–2.231344	–3.356088	2.919581
H	–1.236992	–2.802347	0.722673
H	3.885166	0.000067	1.638801
H	4.206904	0.000044	4.095340
H	2.231751	–0.000064	5.622466
H	–0.072361	–0.000139	4.660363
H	–0.393939	–0.000092	2.195910
H	–2.444484	2.067018	–3.107565
H	–2.422328	4.495834	–3.634507
H	–0.590118	5.948204	–2.749579
H	1.158608	4.978060	–1.287337
H	3.990493	1.490361	–1.354495
H	6.183306	2.617103	–1.679566
H	6.525819	4.943804	–0.851971
H	4.673439	6.134083	0.316997
H	2.497929	5.004841	0.673068
H	2.715519	3.041402	2.457722
H	1.714724	3.603859	4.649894
H	–0.762374	3.756685	4.894644
H	–2.231621	3.356000	2.919520
H	–1.237210	2.802300	0.722627

Complex		**10**···F⁻	
Atom	X	Y	Z
Sb	–0.606538	0.083121	–0.353181
F	–0.436270	0.609774	–2.371702
C	1.553800	–0.013554	–0.446459
C	2.182010	–1.271408	–0.332252
C	1.468577	–2.508310	–0.272911
C	2.119007	–3.711508	–0.139069
C	3.539494	–3.763292	–0.059173
C	4.271377	–2.602512	–0.120852
C	3.631142	–1.331954	–0.255981
C	4.371442	–0.145462	–0.303922
C	3.752616	1.103444	–0.434071
C	4.520848	2.307724	–0.481845
C	3.912415	3.532688	–0.607161
C	2.494145	3.613749	–0.699580
C	1.720884	2.478071	–0.656288
C	2.303747	1.180448	–0.514217
C	–1.888154	–1.506131	–1.023641
C	–2.175280	–2.577048	–0.167676
C	–3.038503	–3.593629	–0.588376
C	–3.623752	–3.535454	–1.857158
C	–3.338397	–2.463143	–2.708560
C	–2.466731	–1.448827	–2.297927
C	–0.710716	–0.411152	1.782773
C	–1.970877	–0.486732	2.396898
C	–2.081375	–0.745845	3.765885
C	–0.927254	–0.926328	4.537727
C	0.331734	–0.843702	3.936163
C	0.437921	–0.586060	2.563289
C	–1.651493	1.940299	–0.119860
C	–1.608543	2.605473	1.111635
C	–2.298520	3.811107	1.273885
C	–3.044588	4.339566	0.215433
C	–3.091674	3.668067	–1.011046

C	–2.387759	2.472025	–1.185827
H	0.381080	–2.506908	–0.351221
H	1.541507	–4.636487	–0.098923
H	4.040459	–4.726777	0.046442
H	5.362068	–2.626845	–0.066492
H	5.461217	–0.194842	–0.234975
H	5.608335	2.228259	–0.416597
H	4.510177	4.444856	–0.642060
H	2.016125	4.588390	–0.811516
H	0.638881	2.569807	–0.747809
H	–1.729938	–2.626893	0.827254
H	–3.253492	–4.430039	0.079094
H	–4.300136	–4.327559	–2.183234
H	–3.791836	–2.415631	–3.700476
H	–2.221551	–0.622413	–2.963489
H	–2.880777	–0.340189	1.808311
H	–3.067296	–0.805365	4.231362
H	–1.011052	–1.127899	5.607291
H	1.235013	–0.978099	4.534856
H	1.427256	–0.519292	2.106991
H	–1.038226	2.191095	1.944247
H	–2.254114	4.335208	2.230337
H	–3.588221	5.276998	0.345717
H	–3.674072	4.078244	–1.838262
H	–2.396814	1.961602	–2.148321

Complex		**$4CH_3{\cdots}F^-$**	
Atom	X	Y	Z
Te	1.764242	0.294919	–0.254142
F	–0.555287	–0.194358	–1.194347
C	–0.754832	3.920554	–0.559322
C	–0.964570	1.653134	0.388458
C	–0.031800	1.337435	2.787427
C	4.186036	–0.771544	1.308726
C	1.326245	–1.774087	–0.025177
C	–0.835873	–1.113346	1.169671
C	0.235805	–2.038421	0.875451
C	3.843886	0.100888	0.268848
C	–0.394233	2.179243	1.584322
C	6.145033	0.820742	0.095970
C	4.814741	0.910946	–0.328634
B	–1.336987	0.069545	0.096602
C	–1.116628	2.572833	–0.694063
C	0.244406	–3.352026	1.467701
C	0.978353	–4.405307	0.815051
C	–0.228410	4.436251	0.627638
C	6.496965	–0.063159	1.120828
C	–0.051646	3.538369	1.682638
C	–1.662611	–1.439878	2.250964
C	–0.514565	–3.562869	2.666847
C	5.516592	–0.854623	1.729172
C	–1.660689	2.174059	–2.051219
C	1.928764	–4.108049	–0.157233
C	–1.453310	–2.608730	3.046175
C	0.119658	5.896558	0.767633
C	2.181594	–2.747645	–0.521848
C	–3.221102	–1.524245	–0.899559
C	2.038110	0.564696	–2.369722
C	–2.193422	–2.616325	–1.122026
C	–2.917930	–0.261418	–0.302254
C	–4.529877	–1.851500	–1.286644
C	–5.607803	–0.984323	–1.091364
C	–5.326044	0.236923	–0.480231

C	–4.025612	0.611255	–0.094627
C	–3.937760	1.991246	0.528091
C	–7.003422	–1.346888	–1.533908
C	3.314811	–2.481314	–1.476544
C	2.720430	–5.196939	–0.841335
C	0.603287	–5.856417	1.041400
C	–0.185604	–4.702507	3.611823
C	–2.293782	–2.810309	4.286046
C	–2.793747	–0.534314	2.669644
H	–0.894421	4.590431	–1.414402
H	–0.905946	0.901816	3.286021
H	0.506722	1.949715	3.524380
H	0.614560	0.488500	2.515712
H	3.426839	–1.402016	1.775638
H	6.905697	1.444018	–0.377400
H	4.554378	1.610207	–1.125650
H	7.535671	–0.133517	1.447641
H	0.391618	3.900397	2.615824
H	5.787054	–1.543330	2.531548
H	–2.076295	3.053341	–2.565046
H	–2.437047	1.403575	–1.977186
H	–0.869470	1.756054	–2.691102
H	0.911938	6.050029	1.514569
H	–0.755201	6.483299	1.094480
H	0.456275	6.322598	–0.188799
H	3.107177	0.603505	–2.600670
H	1.544375	1.510197	–2.615244
H	1.542691	–0.274742	–2.864382
H	–1.989119	–3.156645	–0.184525
H	–1.233336	–2.228575	–1.476318
H	–2.573881	–3.348737	–1.849246
H	–4.710714	–2.828961	–1.746766
H	–6.147936	0.935559	–0.291061
H	–4.915228	2.271778	0.947339
H	–3.670287	2.752008	–0.221692
H	–3.183822	2.074128	1.317848
H	–7.218203	–2.411468	–1.356914
H	–7.139292	–1.166122	–2.613396
H	–7.758763	–0.749110	–1.003773
H	4.279900	–2.788628	–1.045252
H	3.177666	–3.058865	–2.403464
H	3.407208	–1.430124	–1.754264
H	2.632209	–6.158955	–0.326802
H	2.392466	–5.342173	–1.884923
H	3.789121	–4.942737	–0.880759
H	–0.380435	–5.946992	1.511145
H	0.548992	–6.374388	0.073519
H	1.327061	–6.409709	1.660717
H	–0.145885	–4.322251	4.642663
H	–0.924423	–5.520167	3.601594
H	0.795758	–5.135663	3.393886
H	–3.354261	–2.607291	4.078576
H	–2.224999	–3.831451	4.675204
H	–1.995892	–2.122258	5.095971
H	–3.777956	–0.974468	2.439758
H	–2.770540	–0.354082	3.755781
H	–2.742538	0.433015	2.169874

Complex		**4CN**···F^-	
Atom	X	Y	Z
Te	1.618915	0.554988	–0.417224
F	–0.800503	–0.251177	–1.189550
C	–0.180549	3.608935	–0.652385

C	–1.053814	1.581938	0.425070
C	–0.493274	1.256826	2.926406
C	4.075663	–0.372907	1.180941
C	1.214583	–1.551303	–0.047461
C	–1.002006	–1.134319	1.119036
C	0.163003	–1.949498	0.847496
C	3.704324	0.320899	0.023445
C	–0.431198	2.021354	1.626159
C	6.004103	0.895047	–0.410906
C	4.655006	0.971283	–0.768356
B	–1.547918	0.049868	0.091708
C	–0.982146	2.459769	–0.698018
C	0.282976	–3.263032	1.443698
C	1.190678	–4.217308	0.886095
C	0.533755	3.973512	0.494835
C	6.390856	0.180221	0.727521
C	0.346627	3.188719	1.637276
C	–1.830833	–1.556441	2.166668
C	–0.531705	–3.587624	2.569497
C	5.428598	–0.449225	1.523527
C	–1.713089	2.203278	–1.999467
C	2.064490	–3.843417	–0.134268
C	–1.553579	–2.712311	2.950010
C	1.411869	5.196395	0.516719
C	2.128989	–2.476008	–0.542014
C	–3.519779	–1.480115	–0.784099
C	1.782983	0.535190	–2.558291
C	–2.549384	–2.613887	–1.047638
C	–3.135469	–0.236342	–0.201294
C	–4.858288	–1.731068	–1.119977
C	–5.869872	–0.795797	–0.890139
C	–5.499898	0.409743	–0.286904
C	–4.173611	0.701903	0.061952
C	–3.951901	2.032248	0.744869
C	–7.297647	–1.068226	–1.287181
C	3.146983	–2.159452	–1.492698
N	3.968952	–2.004354	–2.303713
C	2.920371	–4.805326	–0.743815
N	3.624142	–5.583802	–1.249598
C	1.197767	–5.597020	1.251273
N	1.245318	–6.746030	1.438612
C	–0.319345	–4.731916	3.390974
N	–0.187084	–5.604709	4.152553
C	–2.348471	–3.011470	4.095851
N	–2.994556	–3.253083	5.034707
C	–3.009043	–0.843334	2.559254
N	–3.937945	–0.346263	3.059729
H	–0.110029	4.236344	–1.546334
H	–1.522510	0.992793	3.201567
H	–0.078113	1.864716	3.741262
H	0.089811	0.324088	2.891849
H	3.332653	–0.866320	1.810339
H	6.753242	1.391182	–1.029636
H	4.366039	1.524937	–1.663033
H	7.446020	0.116182	0.996892
H	0.850101	3.475103	2.565007
H	5.727584	–1.002768	2.414768
H	–2.087218	3.155040	–2.404904
H	–2.557324	1.517046	–1.873819
H	–1.049967	1.763266	–2.758763
H	0.828490	6.092764	0.784353
H	1.861936	5.381732	–0.468638

H	2.217465	5.095941	1.257283
H	2.788579	0.220138	–2.845561
H	1.569983	1.565188	–2.863286
H	1.011281	–0.149816	–2.919734
H	–2.353136	–3.189366	–0.127938
H	–1.586484	–2.264943	–1.434121
H	–2.978261	–3.320123	–1.772019
H	–5.115906	–2.694018	–1.571744
H	–6.274388	1.150384	–0.065293
H	–4.915129	2.444166	1.077436
H	–3.489016	2.768488	0.071618
H	–3.296266	1.948594	1.619196
H	–7.513738	–2.146042	–1.293096
H	–7.502741	–0.687465	–2.301644
H	–8.004649	–0.573264	–0.605921

Complex		**$4NO_2\cdots F^-$**	
Atom	X	Y	Z
Te	1.787356	0.528667	–0.174215
F	–0.555245	–0.263735	–1.114566
C	–0.684741	3.849616	–0.622847
C	–0.996584	1.630057	0.385861
C	–0.117424	1.324990	2.800691
C	4.220948	–0.439586	1.349599
C	1.331866	–1.592133	0.067762
C	–0.893896	–1.078963	1.217645
C	0.282921	–1.911734	1.002304
C	3.878938	0.192151	0.145614
C	–0.424032	2.157525	1.580010
C	6.208166	0.426430	–0.424905
C	4.862651	0.640288	–0.740169
B	–1.389097	0.061689	0.099467
C	–1.114232	2.519145	–0.725046
C	0.409582	–3.166175	1.688152
C	1.257858	–4.178289	1.149776
C	–0.133587	4.367431	0.551237
C	6.559012	–0.225636	0.760803
C	–0.015164	3.497609	1.639696
C	–1.754188	–1.519280	2.220173
C	–0.348589	–3.367776	2.879711
C	5.567078	–0.655607	1.648699
C	–1.687033	2.110744	–2.066323
C	2.189291	–3.872453	0.183282
C	–1.462241	–2.579398	3.098347
C	0.298001	5.807085	0.649262
C	2.248768	–2.552700	–0.318306
C	–3.230122	–1.592915	–0.839154
C	1.848499	1.004019	–2.255910
C	–2.191533	–2.680227	–1.031980
C	–2.947328	–0.309243	–0.277754
C	–4.534793	–1.940754	–1.210918
C	–5.617224	–1.075653	–1.030394
C	–5.348172	0.168688	–0.457887
C	–4.055090	0.568140	–0.086461
C	–3.959419	1.958085	0.501042
C	–7.010175	–1.463446	–1.452089
N	3.275983	–2.269896	–1.354848
O	2.899732	–1.640556	–2.344015
O	4.407908	–2.711649	–1.171763
N	3.075229	–4.919710	–0.412405
O	2.701664	–5.385842	–1.486478
O	4.099964	–5.187455	0.195485
N	0.933247	–5.611096	1.408617

O	–0.251058	–5.870950	1.624237
O	1.838376	–6.435654	1.323995
N	0.177112	–4.219869	3.955523
O	–0.470474	–4.294733	5.002311
O	1.280446	–4.755166	3.783769
N	–3.085879	–0.886904	2.463976
O	–4.062522	–1.636085	2.392860
O	–3.109954	0.288249	2.822648
N	–2.382903	–2.818311	4.248194
O	–3.112831	–3.797824	4.176502
O	–2.377055	–1.962030	5.130106
H	–0.789435	4.501929	–1.495190
H	–1.014695	0.869813	3.234250
H	0.361023	1.942794	3.572209
H	0.585622	0.504383	2.574720
H	3.454217	–0.780069	2.048837
H	6.981243	0.767959	–1.114468
H	4.607228	1.149075	–1.669379
H	7.610292	–0.397334	0.995818
H	0.436003	3.866497	2.565148
H	5.838572	–1.161194	2.576211
H	–2.163743	2.975738	–2.548955
H	–2.421797	1.303017	–1.982844
H	–0.899357	1.753354	–2.745898
H	–0.522354	6.435979	1.032992
H	0.584955	6.207010	–0.333383
H	1.147021	5.924663	1.337637
H	2.826451	0.740884	–2.663203
H	1.654903	2.082375	–2.292276
H	1.042696	0.432287	–2.719718
H	–2.036634	–3.248754	–0.100124
H	–1.220807	–2.293123	–1.354991
H	–2.539707	–3.404328	–1.781402
H	–4.711462	–2.930836	–1.642242
H	–6.176467	0.863557	–0.289575
H	–4.941337	2.264472	0.888226
H	–3.660617	2.694450	–0.261018
H	–3.226656	2.030739	1.309946
H	–7.184828	–2.540664	–1.317396
H	–7.173313	–1.239132	–2.519420
H	–7.769812	–0.910964	–0.881409

Complex		**4OH**···F⁻	
Atom	X	Y	Z
Te	1.502089	0.288205	–0.767480
F	–0.895455	–0.333732	–1.270979
C	–0.175813	3.561006	–0.393938
H	–0.178411	4.297976	–1.203704
C	–0.975434	1.410975	0.491370
C	–0.284403	0.825404	2.913955
H	–1.297060	0.468810	3.143980
H	0.087038	1.388906	3.781994
H	0.347994	–0.067078	2.797743
C	3.967219	0.255608	1.063542
H	3.242952	–0.150396	1.773425
C	1.310632	–1.677907	0.011657
C	–1.021436	–1.334476	1.033750
C	0.210985	–2.075000	0.866683
C	3.601223	0.483284	–0.273062
C	–0.259486	1.707224	1.684546
C	5.832632	1.285481	–0.757135
H	6.558464	1.686215	–1.466429
C	4.528452	1.012185	–1.183069

H	4.250338	1.201094	–2.221061
B	–1.546153	–0.079535	0.089881
C	–0.970806	2.414117	–0.521486
C	0.409012	–3.335316	1.581003
C	1.531014	–4.181832	1.311442
C	0.634258	3.782910	0.725358
C	6.203387	1.045292	0.569379
H	7.221980	1.259175	0.896540
C	0.537811	2.860855	1.771144
H	1.105664	3.038922	2.689729
C	–1.897835	–1.807545	2.009698
C	–0.551941	–3.726827	2.551323
C	5.271924	0.530925	1.478582
H	5.560647	0.343994	2.514071
C	–1.747084	2.281947	–1.814972
H	–2.022225	3.278008	–2.191980
H	–2.656962	1.683351	–1.695292
H	–1.143877	1.788975	–2.593219
C	2.494344	–3.790270	0.396276
C	–1.664813	–2.959022	2.786805
C	1.563247	4.966847	0.802848
H	1.727936	5.281461	1.843274
H	1.170649	5.823623	0.236482
H	2.549341	4.718314	0.376675
C	2.399656	–2.524406	–0.212623
C	–3.654318	–1.255879	–1.021724
C	1.777912	–0.211862	–2.843816
H	2.479221	–1.044890	–2.933913
H	2.134865	0.688173	–3.355647
H	0.776189	–0.484110	–3.190138
C	–2.757034	–2.363199	–1.531164
H	–2.016698	–2.666320	–0.780125
H	–2.190094	–2.040077	–2.416279
H	–3.358881	–3.239203	–1.812528
C	–3.169083	–0.178349	–0.216915
C	–5.006538	–1.333726	–1.375934
H	–5.341376	–2.175956	–1.990152
C	–5.945729	–0.383928	–0.956155
C	–5.488353	0.644477	–0.132472
H	–6.203546	1.382141	0.244237
C	–4.137993	0.762132	0.243648
C	–3.807885	1.914762	1.170247
H	–4.726287	2.283309	1.649149
H	–3.350501	2.753380	0.624725
H	–3.095460	1.634614	1.956119
C	–7.391586	–0.479147	–1.371410
H	–7.771794	–1.506604	–1.267845
H	–7.517724	–0.195262	–2.429032
H	–8.025073	0.187197	–0.769703
O	3.464367	–2.269884	–1.056532
H	3.799460	–1.352154	–0.904474
O	3.564498	–4.603849	0.130544
H	4.146496	–4.079809	–0.461949
O	1.726944	–5.390893	1.910416
H	0.974640	–5.544536	2.533766
O	–0.379942	–4.895406	3.279564
H	–1.210937	–5.084565	3.759878
O	–2.568733	–3.379835	3.732309
H	–3.344232	–2.784491	3.644096
O	–3.089189	–1.208059	2.358903
H	–3.409933	–0.695889	1.567143

Complex **$5CH_3$,H···F⁻**

Atom	X	Y	Z
C	1.875001	–1.588911	4.384443
C	2.959651	–1.336379	3.571232
C	0.552167	–1.461888	3.878248
C	2.755435	–0.891152	2.245226
C	1.489203	–0.682274	1.709835
C	0.345557	–1.032319	2.513693
B	1.386298	0.038110	0.279826
C	–0.994464	–0.988566	2.000391
C	–0.565446	–1.759526	4.702435
C	–1.849253	–1.662099	4.201808
C	–2.047830	–1.298404	2.855508
B	–1.349927	–0.742172	0.462101
C	2.552242	–0.443565	–0.740884
C	0.976136	1.611935	0.227116
C	–2.131294	–2.068939	–0.158888
C	–2.155454	0.665363	0.101445
C	3.671919	0.385958	–1.022181
C	2.543545	–1.733912	–1.340350
C	4.665949	–0.030148	–1.922687
C	3.884644	1.733249	–0.364164
C	3.546549	–2.109455	–2.247822
C	1.502789	–2.782461	–1.013718
C	4.610852	–1.264429	–2.575720
C	5.658345	–1.671525	–3.581606
C	0.563581	2.162630	–1.021666
C	0.982937	2.493566	1.340741
C	0.083379	3.474554	–1.107233
C	0.678475	1.414754	–2.332347
C	0.510171	3.810198	1.211424
C	1.532176	2.128668	2.703174
C	0.021927	4.315888	0.006134
C	–0.558841	5.701958	–0.089644
C	–2.978624	–1.860630	–1.263806
C	–4.058607	–2.678911	–1.631217
C	–4.150790	–3.921282	–0.961852
S	–2.258253	–0.552839	–2.280944
C	–3.204075	–4.271615	0.021189
C	–2.200030	–3.357424	0.425738
C	–2.533352	0.903668	–1.240170
C	–2.437463	1.736026	0.988645
C	–2.972958	2.123960	–1.764204
C	–3.141121	2.887088	0.542790
C	–3.354489	3.110606	–0.828324
C	–3.163726	–0.465670	–3.841203
F	–0.010058	–0.650020	–0.340766
C	–2.970484	2.481516	–3.229856
C	–3.919654	4.406139	–1.360735
C	–3.582054	3.905305	1.568974
C	–1.984014	1.761689	2.427796
C	–1.149363	–3.855361	1.391444
C	–3.292171	–5.628376	0.681564
C	–5.251943	–4.888689	–1.330954
C	–5.184004	–2.244868	–2.542555
H	2.011740	–1.908187	5.421175
H	3.975759	–1.461829	3.953244
H	3.628824	–0.664858	1.627736
H	–0.388108	–2.074160	5.734337
H	–2.707503	–1.892595	4.837432
H	–3.069259	–1.273864	2.464861
H	5.516530	0.633366	–2.110440
H	3.236098	2.509413	–0.796957

H	3.663627	1.707965	0.711193
H	4.929294	2.052879	–0.491433
H	3.504262	–3.108878	–2.693651
H	0.548121	–2.604889	–1.529835
H	1.865105	–3.779379	–1.303537
H	1.276706	–2.792940	0.060462
H	6.621252	–1.180307	–3.379612
H	5.816637	–2.759985	–3.578959
H	5.356964	–1.390000	–4.604584
H	–0.253522	3.851018	–2.078284
H	0.388099	0.362794	–2.259898
H	0.060298	1.899274	–3.102029
H	1.720949	1.425172	–2.690165
H	0.517009	4.458421	2.093665
H	1.510170	3.008987	3.361427
H	0.965996	1.325429	3.193230
H	2.570999	1.772620	2.644472
H	–1.646376	5.683698	0.088803
H	–0.117688	6.377724	0.657444
H	–0.403977	6.136313	–1.088289
H	–4.107254	0.077193	–3.773071
H	–2.483308	0.001055	–4.558990
H	–3.321828	–1.509332	–4.131793
H	–2.257718	1.880211	–3.801255
H	–3.959899	2.397603	–3.705987
H	–2.652744	3.525929	–3.346993
H	–3.128689	5.013571	–1.831277
H	–4.683473	4.227359	–2.131509
H	–4.371628	5.022161	–0.577985
H	–4.426035	4.508406	1.216767
H	–3.893141	3.417108	2.501583
H	–2.765851	4.600625	1.829384
H	–2.758140	1.386677	3.117853
H	–1.097613	1.148772	2.577285
H	–1.735124	2.787392	2.725676
H	–1.524064	–3.960079	2.421041
H	–0.798018	–4.846231	1.065019
H	–0.287259	–3.187272	1.426082
H	–4.334608	–5.953276	0.792173
H	–2.773377	–6.402023	0.089330
H	–2.838461	–5.624935	1.679014
H	–5.658095	–4.688411	–2.328688
H	–4.881352	–5.922057	–1.330202
H	–6.091340	–4.845774	–0.615967
H	–5.117926	–2.653459	–3.563256
H	–6.138231	–2.590974	–2.124080
H	–5.252605	–1.155314	–2.607050

Complex		**5H**,$\mathbf{CH_3}$···$\mathbf{F^-}$	
Atom	X	Y	Z
C	1.644632	–2.064546	4.323265
C	2.784520	–1.895939	3.547168
C	0.430532	–1.406756	3.924590
C	2.736878	–1.098181	2.360504
C	1.517532	–0.719448	1.791447
C	0.311687	–0.942696	2.564529
B	1.478469	0.011619	0.341807
C	–1.008230	–0.672212	2.053699
C	–0.657163	–1.185223	4.836851
C	–1.909355	–0.840156	4.338239
C	–2.097697	–0.686468	2.930742
B	–1.300866	–0.534124	0.489990
C	2.526140	–0.580082	–0.755158

C	1.137101	1.598005	0.256578
C	–2.088676	–1.817569	–0.123993
C	–1.994353	0.844600	0.004097
C	3.568992	0.195937	–1.335271
C	2.443995	–1.943583	–1.158362
C	4.422525	–0.356993	–2.301868
C	3.877609	1.628573	–0.943270
C	3.312519	–2.458374	–2.134706
C	1.450904	–2.927060	–0.572432
C	4.301660	–1.679172	–2.739109
C	5.202763	–2.239698	–3.810780
C	0.721003	2.159060	–0.989146
C	1.191538	2.483891	1.365810
C	0.332304	3.499818	–1.081105
C	0.705041	1.398688	–2.300002
C	0.802860	3.827918	1.229454
C	1.673992	2.081510	2.743248
C	0.350022	4.357484	0.021099
C	–0.128265	5.781261	–0.092209
C	–2.594515	–1.819840	–1.431323
C	–3.213313	–2.922688	–2.031225
C	–3.367236	–4.086741	–1.276943
S	–2.269918	–0.360497	–2.440200
C	–2.891669	–4.130549	0.037863
C	–2.266810	–3.013700	0.594289
C	–2.513967	1.003059	–1.287363
C	–2.133933	1.956688	0.852730
C	–3.091958	2.186856	–1.760677
C	–2.721265	3.145352	0.427638
C	–3.199328	3.264638	–0.881939
C	–3.705975	–0.263291	–3.532809
F	0.037267	–0.621499	–0.284294
C	4.071135	–0.691673	1.776579
C	4.098887	–2.530719	3.942052
C	1.654981	–3.041862	5.482691
C	–0.416618	–1.146406	6.335356
C	–3.089884	–0.627019	5.256766
C	–3.521724	–0.509339	2.448320
H	5.221731	0.267278	–2.715258
H	3.290176	2.350621	–1.531102
H	3.655704	1.846647	0.107663
H	4.941297	1.842296	–1.125164
H	3.220976	–3.512948	–2.415939
H	0.477731	–2.877666	–1.083877
H	1.831249	–3.953753	–0.678911
H	1.257798	–2.730051	0.489195
H	6.199529	–1.775601	–3.781428
H	5.323182	–3.327674	–3.705027
H	4.787959	–2.053741	–4.815769
H	–0.008869	3.882910	–2.048198
H	0.556953	0.323717	–2.182747
H	–0.084803	1.796157	–2.954480
H	1.660944	1.528349	–2.833408
H	0.847519	4.478826	2.108730
H	1.795449	2.976149	3.371315
H	0.967692	1.404407	3.244401
H	2.635735	1.552936	2.710475
H	–1.223113	5.815654	–0.220292
H	0.122009	6.362110	0.806725
H	0.311303	6.288024	–0.965061
H	–3.576617	–2.896135	–3.057404
H	–3.858068	–4.953303	–1.722004

H	–3.005023	–5.043007	0.626384
H	–1.895955	–3.052388	1.620635
H	–1.746251	1.871241	1.868821
H	–3.457998	2.286447	–2.781311
H	–2.794399	3.992579	1.111587
H	–3.653319	4.194557	–1.227080
H	–4.630911	–0.263896	–2.947322
H	–3.594033	0.652779	–4.122000
H	–3.649001	–1.119112	–4.213273
H	4.793523	–0.485866	2.580623
H	4.514304	–1.470867	1.134798
H	3.987783	0.212195	1.170669
H	3.962263	–3.374545	4.627850
H	4.653220	–2.894302	3.064877
H	4.757053	–1.807249	4.453631
H	0.639476	–3.300030	5.799417
H	2.140755	–3.979786	5.173830
H	2.202847	–2.679272	6.367712
H	–0.902930	–0.258479	6.765125
H	–0.813776	–2.020543	6.876760
H	0.650873	–1.069220	6.566384
H	–3.943823	–1.251387	4.951341
H	–2.862654	–0.872788	6.299138
H	–3.445513	0.417054	5.225532
H	–3.595539	–0.432969	1.360692
H	–4.149900	–1.359147	2.762872
H	–3.983280	0.397110	2.873853

Complex		**5CN**,**H**···F⁻	
Atom	X	Y	Z
C	1.807212	–1.550523	4.398908
C	2.916606	–1.393918	3.594707
C	0.504284	–1.362418	3.866365
C	2.758267	–0.983056	2.253369
C	1.511741	–0.709685	1.693623
C	0.341704	–0.966813	2.490550
B	1.552581	0.018920	0.283925
C	–0.987894	–0.881518	1.966158
C	–0.640113	–1.568245	4.684651
C	–1.912915	–1.421019	4.175988
C	–2.074642	–1.103430	2.814596
B	–1.314351	–0.670000	0.428561
C	2.619135	–0.557942	–0.750842
C	1.066338	1.541846	0.155069
C	–2.258692	–1.905784	–0.142554
C	–2.068175	0.774587	0.124536
C	3.701722	0.250997	–1.197783
C	2.574990	–1.905165	–1.206089
C	4.634295	–0.255227	–2.112738
C	3.941842	1.656394	–0.687291
C	3.517865	–2.367039	–2.137271
C	1.545966	–2.908860	–0.733145
C	4.546514	–1.555452	–2.622425
C	5.529479	–2.061876	–3.646665
C	0.596901	2.038455	–1.099232
C	1.102092	2.461221	1.243076
C	0.086221	3.338115	–1.203980
C	0.691651	1.267621	–2.397535
C	0.609705	3.766170	1.085882
C	1.723477	2.142685	2.582095
C	0.078945	4.225636	–0.122698
C	–0.415229	5.638504	–0.278974
C	–3.011981	–1.734881	–1.311044

C	–3.988532	–2.646620	–1.755925
C	–4.115308	–3.870645	–1.051954
S	–2.383254	–0.342774	–2.280412
C	–3.252736	–4.155148	0.023635
C	–2.342196	–3.168806	0.480866
C	–2.657553	1.022383	–1.127786
C	–2.147859	1.819766	1.071662
C	–3.279362	2.231161	–1.489517
C	–2.734412	3.067236	0.739819
C	–3.311296	3.269365	–0.528186
C	–3.364255	–0.146392	–3.767711
F	–0.124011	–0.726144	–0.435756
C	–1.447829	–3.581486	1.523324
N	–0.734751	–4.141928	2.257541
C	–3.316676	–5.433472	0.651442
N	–3.377666	–6.479561	1.159716
C	–5.097003	–4.823918	–1.450247
N	–5.897081	–5.606857	–1.771410
C	–4.911329	–2.429045	–2.820661
N	–5.718997	–2.313849	–3.652065
C	–1.654623	1.746608	2.417104
N	–1.375332	1.932782	3.534849
C	–2.774902	4.129004	1.690476
N	–2.826473	5.010655	2.449555
C	–3.922784	4.516507	–0.841886
N	–4.423122	5.538244	–1.092716
C	–3.864253	2.536096	–2.752841
N	–4.353088	2.878855	–3.753087
H	1.909681	–1.840040	5.447448
H	3.917543	–1.568613	3.994594
H	3.651561	–0.831161	1.642462
H	–0.487797	–1.854645	5.728193
H	–2.786899	–1.577421	4.810210
H	–3.090618	–1.033985	2.413090
H	5.464309	0.384973	–2.427316
H	3.250148	2.385272	–1.134987
H	3.814897	1.729548	0.401464
H	4.965518	1.974363	–0.930082
H	3.455261	–3.405553	–2.477228
H	0.622327	–2.853259	–1.328918
H	1.941719	–3.929558	–0.832287
H	1.264752	–2.745054	0.314121
H	6.532798	–1.642622	–3.482629
H	5.601392	–3.158512	–3.625175
H	5.219891	–1.772741	–4.664787
H	–0.296391	3.676624	–2.171613
H	0.604978	0.185667	–2.282033
H	–0.069265	1.621113	–3.109832
H	1.671785	1.456001	–2.866069
H	0.645106	4.446098	1.941411
H	1.785779	3.055039	3.190238
H	1.142910	1.401896	3.147735
H	2.737081	1.733099	2.472233
H	–1.212930	5.705867	–1.032276
H	–0.789399	6.044146	0.670701
H	0.401269	6.297215	–0.617351
H	–4.417260	0.064250	–3.577847
H	–2.869460	0.654877	–4.327772
H	–3.219994	–1.088043	–4.312098

Complex		**5H**,**CN**···F⁻	
Atom	X	Y	Z
C	1.665765	–1.780940	4.408991

C	2.793073	–1.694392	3.588459
C	0.403967	–1.320080	3.923216
C	2.701977	–1.118275	2.285473
C	1.476821	–0.730766	1.731366
C	0.292534	–0.914915	2.541307
B	1.461903	–0.026685	0.264772
C	–1.004537	–0.676455	1.982871
C	–0.742206	–1.243316	4.772754
C	–1.989393	–0.913748	4.231789
C	–2.116280	–0.692592	2.833947
B	–1.307677	–0.518579	0.417868
C	2.537127	–0.649922	–0.761567
C	1.168836	1.561622	0.204519
C	–2.139106	–1.778005	–0.159062
C	–1.990961	0.884991	0.029641
C	3.604761	0.118288	–1.304958
C	2.441476	–2.013273	–1.159673
C	4.466039	–0.444478	–2.253432
C	3.936997	1.524713	–0.855224
C	3.327867	–2.538870	–2.112763
C	1.415138	–2.977551	–0.604440
C	4.335530	–1.766821	–2.693408
C	5.255427	–2.334925	–3.742926
C	0.734185	2.114445	–1.038661
C	1.280094	2.450202	1.304544
C	0.348803	3.455903	–1.119928
C	0.714846	1.353112	–2.347927
C	0.893770	3.794239	1.175577
C	1.854682	2.058317	2.648314
C	0.400017	4.316413	–0.019740
C	–0.069454	5.742372	–0.127743
C	–2.742329	–1.726377	–1.425216
C	–3.422561	–2.801874	–2.004065
C	–3.535918	–3.987944	–1.276910
S	–2.464160	–0.250507	–2.420682
C	–2.952605	–4.086660	–0.011409
C	–2.266689	–2.998044	0.528660
C	–2.594927	1.083108	–1.220581
C	–2.050161	1.975679	0.914300
C	–3.180009	2.289005	–1.618231
C	–2.649153	3.182935	0.563318
C	–3.211895	3.343544	–0.705447
C	–3.968359	–0.097582	–3.408954
F	0.029623	–0.637846	–0.333740
C	–3.441539	–0.503609	2.326724
N	–4.543673	–0.369304	1.972384
C	–3.136425	–0.820499	5.073541
N	–4.083073	–0.740086	5.747954
C	–0.688670	–1.408379	6.188271
N	–0.742641	–1.474615	7.350831
C	1.841574	–2.412702	5.675119
N	2.073556	–2.984212	6.664328
C	4.046862	–2.175435	4.070674
N	5.067927	–2.572153	4.467451
C	3.967723	–0.944561	1.635627
N	5.086199	–0.837608	1.321187
H	5.287302	0.164723	–2.643158
H	3.299117	2.280354	–1.336792
H	3.815929	1.654891	0.226829
H	4.980856	1.756313	–1.110093
H	3.231766	–3.591167	–2.397309
H	0.457083	–2.907003	–1.140483

H	1.776495	–4.010570	–0.703520
H	1.194051	–2.798777	0.455927
H	6.278855	–1.947909	–3.631891
H	5.289565	–3.432369	–3.694505
H	4.913571	–2.059643	–4.754497
H	–0.010591	3.839833	–2.079270
H	0.493518	0.288593	–2.244937
H	–0.020001	1.800337	–3.032323
H	1.699215	1.419086	–2.839503
H	0.980755	4.451180	2.045969
H	2.018032	2.955123	3.261009
H	1.188527	1.397408	3.221109
H	2.822567	1.546540	2.553375
H	–1.163257	5.782058	–0.259365
H	0.182611	6.317886	0.773471
H	0.375366	6.247498	–0.998570
H	–3.866503	–2.738007	–2.995758
H	–4.077716	–4.830393	–1.708049
H	–3.027558	–5.017048	0.553379
H	–1.810298	–3.101523	1.514605
H	–1.591828	1.880611	1.899052
H	–3.612782	2.422772	–2.607906
H	–2.663002	4.008989	1.275348
H	–3.675970	4.287233	–0.993921
H	–4.850873	–0.099311	–2.761284
H	–3.875899	0.832685	–3.979039
H	–3.969363	–0.934255	–4.115192

Complex		**$5NO_2$,H**···F⁻	
Atom	X	Y	Z
C	2.018927	–1.573732	4.337040
C	3.087665	–1.411993	3.481392
C	0.689935	–1.396551	3.870100
C	2.856111	–0.998107	2.153526
C	1.580349	–0.724242	1.657091
C	0.445725	–0.999224	2.504301
B	1.604269	0.061307	0.284621
C	–0.919784	–0.939411	2.057543
C	–0.399434	–1.617087	4.758462
C	–1.698812	–1.496512	4.322590
C	–1.941280	–1.191460	2.967088
B	–1.346909	–0.736720	0.542600
C	2.635941	–0.450788	–0.812415
C	1.046693	1.550499	0.188790
C	–2.306433	–1.996447	–0.043653
C	–2.196309	0.699815	0.227695
C	3.687693	0.406581	–1.247690
C	2.594605	–1.764647	–1.353346
C	4.596958	–0.025968	–2.220734
C	3.915730	1.786146	–0.666836
C	3.511396	–2.150567	–2.343802
C	1.585559	–2.802463	–0.921657
C	4.512034	–1.293939	–2.807976
C	5.468920	–1.717786	–3.892457
C	0.534537	2.046486	–1.045894
C	1.083464	2.455037	1.288968
C	–0.025649	3.329073	–1.120556
C	0.643699	1.297254	–2.354986
C	0.548790	3.742092	1.161972
C	1.764937	2.133463	2.597976
C	–0.032406	4.198413	–0.026024
C	–0.569529	5.600090	–0.136393
C	–2.972289	–1.791956	–1.269738

C	–3.942128	–2.661698	–1.770247
C	–4.182834	–3.863696	–1.106414
S	–2.208778	–0.431791	–2.190672
C	–3.445109	–4.170761	0.030273
C	–2.533745	–3.245482	0.550648
C	–2.668855	0.931668	–1.089040
C	–2.520192	1.721064	1.135700
C	–3.336825	2.089623	–1.485061
C	–3.169125	2.899985	0.762151
C	–3.559213	3.108061	–0.556559
C	–2.878016	–0.311992	–3.854382
F	–0.225417	–0.739346	–0.380409
N	–2.300700	1.612887	2.617367
O	–3.332345	1.427185	3.268159
O	–1.179000	1.769782	3.061892
N	–3.565907	3.880203	1.818666
O	–4.771484	4.014213	1.999474
O	–2.658445	4.425516	2.436478
N	–4.201081	4.381437	–0.951856
O	–5.018422	4.341017	–1.869928
O	–3.860024	5.386442	–0.331198
N	–3.812066	2.290579	–2.884970
O	–4.864820	1.733615	–3.177911
O	–3.097466	2.962127	–3.621371
N	–1.744914	–3.740125	1.721800
O	–2.383648	–4.140116	2.695311
O	–0.531135	–3.807976	1.567154
N	–3.651571	–5.489721	0.695677
O	–2.694265	–6.255829	0.681280
O	–4.754451	–5.684352	1.193408
N	–5.205443	–4.811366	–1.619330
O	–4.863530	–5.985397	–1.723385
O	–6.303343	–4.334732	–1.894325
N	–4.763440	–2.350443	–2.970002
O	–5.513620	–1.383235	–2.863355
O	–4.618655	–3.069601	–3.953496
H	2.172317	–1.862707	5.379532
H	4.108376	–1.581913	3.829751
H	3.715483	–0.835472	1.498569
H	–0.179566	–1.895128	5.791995
H	–2.534546	–1.671768	5.001517
H	–2.980170	–1.171789	2.624677
H	5.405302	0.647286	–2.522371
H	3.191546	2.520539	–1.049430
H	3.825410	1.795701	0.428024
H	4.923087	2.141268	–0.925735
H	3.449388	–3.165075	–2.749905
H	0.655544	–2.727720	–1.506226
H	1.991216	–3.812476	–1.076947
H	1.305831	–2.693841	0.131392
H	6.479735	–1.323122	–3.713402
H	5.529646	–2.812620	–3.967523
H	5.142654	–1.337468	–4.874708
H	–0.436472	3.671446	–2.075245
H	0.578276	0.211467	–2.255265
H	–0.118343	1.650804	–3.065168
H	1.620117	1.505801	–2.822328
H	0.590572	4.414851	2.022890
H	1.783987	3.025200	3.239303
H	1.259764	1.330726	3.148429
H	2.802421	1.803254	2.442886
H	–1.145195	5.739203	–1.060831

H	–1.214679	5.849844	0.717819
H	0.255831	6.330542	–0.141612
H	–3.951995	–0.134034	–3.916537
H	–2.293424	0.487522	–4.326049
H	–2.575263	–1.260661	–4.317610

Complex		**5H,NO_2···F^-**	
Atom	X	Y	Z
C	1.550854	–1.158577	4.545311
C	2.689807	–1.083030	3.777110
C	0.281504	–1.263508	3.907580
C	2.595749	–0.957195	2.381012
C	1.398998	–0.700101	1.724052
C	0.188352	–0.941880	2.495181
B	1.431825	–0.059475	0.220209
C	–1.107920	–0.899155	1.867553
C	–0.885815	–1.680217	4.601231
C	–2.113912	–1.658531	3.978608
C	–2.209159	–1.230112	2.648603
B	–1.364710	–0.555517	0.307663
C	2.549039	–0.713783	–0.757558
C	1.205977	1.544428	0.110768
C	–2.127835	–1.722599	–0.489202
C	–1.946994	0.924936	0.107783
C	3.634217	0.026009	–1.310527
C	2.464555	–2.094096	–1.100550
C	4.530383	–0.591824	–2.196302
C	3.935683	1.474245	–0.993733
C	3.373522	–2.666901	–1.998611
C	1.428069	–3.028953	–0.525185
C	4.411353	–1.930085	–2.575920
C	5.363276	–2.555830	–3.561556
C	0.781954	2.054300	–1.154742
C	1.405696	2.486691	1.153217
C	0.543585	3.422671	–1.324946
C	0.558114	1.197996	–2.381808
C	1.168129	3.851732	0.932466
C	1.880110	2.127245	2.543027
C	0.720180	4.345794	–0.293119
C	0.401595	5.803736	–0.487171
C	–2.869489	–1.495206	–1.654721
C	–3.357535	–2.518575	–2.478724
C	–3.145612	–3.842712	–2.100028
S	–3.320461	0.144977	–2.213022
C	–2.446200	–4.120132	–0.921150
C	–1.941398	–3.076481	–0.146782
C	–2.705183	1.309458	–1.003962
C	–1.698267	1.945522	1.045445
C	–3.116559	2.628178	–1.249845
C	–2.131962	3.254528	0.860419
C	–2.825140	3.605766	–0.303666
C	–5.093450	0.140422	–1.781287
H	5.360934	–0.000869	–2.593811
H	3.302409	2.159147	–1.577390
H	3.770910	1.721010	0.060372
H	4.983995	1.693706	–1.240700
H	3.278574	–3.730878	–2.236027
H	0.481123	–2.974049	–1.080032
H	1.782744	–4.067507	–0.575771
H	1.194744	–2.806092	0.524256
H	6.331748	–2.036175	–3.569231
H	5.536640	–3.617411	–3.333471
H	4.955645	–2.505835	–4.584959

H	0.207858	3.776217	–2.304351
H	–0.464706	0.791601	–2.401585
H	0.680069	1.805302	–3.289115
H	1.240602	0.343088	–2.436313
H	1.327507	4.550761	1.758587
H	1.972823	3.034971	3.153742
H	1.178009	1.461866	3.067775
H	2.862907	1.636278	2.532892
H	–0.685161	5.975190	–0.408012
H	0.891341	6.428162	0.272888
H	0.710817	6.155216	–1.482392
H	–3.897866	–2.289509	–3.399009
H	–3.525504	–4.650709	–2.725882
H	–2.280470	–5.153925	–0.614917
H	–1.375104	–3.316237	0.755278
H	–1.140936	1.699603	1.949205
H	–3.664261	2.885720	–2.158195
H	–1.912363	4.010582	1.614586
H	–3.142905	4.634725	–0.474730
H	–5.187379	–0.100931	–0.716850
H	–5.479786	1.139465	–2.010371
H	–5.573686	–0.610394	–2.418300
F	0.031205	–0.634054	–0.387235
N	3.924207	–0.977634	1.690781
O	4.311234	–2.071081	1.293464
O	4.574593	0.070287	1.689196
N	4.034477	–0.965828	4.411664
O	4.777311	–1.936155	4.302195
O	4.296054	0.109006	4.943351
N	1.686039	–1.019130	6.006008
O	2.629898	–1.584832	6.558237
O	0.852432	–0.301956	6.568190
N	–0.824418	–2.268009	5.958307
O	0.045765	–3.120752	6.149637
O	–1.658528	–1.894688	6.781086
N	–3.335375	–2.140124	4.678878
O	–3.370754	–3.325456	4.991075
O	–4.215527	–1.301999	4.859291
N	–3.575683	–1.288236	2.049426
O	–4.128691	–2.389351	2.052119
O	–4.050689	–0.246819	1.605566

Complex		**5OH,H**···F⁻	
Atom	X	Y	Z
C	1.614044	–1.436738	4.470923
C	2.707348	–1.222196	3.658210
C	0.299183	–1.311995	3.947094
C	2.518057	–0.819895	2.318045
C	1.259868	–0.615709	1.759785
C	0.108939	–0.930664	2.565545
B	1.191782	0.017897	0.280561
C	–1.231780	–0.891201	2.045234
C	–0.827096	–1.566581	4.776377
C	–2.106784	–1.485811	4.269066
C	–2.294543	–1.169751	2.904819
B	–1.597042	–0.594269	0.514344
C	2.352189	–0.629088	–0.667293
C	0.942533	1.619208	0.094679
C	–2.299913	–1.820074	–0.277617
C	–2.247451	0.857877	0.236831
C	3.538697	0.084580	–0.995459
C	2.266468	–1.972697	–1.129663
C	4.524427	–0.497626	–1.809261

C	3.841913	1.476370	–0.479677
C	3.266475	–2.515911	–1.951587
C	1.132943	–2.897642	–0.749576
C	4.400133	–1.789821	–2.326293
C	5.446033	–2.377243	–3.240434
C	0.568674	2.096731	–1.193718
C	1.094342	2.593550	1.119291
C	0.348099	3.464791	–1.420339
C	0.401697	1.192616	–2.394682
C	0.869952	3.951941	0.852375
C	1.534929	2.263846	2.527997
C	0.495358	4.416745	–0.411365
C	0.284791	5.887804	–0.671492
C	–2.889188	–1.635358	–1.544097
C	–3.226799	–2.683682	–2.412898
C	–2.993451	–4.009325	–2.026422
S	–3.279422	–0.046316	–2.233803
C	–2.472407	–4.248948	–0.752031
C	–2.129448	–3.170107	0.088772
C	–2.804114	1.164010	–1.025825
C	–2.134042	1.940275	1.125615
C	–3.096564	2.467572	–1.452617
C	–2.495224	3.249280	0.743403
C	–2.914091	3.519345	–0.553685
C	–5.095135	0.003358	–2.016580
H	1.737497	–1.723616	5.518413
H	3.719228	–1.346453	4.051315
H	3.400225	–0.629623	1.701497
H	–0.656019	–1.841229	5.820493
H	–2.970321	–1.686540	4.906532
H	–3.313275	–1.148933	2.504916
H	5.426690	0.080203	–2.035103
H	3.261530	2.248223	–1.005924
H	3.604132	1.583093	0.586942
H	4.909988	1.700892	–0.615409
H	3.161772	–3.551918	–2.290823
H	0.225360	–2.703961	–1.339150
H	1.424046	–3.944760	–0.916569
H	0.849732	–2.780153	0.304492
H	6.439709	–1.950631	–3.040375
H	5.508470	–3.469699	–3.129550
H	5.209997	–2.170962	–4.297927
H	0.062114	3.792351	–2.425366
H	–0.564393	0.667703	–2.371241
H	0.436785	1.779908	–3.323113
H	1.176341	0.416240	–2.435606
H	0.995285	4.673118	1.666210
H	1.537564	3.175420	3.143073
H	0.877880	1.525525	3.003366
H	2.549232	1.837532	2.552717
H	–0.402946	6.337486	0.062264
H	1.230461	6.448510	–0.594602
H	–0.114556	6.064403	–1.681465
H	–5.318002	–0.220811	–0.968603
H	–5.410142	1.013963	–2.298786
H	–5.528008	–0.736246	–2.697095
F	–0.216830	–0.567862	–0.300550
O	–2.368131	4.233872	1.680154
H	–2.641557	5.080693	1.271758
O	–1.652954	1.781897	2.397394
H	–1.488798	2.677602	2.756071
O	–3.238452	4.819556	–0.930100

H	–2.450215	5.245266	–1.324399
O	–3.574497	2.696691	–2.714201
H	–3.815867	3.645350	–2.767609
O	–3.713751	–2.416161	–3.687966
H	–4.620052	–2.770086	–3.783200
O	–3.262882	–5.066339	–2.848481
H	–3.416832	–4.714505	–3.748628
O	–2.243917	–5.531830	–0.350938
H	–1.860207	–5.467426	0.550652
O	–1.560461	–3.598100	1.259991
H	–1.453352	–2.810697	1.854870
Complex		**5H**,**OH**···F⁻	
Atom	X	Y	Z
C	1.839555	–1.631904	4.499247
C	2.922563	–1.627069	3.639786
C	0.550199	–1.263162	4.001885
C	2.766317	–1.192872	2.300516
C	1.553869	–0.776251	1.761380
C	0.394616	–0.880849	2.610934
B	1.509285	–0.045624	0.332543
C	–0.916351	–0.589504	2.100334
C	–0.594764	–1.245427	4.843536
C	–1.831993	–0.875593	4.360866
C	–1.980808	–0.572735	2.992625
B	–1.265915	–0.504127	0.544485
C	2.572586	–0.603682	–0.766129
C	1.180012	1.541798	0.266839
C	–2.126759	–1.777878	0.015088
C	–1.984074	0.866771	0.064214
C	3.671317	0.183826	–1.221681
C	2.442766	–1.914366	–1.316059
C	4.518526	–0.292049	–2.233471
C	4.020377	1.530729	–0.623759
C	3.302242	–2.345009	–2.336313
C	1.413857	–2.911362	–0.827724
C	4.334503	–1.541859	–2.831576
C	5.223345	–2.012739	–3.953878
C	0.761959	2.112093	–0.973605
C	1.260333	2.420575	1.378964
C	0.362789	3.450597	–1.050515
C	0.775381	1.363131	–2.290570
C	0.859081	3.762341	1.258285
C	1.806641	2.020089	2.732571
C	0.381358	4.296719	0.061493
C	–0.102910	5.719593	–0.035755
C	–2.665965	–1.806296	–1.279859
C	–3.357361	–2.895802	–1.818426
C	–3.553171	–4.017582	–1.010316
S	–2.290925	–0.395028	–2.339197
C	–3.048581	–4.032765	0.293735
C	–2.350498	–2.929549	0.788977
C	–2.529340	0.999475	–1.223148
C	–2.115365	1.991445	0.897905
C	–3.120790	2.169376	–1.703680
C	–2.727984	3.167750	0.464413
C	–3.226460	3.260188	–0.836970
C	–3.698854	–0.299579	–3.464314
F	0.026889	–0.641924	–0.284500
O	3.975136	–1.171544	1.629871
O	4.166983	–2.007292	4.093750
O	2.072268	–2.011925	5.799782
O	–0.472789	–1.586054	6.184570

O	–2.899413	–0.861257	5.235511
O	–3.300510	–0.331097	2.638415
H	5.357011	0.333704	–2.554413
H	3.398634	2.336316	–1.041760
H	3.870974	1.554544	0.463304
H	5.072606	1.770998	–0.833174
H	3.174355	–3.354524	–2.739752
H	0.448426	–2.784547	–1.340212
H	1.762753	–3.935917	–1.020863
H	1.217945	–2.797080	0.246033
H	6.218536	–1.549075	–3.899450
H	5.345022	–3.105371	–3.938278
H	4.791587	–1.747128	–4.933186
H	0.018272	3.842478	–2.012701
H	0.560761	0.296482	–2.193569
H	0.047021	1.806529	–2.985347
H	1.767861	1.441180	–2.764731
H	0.920987	4.409267	2.139314
H	2.000086	2.918945	3.335785
H	1.107273	1.380648	3.290325
H	2.744298	1.454048	2.650929
H	–1.190782	5.750980	–0.212283
H	0.104326	6.278131	0.887740
H	0.371554	6.251645	–0.874837
H	–3.746156	–2.890914	–2.835500
H	–4.101091	–4.873779	–1.405890
H	–3.196968	–4.912088	0.923228
H	–1.954967	–2.948566	1.806699
H	–1.686213	1.938327	1.900279
H	–3.503649	2.251182	–2.719588
H	–2.797397	4.024344	1.136424
H	–3.696161	4.179404	–1.189067
H	–4.637200	–0.263230	–2.901706
H	–3.551899	0.595651	–4.077761
H	–3.643667	–1.176766	–4.117509
H	3.781412	–1.014096	0.669625
H	4.762651	–1.909951	3.320863
H	1.210101	–1.974966	6.275153
H	–1.360364	–1.558347	6.593418
H	–3.686357	–0.595027	4.718710
H	–3.319623	0.112262	1.764838

Complex		**$6CH_3\cdots F^-$**	
Atom	X	Y	Z
C	–0.040189	–2.049987	4.142840
C	–1.389839	–1.662206	3.997855
C	0.894966	–1.709749	3.143594
C	–1.811685	–0.924705	2.871813
C	0.437930	–0.931536	2.063614
C	–0.898905	–0.567662	1.850612
Sb	1.901007	–0.239388	0.653490
B	–1.353068	0.025061	0.389059
C	1.886922	1.591110	–0.435720
C	2.061209	1.542863	–1.822537
C	1.893656	2.813940	0.242615
C	2.224829	2.733838	–2.537392
C	2.055215	3.998333	–0.479107
C	2.221481	3.960045	–1.867048
C	2.652730	–1.698663	–0.708889
C	1.868193	–2.176956	–1.768041
C	3.966155	–2.158262	–0.542289
C	2.401567	–3.118981	–2.653089
C	4.490970	–3.104367	–1.428996

C	3.709128	–3.585520	–2.483435
C	–2.681303	–0.790492	–0.154786
C	–3.933749	–0.186198	–0.460625
C	–2.610248	–2.208172	–0.311769
C	–5.007622	–0.952560	–0.945817
C	–3.700944	–2.935941	–0.813820
C	–4.912880	–2.329376	–1.153961
C	–1.306910	1.646100	0.177186
C	–1.312801	2.141883	–1.161269
C	–1.228268	2.615086	1.211688
C	–1.263649	3.514852	–1.424435
C	–1.189755	3.987817	0.907238
C	–1.203747	4.465567	–0.402512
C	3.649511	0.289457	1.812136
C	–4.234235	1.287294	–0.273486
C	–6.061133	–3.124563	–1.723078
C	–1.104166	5.936446	–0.711470
C	–1.157783	2.278135	2.686624
C	–1.374045	1.235162	–2.369649
F	–0.198231	–0.460278	–0.536356
C	2.294399	–2.275246	3.216559
C	0.404403	–2.826098	5.362670
C	–2.401209	–2.075504	5.042522
C	–3.259554	–0.499900	2.794389
C	–1.407025	–3.035517	0.095441
H	2.076281	0.587618	–2.349846
H	1.757703	2.857515	1.323719
H	2.354462	2.699218	–3.620716
H	2.041861	4.954466	0.046247
H	2.344592	4.888800	–2.426855
H	0.850268	–1.813698	–1.903399
H	4.592096	–1.785783	0.269960
H	1.790179	–3.488428	–3.478346
H	5.513022	–3.462374	–1.293985
H	4.120054	–4.323031	–3.174939
H	–5.955311	–0.447898	–1.161515
H	–3.600986	–4.020832	–0.925285
H	–1.269687	3.852186	–2.466075
H	–1.126123	4.706539	1.730779
H	4.280201	0.911288	1.166189
H	3.307063	0.876838	2.673348
H	4.205047	–0.583370	2.165690
H	–5.322095	1.440713	–0.220408
H	–3.778012	1.706989	0.631435
H	–3.850632	1.892732	–1.108397
H	–7.027796	–2.651914	–1.496005
H	–5.985980	–3.202238	–2.820806
H	–6.075105	–4.150534	–1.326630
H	–1.263732	6.548000	0.187897
H	–0.106692	6.184626	–1.112053
H	–1.838812	6.241814	–1.472329
H	–0.286257	1.653826	2.927630
H	–1.086388	3.202785	3.277332
H	–2.039603	1.726198	3.037264
H	–1.730664	1.793473	–3.247657
H	–0.376523	0.836442	–2.606448
H	–2.028697	0.369564	–2.207006
H	2.272571	–3.304787	3.597766
H	2.764104	–2.332129	2.225693
H	2.959185	–1.697213	3.877229
H	–0.129602	–2.489782	6.261218
H	0.212355	–3.907919	5.257729

H	1.476447	–2.701378	5.555546
H	–3.395219	–2.222344	4.602281
H	–2.115836	–3.011609	5.537889
H	–2.507113	–1.308791	5.829723
H	–3.406395	0.274867	2.039034
H	–3.924238	–1.339008	2.530745
H	–3.603884	–0.102088	3.761350
H	–0.469330	–2.648828	–0.315740
H	–1.285620	–3.041873	1.189466
H	–1.533063	–4.075932	–0.236879
Complex		**6CN**···F⁻	
Atom	X	Y	Z
C	0.015469	–1.850912	4.198309
C	–1.330225	–1.473916	4.029908
C	0.951332	–1.514730	3.188875
C	–1.737469	–0.827507	2.838422
C	0.531716	–0.808570	2.046662
C	–0.820042	–0.498829	1.809859
Sb	2.014641	–0.291681	0.543901
B	–1.286266	0.023436	0.324357
C	1.978081	1.487714	–0.606406
C	2.144407	1.387844	–1.991074
C	1.982971	2.727261	0.040083
C	2.297575	2.557784	–2.741746
C	2.136310	3.886860	–0.721625
C	2.293179	3.803211	–2.108713
C	2.530984	–1.972646	–0.638341
C	1.832768	–2.273000	–1.815689
C	3.609444	–2.763149	–0.221477
C	2.226922	–3.374169	–2.580414
C	3.987054	–3.869142	–0.989383
C	3.298691	–4.172419	–2.167527
C	–2.648689	–0.781397	–0.102946
C	–3.909912	–0.152427	–0.305273
C	–2.600440	–2.197771	–0.267266
C	–5.027575	–0.907481	–0.688781
C	–3.746713	–2.916537	–0.643079
C	–4.972992	–2.291970	–0.875162
C	–1.224152	1.628299	0.056429
C	–1.229547	2.051399	–1.304801
C	–1.162262	2.639514	1.046364
C	–1.167696	3.410553	–1.629869
C	–1.104010	3.994502	0.679763
C	–1.098994	4.407036	–0.652754
C	3.788215	0.176103	1.668467
C	–4.161785	1.324227	–0.093918
C	–6.185448	–3.073247	–1.312221
C	–0.987571	5.860263	–1.031071
C	–1.176754	2.359922	2.532508
C	–1.319311	1.085008	–2.463056
F	–0.153364	–0.541490	–0.539029
C	2.281162	–2.006744	3.356729
N	3.340470	–2.469749	3.503589
C	0.423121	–2.571312	5.356316
N	0.759476	–3.159526	6.304545
C	–2.274406	–1.779962	5.054199
N	–3.039513	–2.031457	5.895854
C	–3.129763	–0.504526	2.759910
N	–4.259482	–0.238260	2.872398
C	–1.346408	–3.022516	–0.074433
H	2.166107	0.418130	–2.489568
H	1.852369	2.803162	1.119539

H	2.421539	2.489516	–3.823653
H	2.124225	4.858717	–0.226814
H	2.409387	4.713839	–2.698394
H	0.985090	–1.666266	–2.129946
H	4.156209	–2.536522	0.694274
H	1.688723	–3.608966	–3.499983
H	4.821374	–4.491472	–0.662646
H	3.597498	–5.034502	–2.765878
H	–5.983753	–0.392762	–0.825303
H	–3.673530	–4.003124	–0.751679
H	–1.173629	3.698752	–2.685613
H	–1.053953	4.751043	1.468815
H	4.411164	0.753988	0.975584
H	3.506868	0.796725	2.527279
H	4.312514	–0.719423	2.008566
H	–5.243734	1.511057	–0.040613
H	–3.703897	1.697931	0.829094
H	–3.752317	1.933641	–0.912666
H	–7.108090	–2.655842	–0.883256
H	–6.297148	–3.046326	–2.408990
H	–6.109647	–4.129195	–1.016336
H	–1.141513	6.514866	–0.161935
H	0.011055	6.080509	–1.444127
H	–1.720492	6.133163	–1.805432
H	–0.325771	1.744855	2.857747
H	–1.130963	3.302411	3.095108
H	–2.093975	1.840688	2.848515
H	–1.672171	1.604456	–3.365186
H	–0.334415	0.651221	–2.691281
H	–1.994357	0.245734	–2.250470
H	–0.780273	–2.741348	0.822127
H	–1.603548	–4.087242	0.012187
H	–0.654749	–2.910138	–0.920539

Complex		**$6NO_2 \cdots F^-$**	
Atom	X	Y	Z
C	–0.175088	–1.806997	4.258214
C	–1.508826	–1.500063	4.013097
C	0.771800	–1.479642	3.285551
C	–1.870262	–0.887740	2.813340
C	0.411204	–0.829421	2.106446
C	–0.939991	–0.527037	1.825230
Sb	1.947450	–0.307358	0.632303
B	–1.337094	0.008858	0.317528
C	1.957904	1.483059	–0.508090
C	2.125221	1.371190	–1.892326
C	2.015924	2.724536	0.131591
C	2.331412	2.529143	–2.648107
C	2.220372	3.873186	–0.635277
C	2.377735	3.776996	–2.021248
C	2.557752	–1.906293	–0.620059
C	1.828449	–2.254731	–1.764254
C	3.763368	–2.549355	–0.313663
C	2.312663	–3.264416	–2.600806
C	4.234608	–3.561264	–1.155607
C	3.510316	–3.918816	–2.296576
C	–2.679256	–0.785001	–0.178740
C	–3.930531	–0.150645	–0.430084
C	–2.633434	–2.204177	–0.330433
C	–5.047770	–0.908520	–0.812173
C	–3.773956	–2.920456	–0.719980
C	–4.997095	–2.295183	–0.972130
C	–1.220415	1.614980	0.081674

C	–1.217052	2.054594	–1.275478
C	–1.095537	2.611289	1.083494
C	–1.126365	3.414782	–1.586862
C	–1.018439	3.968900	0.727584
C	–1.032596	4.398173	–0.599060
C	3.679585	0.179893	1.814471
C	–1.391703	–3.038184	–0.097443
C	–4.167291	1.337624	–0.307447
C	–6.206002	–3.080699	–1.409840
C	–0.898469	5.853352	–0.961221
C	–1.008176	2.324916	2.567376
C	–1.305816	1.102453	–2.445273
H	2.108503	0.398944	–2.385960
H	1.890594	2.813063	1.210576
H	2.456687	2.449812	–3.729119
H	2.248901	4.846884	–0.144575
H	2.535077	4.679148	–2.614396
H	0.893706	–1.750776	–2.002072
H	4.339326	–2.279242	0.571432
H	1.747307	–3.537851	–3.493003
H	5.170347	–4.068162	–0.915521
H	3.881320	–4.708633	–2.951576
H	–5.996806	–0.390447	–0.981145
H	–3.704186	–4.008513	–0.814002
H	–1.128018	3.714054	–2.639466
H	–0.924084	4.714470	1.522865
H	4.373674	0.647949	1.106448
H	3.382330	0.908131	2.577851
H	4.144669	–0.693548	2.279315
H	–1.663310	–4.098242	–0.000077
H	–0.683323	–2.949355	–0.932389
H	–0.838782	–2.752143	0.805261
H	–5.246382	1.538865	–0.250146
H	–3.682216	1.771589	0.573246
H	–3.769560	1.881548	–1.177760
H	–7.137736	–2.601327	–1.077011
H	–6.251078	–3.152860	–2.509379
H	–6.180808	–4.107295	–1.017165
H	–1.016817	6.499415	–0.080273
H	0.094896	6.056053	–1.395470
H	–1.643383	6.152585	–1.714120
H	–0.104943	1.754951	2.832927
H	–0.963875	3.268974	3.127755
H	–1.872431	1.760382	2.937669
H	–1.634722	1.636094	–3.347948
H	–0.322598	0.657892	–2.660839
H	–1.993951	0.268750	–2.255418
F	–0.169542	–0.566765	–0.496186
N	2.179978	–1.859079	3.546944
O	2.701609	–2.597565	2.707310
O	2.722218	–1.400125	4.548046
O	0.925286	–3.490032	5.397372
O	–0.213601	–2.013502	6.558147
N	0.212164	–2.494039	5.508872
N	–2.544405	–1.889463	5.005360
O	–2.624662	–3.083033	5.282748
O	–3.237558	–0.980395	5.455489
N	–3.337693	–0.685139	2.627587
O	–4.042298	–1.695229	2.646578
O	–3.739030	0.474582	2.568425

Complex		**6OH**···F⁻	
Atom	X	Y	Z

C	0.140502	–1.369523	4.380700
C	–1.220276	–1.259990	4.104175
C	1.075140	–1.082245	3.376874
C	–1.650251	–0.840247	2.836457
C	0.620400	–0.655132	2.119838
C	–0.752592	–0.505165	1.818164
Sb	2.056470	–0.342396	0.584768
B	–1.241118	–0.005755	0.339812
C	2.063281	1.486843	–0.491944
C	2.320460	1.491389	–1.866759
C	1.948435	2.686340	0.218395
C	2.445300	2.712748	–2.537580
C	2.078788	3.900515	–0.458360
C	2.325896	3.914559	–1.834718
C	2.430794	–1.985759	–0.720795
C	1.801369	–2.106947	–1.967124
C	3.361391	–2.946808	–0.304626
C	2.113772	–3.187857	–2.796761
C	3.656375	–4.034893	–1.133205
C	3.036459	–4.153257	–2.380476
C	–2.606666	–0.808256	–0.129387
C	–3.887397	–0.199590	–0.284563
C	–2.531377	–2.212786	–0.388173
C	–4.989867	–0.950925	–0.730913
C	–3.653044	–2.922322	–0.836906
C	–4.895283	–2.309453	–1.034321
C	–1.228637	1.610360	0.081684
C	–1.207017	2.059797	–1.270159
C	–1.231689	2.611435	1.086648
C	–1.170687	3.425564	–1.576218
C	–1.196233	3.973060	0.741573
C	–1.154730	4.408259	–0.583581
C	3.997801	–0.106125	1.477836
C	–1.265102	–3.016308	–0.187290
C	–4.168089	1.253746	0.039524
C	–6.080417	–3.088859	–1.544866
C	–1.057854	5.870196	–0.933912
C	–1.300839	2.309920	2.568335
C	–1.239198	1.111268	–2.448086
H	2.429680	0.557817	–2.420624
H	1.739884	2.684120	1.289264
H	2.636959	2.720755	–3.612117
H	1.974641	4.837154	0.090879
H	2.420219	4.865836	–2.361274
H	1.058247	–1.376623	–2.283120
H	3.858544	–2.863325	0.663112
H	1.626927	–3.277582	–3.769472
H	4.373496	–4.787577	–0.801269
H	3.271275	–4.999435	–3.028414
H	–5.957567	–0.450079	–0.833834
H	–3.555287	–3.997090	–1.021790
H	–1.153624	3.730024	–2.627885
H	–1.196521	4.718787	1.543395
H	4.683195	0.149822	0.660307
H	3.938173	0.717843	2.198089
H	4.311108	–1.019287	1.989779
H	–1.503502	–4.087483	–0.119663
H	–0.561427	–2.877146	–1.019848
H	–0.728791	–2.715715	0.721841
H	–5.253520	1.420329	0.092650
H	–3.724524	1.561398	0.995053
H	–3.753132	1.929765	–0.721709

H	–7.021971	–2.554014	–1.357251
H	–6.004229	–3.255777	–2.632005
H	–6.143489	–4.080081	–1.071469
H	–1.333494	6.507577	–0.081666
H	–0.027608	6.134797	–1.226856
H	–1.707894	6.127254	–1.783953
H	–0.410608	1.771212	2.923953
H	–1.381813	3.246651	3.138485
H	–2.169322	1.685258	2.823640
H	–1.602338	1.631897	–3.346315
H	–0.232005	0.725906	–2.668306
H	–1.879799	0.239671	–2.261133
F	–0.116991	–0.517619	–0.552630
O	–3.026643	–0.750946	2.723224
H	–3.239546	–0.769952	1.753996
O	–2.108621	–1.584633	5.096600
H	–3.003946	–1.499068	4.705856
O	0.622336	–1.793244	5.600214
H	–0.137385	–2.024780	6.168828
O	2.411765	–1.255289	3.646848
H	2.485785	–1.591514	4.562559

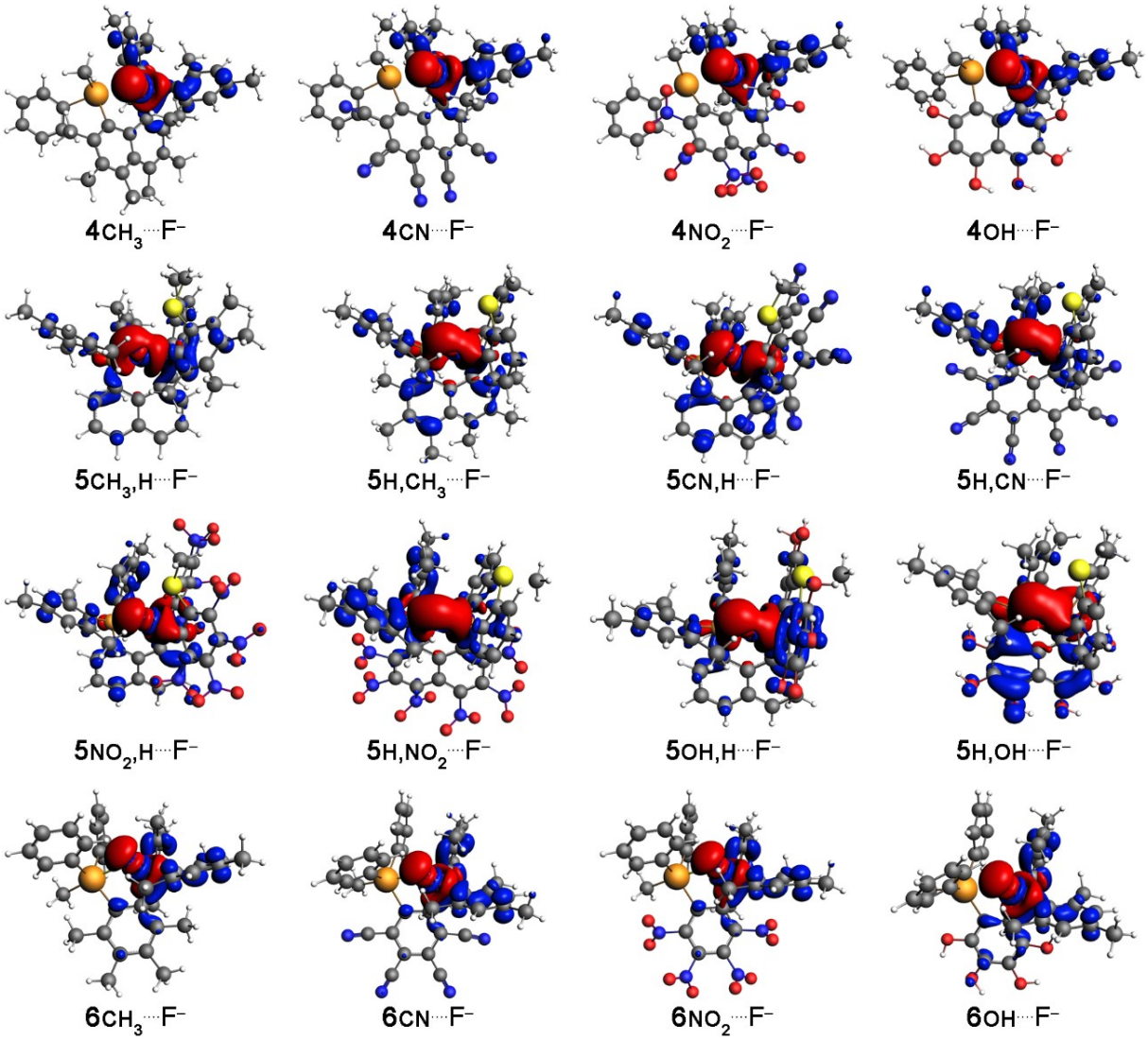

Figure S1. The first density deformation channels surface plots, $\Delta\rho_1$, for the structures designed from the (**4**–**6**)···F⁻ complexes. Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is 0.001 a.u. Atoms color code: H = white; C = gray; N = blue; O = red; S = yellow; Sb = tangerine; and Te = orange.

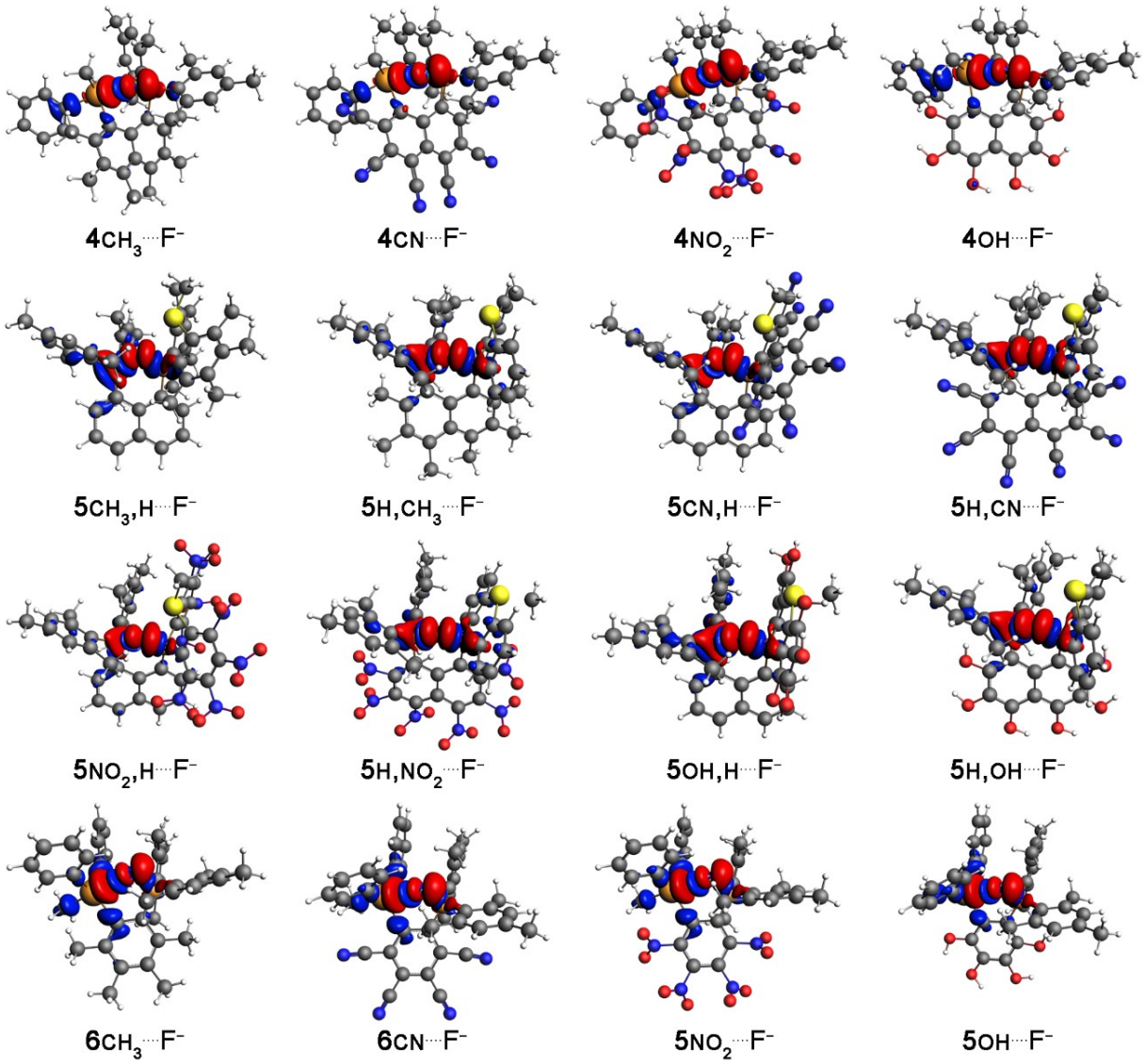

Figure S2. The second density deformation channels surface plots, $\Delta\rho_2$, for the structures designed from the (**4**–**6**)···F⁻ complexes. Red and blue regions indicate the electronic density outflow and inflow, respectively. The isovalue used to represent these surfaces is 0.001 a.u. Atoms color code: H = white; C = gray; N = blue; O = red; S = yellow; Sb = tangerine; and Te = orange.

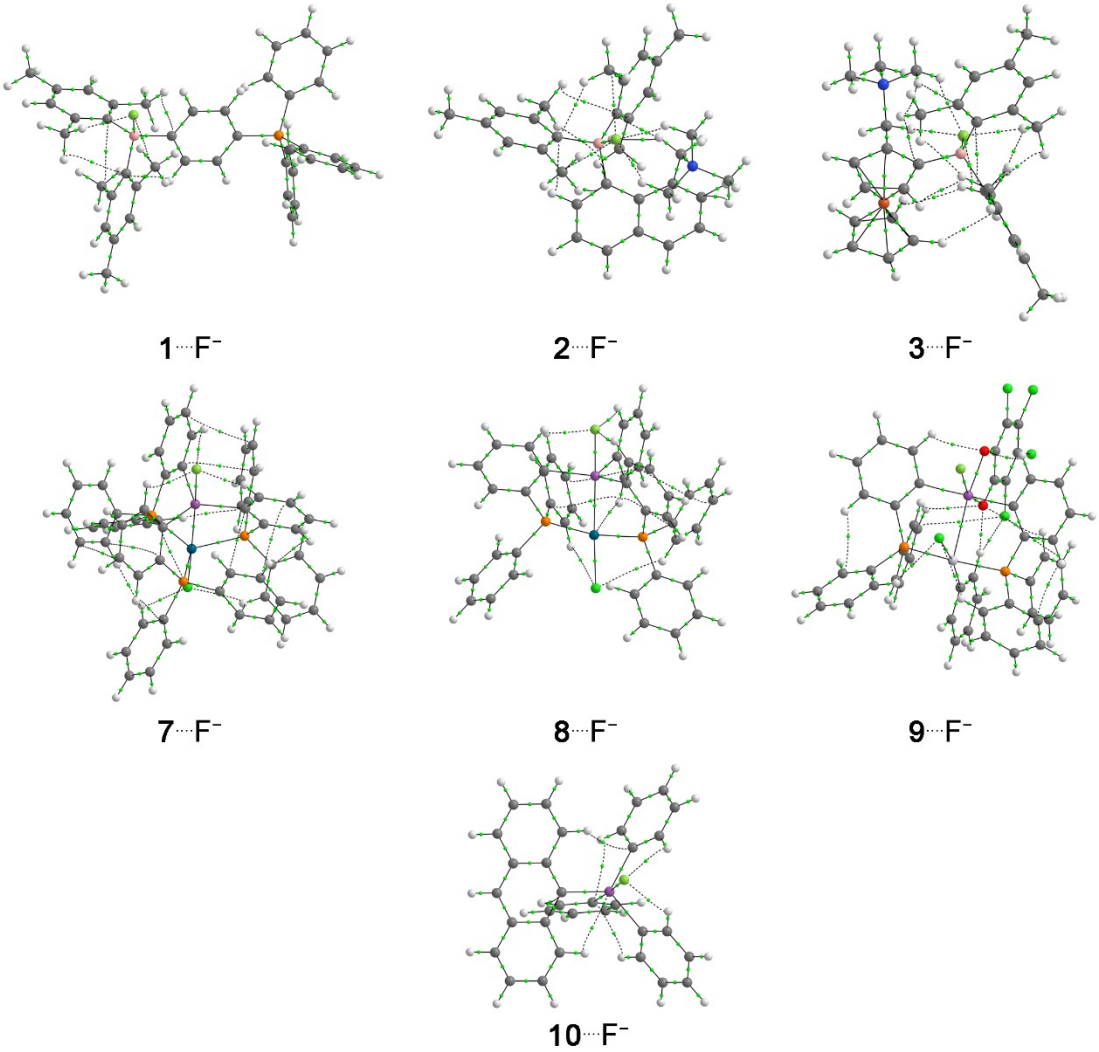

Figure S3. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the complexes (**1**–**3** and **7**–**10**)···F⁻. Atoms color code: H = white; B = pink; C = gray; N = blue; O = red; F = green; P = orange; Cl = light green; Fe = brown; Pd = turquoise; Sb = purple; and Pt = silver.

Table S2. Ratio between the kinetic energy density, G_b, and potential energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions between the receptors **1**–**10** and the anion F^-. The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
1···F^-	B···F^-	0.734	0.129
	C–H···F^-	1.271	0.015
	C···F^-	1.267	0.014
2···F^-	B···F^-	0.736	0.123
	C–H···F^-	1.117	0.027
	C–H···F^-	1.233	0.019
	C–H···F^-	1.307	0.012
	C···F^-	1.265	0.014
	C···F^-	1.253	0.015
3···F^-	B···F^-	0.735	0.128
	C–H···F^-	1.239	0.016
	C–H···F^-	1.243	0.017
	C–H···F^-	1.293	0.013
	C–H···F^-	1.256	0.015
4···F^-	B···F^-	0.739	0.111
	Te···F^-	0.914	0.039
	C–H···F^-	1.285	0.012
	C···F^-	1.268	0.014
5···F^-	B···F^-[a]	0.715	0.071
	B···F^-[b]	0.751	0.102
	C–H···F^-	1.280	0.015
	C···F^-	1.278	0.014
6···F^-	B···F^-	0.743	0.111
	Sb···F^-	0.913	0.039
	C–H···F^-	1.286	0.012
	C···F^-	1.265	0.014
7···F^-	Sb···F^-	0.800	0.091
	C–H···F^-	1.287	0.012
	C–H···F^-	1.277	0.013
	C–H···F^-	1.269	0.014
8···F^-	Sb···F^-	0.802	0.087
	C–H···F^-	1.263	0.015
	C–H···F^-	1.263	0.015
	C–H···F^-	1.261	0.015
9···F^-	Sb···F^-	0.792	0.103
10···F^-	Sb···F^-	0.798	0.086
	C–H···F^-	1.256	0.015
	C–H···F^-	1.278	0.012

[a] Interaction related to boron atom localized in the left position in the respective structure of the Scheme 1; and [b] Interaction related to boron atom localized in the right position in the respective structure of the Scheme 1.

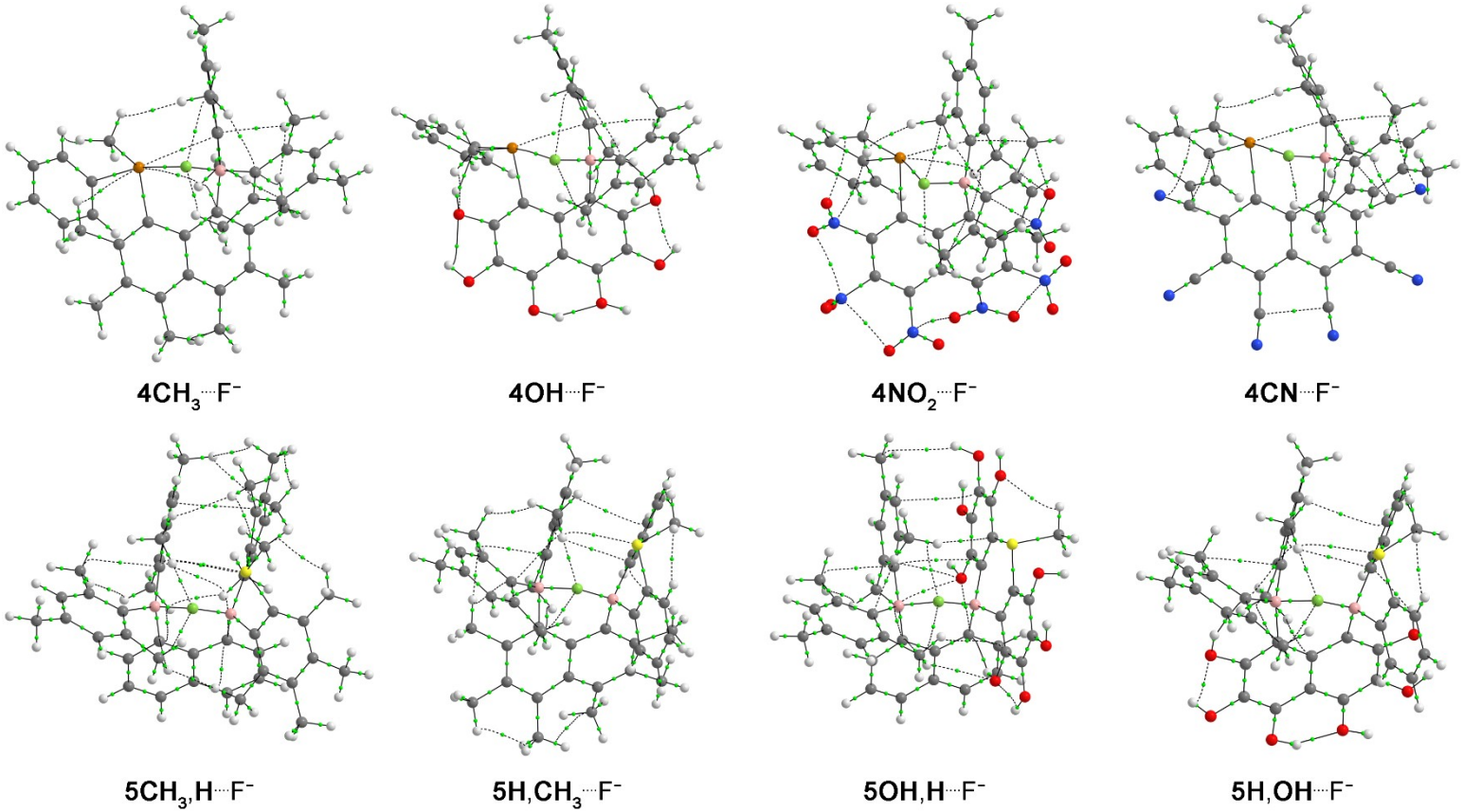

Figure S4. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the complexes **4CH$_3$**···F$^-$, **4OH**···F$^-$, **4NO$_2$**···F$^-$, **4CN**···F$^-$, **5CH$_3$,H**···F$^-$, **5H,CH$_3$**···F$^-$, **5OH,H**···F$^-$, and **5H,OH**···F$^-$. Atoms color code: H = white; B = pink; C = gray; N = blue; O = red; F = green; S = yellow; Cl = light green; and Te = brown.

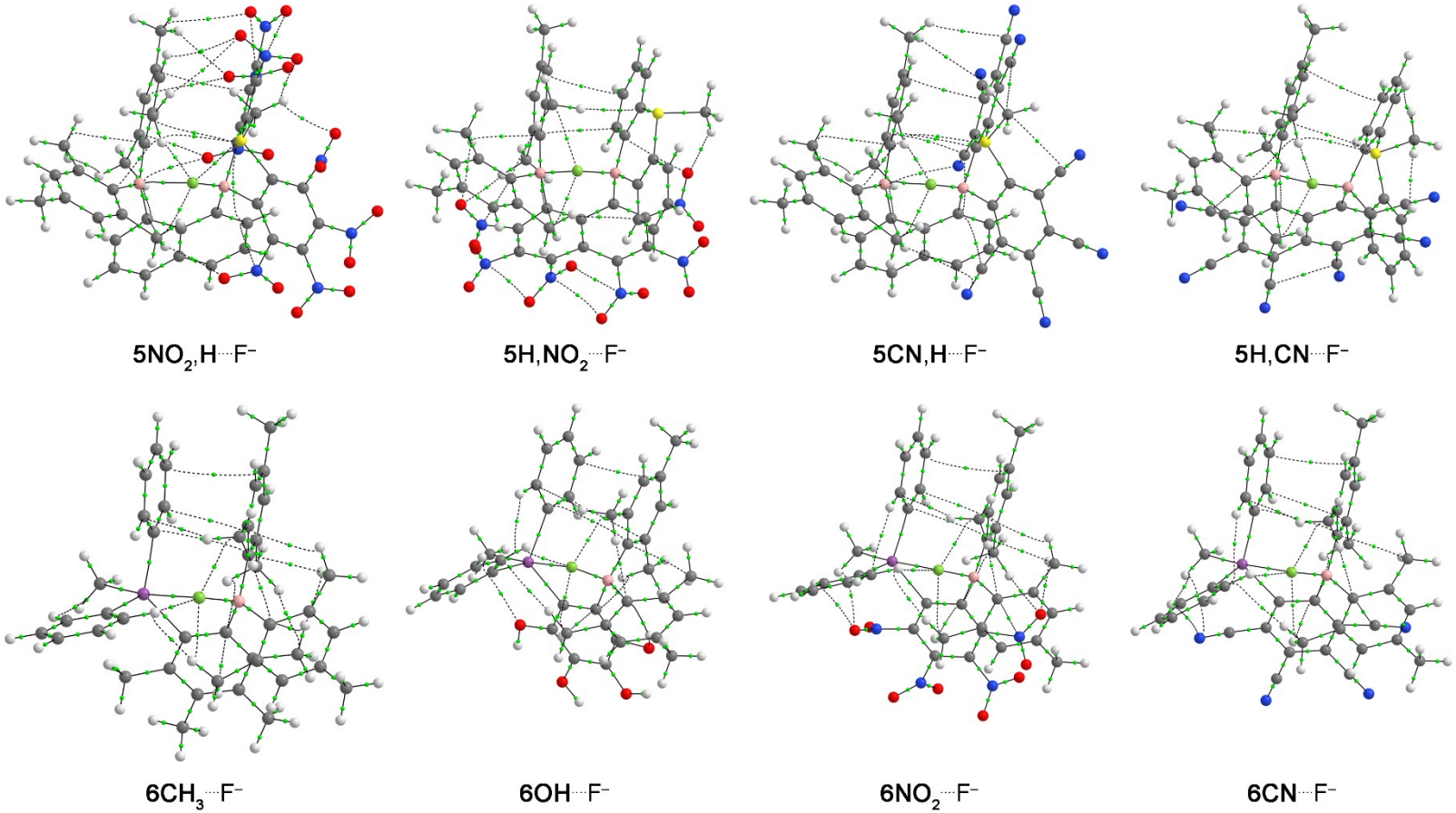

Figure S5. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small light green points), for the complexes **5NO$_2$,H**···F$^-$, **5H,NO$_2$**···F$^-$, **5CN,H**···F$^-$, **5H,CN**···F$^-$, **6CH$_3$**···F$^-$, **6OH**···F$^-$, **6NO$_2$**···F$^-$, and **6CN**···F$^-$. Atoms color code: H = white; B = pink; C = gray; N = blue; O = red; F = green; S = yellow; Cl = light green; and Sb = purple.

Table S3. Ratio between the kinetic energy density, G_b, and potential energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions between the designed receptors from the compound **4** and the anion F^-. The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
4CH$_3$···F$^-$	B···F$^-$	0.737	0.114
	Te···F$^-$	0.942	0.035
	C–H···F$^-$	1.244	0.017
	C···F$^-$	1.276	0.013
4OH···F$^-$	B···F$^-$	0.737	0.114
	Te···F$^-$	0.921	0.038
	C···F$^-$	1.285	0.012
	C···F$^-$	1.283	0.013
4NO$_2$···F$^-$	B···F$^-$	0.734	0.122
	Te···F$^-$	1.005	0.029
	C–H···F$^-$	1.236	0.018
	C···F$^-$	1.289	0.012
4CN···F$^-$	B···F$^-$	0.734	0.120
	Te···F$^-$	1.011	0.028
	C–H···F$^-$	1.249	0.017

Table S4. Ratio between the kinetic energy density, G_b, and potential energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions between the designed receptors from the compound **5** and the anion F^-. The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
5CH$_3$,H···F$^-$	B···F$^-$[a]	0.732	0.075
	B···F$^-$[b]	0.748	0.101
	C–H···F$^-$	1.274	0.015
	C···F$^-$	1.271	0.015
5H,CH$_3$···F$^-$	B···F$^-$[a]	0.731	0.072
	B···F$^-$[b]	0.755	0.105
	C–H···F$^-$	1.260	0.016
	C···F$^-$	1.286	0.014
5OH,H···F$^-$	B···F$^-$[a]	0.746	0.083
	B···F$^-$[b]	0.735	0.092
	C–H···F$^-$	1.301	0.012
	C···F$^-$	1.284	0.014
5H,OH···F$^-$	B···F$^-$[a]	0.705	0.070
	B···F$^-$[b]	0.753	0.107
	C–H···F$^-$	1.264	0.016
	C···F$^-$	1.285	0.014
5NO$_2$,H···F$^-$	B···F$^-$[a]	0.828	0.034
	B···F$^-$[b]	0.739	0.142
	C–H···F$^-$	1.292	0.014
	C···F$^-$	1.306	0.012
	S···F$^-$	1.143	0.021
5H,NO$_2$···F$^-$	B···F$^-$[a]	0.742	0.084
	B···F$^-$[b]	0.746	0.102
	C···F$^-$	1.305	0.012
	C···F$^-$	1.303	0.012
5CN,H···F$^-$	B···F$^-$[a]	0.712	0.043
	B···F$^-$[b]	0.743	0.133
	C–H···F$^-$	1.266	0.016
	C···F$^-$	1.293	0.013
5H,CN···F$^-$	B···F$^-$[a]	0.735	0.077
	B···F$^-$[b]	0.752	0.108
	C–H···F$^-$	1.257	0.016
	C···F$^-$	1.291	0.013

[a] Interaction related to boron atom localized in the left position in the respective structure of the Scheme 2; and [b] Interaction related to boron atom localized in the right position in the respective structure of the Scheme 2.

Table S5. Ratio between the kinetic energy density, G_b, and potential energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at BCPs related to interactions between the designed receptors from the compound **6** and the anion F^-. The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
	B···F⁻	0.743	0.105
	Sb···F⁻	0.895	0.042
6CH$_3$···F⁻	C–H···F⁻	1.274	0.015
	C–H···F⁻	1.241	0.016
	C···F⁻	1.283	0.013
	B···F⁻	0.745	0.115
	Sb···F⁻	0.915	0.039
6OH···F⁻	C–H···F⁻	1.283	0.014
	C···F⁻	1.282	0.013
	C···F⁻	1.281	0.013
	B···F⁻	0.742	0.111
	Sb···F⁻	0.892	0.043
6NO$_2$···F⁻	C–H···F⁻	1.275	0.015
	C···F⁻	1.286	0.012
	C···F⁻	1.300	0.012
	B···F⁻	0.743	0.112
	Sb···F⁻	0.902	0.041
6CN···F⁻	C–H···F⁻	1.291	0.013
	C···F⁻	1.291	0.013
	C···F⁻	1.283	0.013