ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Does induced current density explain the C–H and C–F Perlin effects?

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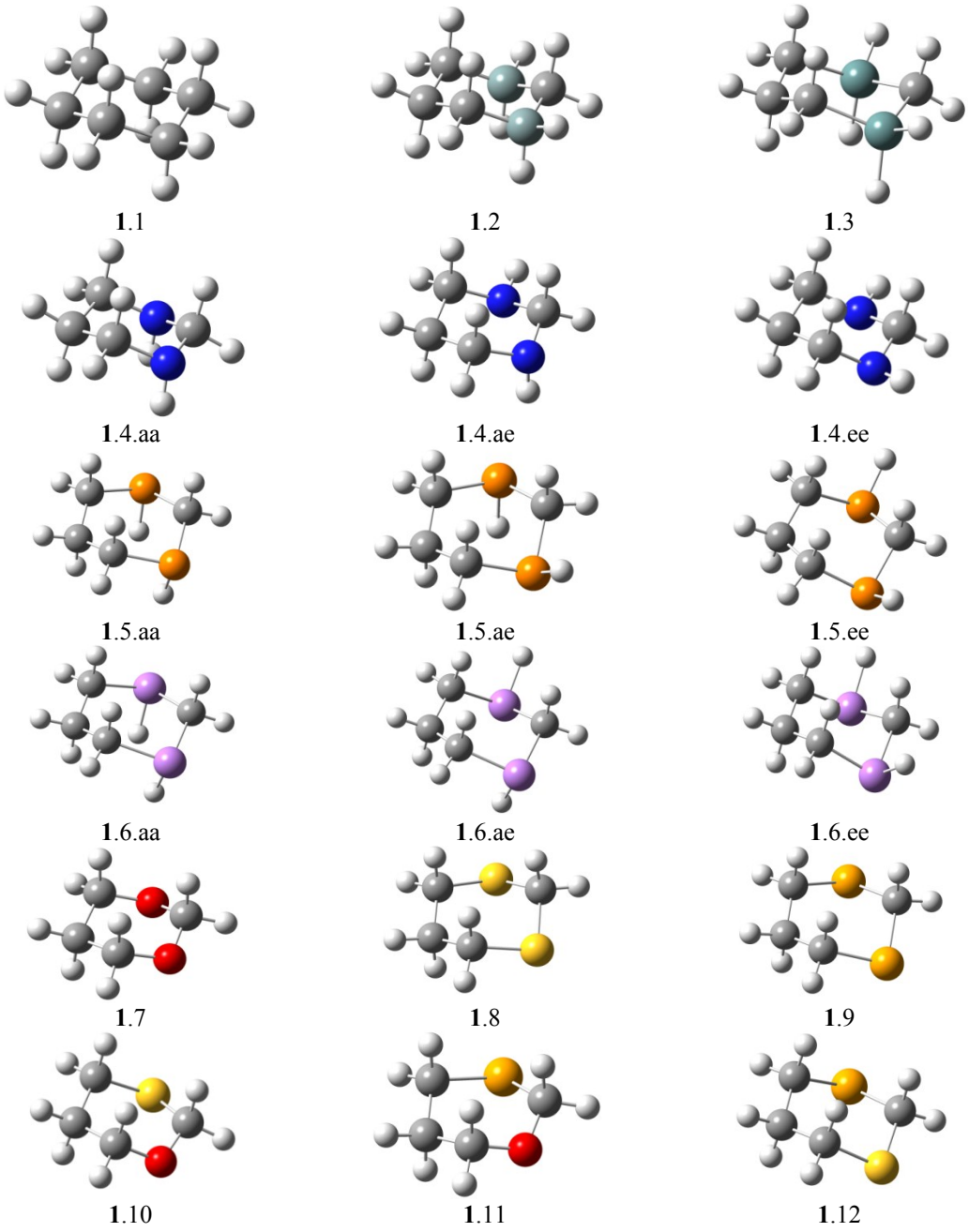

Figure S1. Hydrogenated compounds**1**. Atom colors: H = white, C = grey, Si = green-grey (smaller sphere), Ge = green-grey (larger sphere), N = blue, P = orange, As = light purple, O = red, S = yellow, Se = dark yellow.

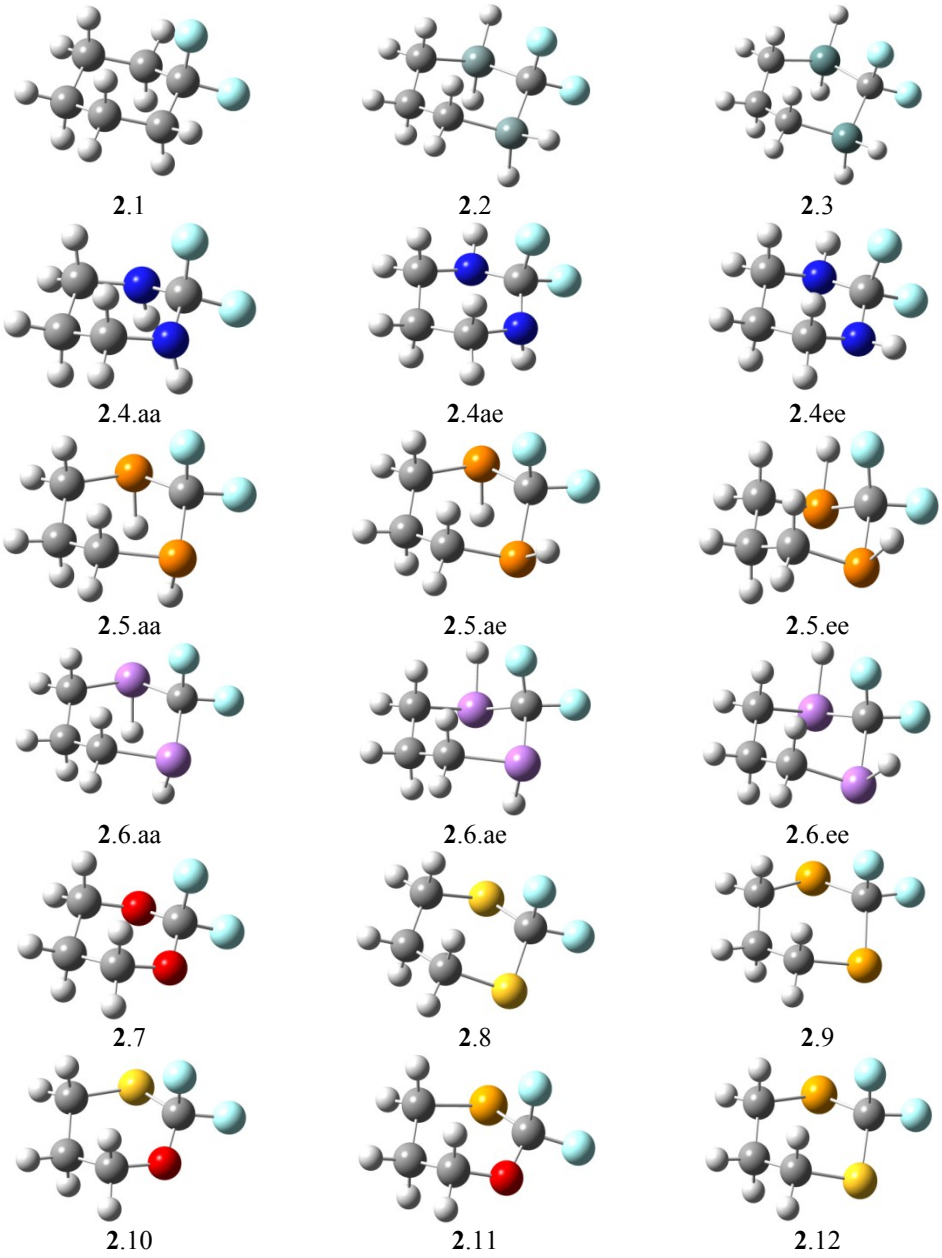

Figure S2. Fluorinated compounds**2**.Atom colors: H = white, C = grey, Si = green-grey (smaller sphere), Ge = green-grey (larger sphere), N = blue, P = orange, As = light purple, O = red, S = yellow, Se = dark yellow.

Standard coordinates (molecular geometries)

1.2 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.136991	-0.456246	-1.160535
2	6	0	-0.615706	-0.583790	-1.209641
3	6	0	0.033442	0.023576	0.032364
4	6	0	-0.533628	-0.587000	1.312163
5	6	0	-2.054913	-0.459457	1.361269
6	6	0	-2.704061	-1.066823	0.119264
7	1	0	1.116017	-0.110191	-0.003888
8	1	0	-0.348183	-1.643739	-1.272109
9	1	0	-0.224426	-0.108631	-2.110882
10	1	0	-2.407729	0.603954	-1.202478
11	1	0	-2.584885	-0.928729	-2.036450
12	1	0	-0.262890	-1.647200	1.354106
13	1	0	-0.085734	-0.114516	2.188078
14	1	0	-2.446193	-0.934615	2.262509
15	1	0	-2.322437	0.600493	1.423736
16	1	0	-2.520416	-2.146313	0.111665
17	1	0	-3.786636	-0.933057	0.155515
18	1	0	-0.150202	1.103066	0.039962

1.2 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.506757	-0.511755	-0.937846
2	6	0	0.326497	0.098782	0.018162
3	6	0	-2.249022	-0.244795	1.612969
4	6	0	-2.908271	-1.016964	0.457758
5	1	0	1.387826	-0.136401	-0.066593
6	1	0	-0.351177	-2.172551	-1.388633
7	1	0	-0.376400	-0.138526	-2.678202
8	1	0	-2.760697	0.549264	-1.028539
9	1	0	-3.092979	-1.028325	-1.701207
10	1	0	-0.021931	-1.835950	1.949136
11	1	0	0.178525	0.410920	2.794094
12	1	0	-2.667262	-0.577212	2.565646
13	1	0	-2.496774	0.818073	1.527035
14	1	0	-2.663380	-2.079783	0.545208
15	1	0	-3.993724	-0.950767	0.561676
16	1	0	0.220444	1.182431	-0.082562
17	14	0	-0.372835	-0.412652	1.684329
18	14	0	-0.677219	-0.720011	-1.341989

1.3 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.312550	-0.588494	-1.010734
2	6	0	0.356738	0.150078	0.043860
3	6	0	-2.171150	-0.331541	1.509513
4	6	0	-2.797776	-1.069749	0.342568
5	1	0	1.433976	0.097837	-0.012602
6	1	0	-2.520554	0.478066	-1.098316
7	1	0	-2.899047	-1.080407	-1.780091
8	1	0	-2.666083	-0.650101	2.421217
9	1	0	-2.378532	0.733070	1.400175
10	1	0	-2.591471	-2.138789	0.441100
11	1	0	-3.884490	-0.971079	0.394776
12	1	0	0.088105	1.198568	-0.048216
13	1	0	0.021676	-1.913477	1.806929
14	1	0	-0.146178	-2.219743	-1.225482
15	32	0	-0.309474	-0.489703	1.685394
16	32	0	-0.479114	-0.797029	-1.353716
17	1	0	0.135517	0.372790	2.785463
18	1	0	-0.167651	-0.174778	-2.645162

1.4aa orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.173943	-0.589065	-1.016468
2	6	0	-0.073311	-0.082685	0.047431
3	6	0	-1.979296	-0.454563	1.472926
4	6	0	-2.717948	-1.120761	0.310559
5	1	0	1.000942	-0.244705	-0.029077
6	1	0	-2.445232	0.466575	-1.120086
7	1	0	-2.617137	-1.112191	-1.863906
8	1	0	-2.279875	-0.884791	2.428329
9	1	0	-2.242771	0.607556	1.506341
10	1	0	-2.564488	-2.203657	0.357981
11	1	0	-3.792621	-0.940749	0.386318
12	1	0	-0.251261	0.995730	0.000803
13	7	0	-0.527969	-0.540829	1.351135
14	7	0	-0.720801	-0.676450	-1.112565
15	1	0	-0.226449	-1.494901	1.503422
16	1	0	-0.440027	-1.644598	-1.203626

1.4ae orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.085931	-0.588394	-1.126197
2	6	0	-0.048738	-0.000491	0.013984
3	6	0	-1.985308	-0.409246	1.364219
4	6	0	-2.667517	-1.104103	0.184846
5	1	0	1.034385	-0.110698	-0.028383
6	1	0	-0.226449	-0.453484	-1.971523
7	1	0	-2.382026	0.466493	-1.255381
8	1	0	-2.486967	-1.146627	-1.972151
9	1	0	-2.308831	-0.839939	2.311796
10	1	0	-2.272901	0.646940	1.379471
11	1	0	-2.497023	-2.181290	0.249578
12	1	0	-3.745357	-0.933194	0.213550
13	1	0	-0.284626	1.074236	-0.046677
14	7	0	-0.528203	-0.465237	1.294459
15	7	0	-0.637462	-0.744303	-1.095811
16	1	0	-0.222008	-1.420701	1.428176

1.4ee orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.078244	-0.454515	-1.280947
2	6	0	-0.088197	-0.008362	-0.012105
3	6	0	-2.079353	-0.566442	1.210029
4	6	0	-2.696014	-1.130044	-0.063486
5	1	0	0.995273	-0.124752	-0.017142
6	1	0	-0.195974	-0.180241	-2.030538
7	1	0	-2.387587	0.604921	-1.293346
8	1	0	-2.441259	-0.914258	-2.199982
9	1	0	-0.197567	-0.361324	1.982384
10	1	0	-2.442489	-1.105740	2.084712
11	1	0	-2.387747	0.487783	1.317151
12	1	0	-2.501317	-2.201981	-0.112368
13	1	0	-3.775782	-0.974730	-0.056879
14	1	0	-0.319952	1.078204	0.037779
15	7	0	-0.631246	-0.704235	1.138089
16	7	0	-0.630320	-0.597374	-1.220744

1.5aa orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.161224	-0.478524	-1.505257
2	6	0	0.234340	0.027602	-0.022292
3	6	0	-2.334090	-0.653506	1.048275
4	6	0	-2.756649	-1.214023	-0.307168
5	1	0	1.313040	-0.120338	0.042317
6	1	0	-2.447826	0.576972	-1.479494
7	1	0	-2.575678	-0.878326	-2.432083
8	1	0	-2.861563	-1.172928	1.850035
9	1	0	-2.627200	0.397303	1.129850
10	1	0	-2.486780	-2.271626	-0.362221
11	1	0	-3.846958	-1.167697	-0.379033
12	1	0	0.081954	1.107678	0.041330
13	15	0	-0.534169	-0.728779	1.486779
14	1	0	-0.324121	-2.086129	1.126860
15	15	0	-0.318727	-0.514488	-1.707770
16	1	0	-0.148475	-1.909280	-1.504075

1.5ae orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.139493	-0.331760	-1.518424
2	6	0	0.260030	0.108547	-0.016962
3	6	0	-2.280570	-0.541918	1.027985
4	6	0	-2.758874	-1.062632	-0.327449
5	1	0	1.345110	0.012379	0.015970
6	1	0	-2.403939	0.729054	-1.484705
7	1	0	-2.556237	-0.715897	-2.450984
8	1	0	-2.845842	-1.018906	1.829451
9	1	0	-2.461491	0.533086	1.098485
10	1	0	-2.544654	-2.131456	-0.408307
11	1	0	-3.845419	-0.957865	-0.381374
12	1	0	0.023934	1.167829	0.098294
13	15	0	-0.486873	-0.920229	1.329607
14	15	0	-0.294508	-0.396936	-1.715754
15	1	0	-0.149616	-1.798904	-1.541078
16	1	0	-0.298758	-0.021160	2.412187

1.5ee orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.245695	-0.502548	-1.141523
2	6	0	0.262739	0.080796	0.012917
3	6	0	-2.134299	-0.411545	1.413502
4	6	0	-2.748784	-1.084220	0.182594
5	1	0	1.349442	0.014033	-0.033310
6	1	0	-2.430979	0.573561	-1.164181
7	1	0	-2.794846	-0.945890	-1.972865
8	1	0	-2.610963	-0.790434	2.318121
9	1	0	-2.316125	0.664631	1.372847
10	1	0	-2.551226	-2.159277	0.213064
11	1	0	-3.833493	-0.966646	0.226497
12	1	0	-0.027639	1.131397	-0.009438
13	15	0	-0.312489	-0.754987	1.568869
14	15	0	-0.441519	-0.854433	-1.429576
15	1	0	-0.005578	0.294775	2.471072
16	1	0	-0.220295	0.135446	-2.420330

1.6aa orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.162060	-0.406663	-1.425284
2	6	0	0.232348	0.037279	-0.023273
3	6	0	-2.302853	-0.572144	1.036522
4	6	0	-2.810417	-1.094940	-0.268050
5	1	0	1.309088	-0.098726	0.030173
6	1	0	-2.429810	0.646944	-1.380424
7	1	0	-2.639328	-0.695662	-2.353999
8	1	0	-2.874589	-0.984253	1.859570
9	1	0	-2.577506	0.478207	1.106979
10	1	0	-2.515331	-2.140243	-0.321576
11	1	0	-3.893248	-1.013285	-0.325318
12	1	0	0.185931	1.115804	0.044977
13	33	0	-0.560389	-0.701432	1.496320
14	33	0	-0.379533	-0.492760	-1.704522
15	1	0	-0.308205	-2.020117	1.238924
16	1	0	-0.150814	-1.835978	-1.591037

1.6ae orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.275042	-0.511398	-1.033050
2	6	0	0.236415	0.053904	-0.010360
3	6	0	-2.188443	-0.326613	1.381686
4	6	0	-2.873354	-1.001856	0.235130
5	1	0	1.316807	-0.029277	-0.024398
6	1	0	-2.404477	0.564156	-1.058229
7	1	0	-2.855614	-0.843445	-1.889346
8	1	0	-2.676087	-0.558091	2.323579
9	1	0	-2.369389	0.742564	1.299211
10	1	0	-2.680252	-2.070684	0.321110
11	1	0	-3.946044	-0.823177	0.226788
12	1	0	0.092150	1.125160	-0.038747
13	1	0	-0.550700	0.389091	-2.317969
14	33	0	-0.411238	-0.554599	1.634432
15	33	0	-0.533671	-0.723422	-1.534116
16	1	0	-0.299605	-1.907579	1.448383

1.6ee orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.166691	-0.711478	-1.183347
2	6	0	0.259504	-0.074231	0.030702
3	6	0	-2.192145	-0.651591	1.222652
4	6	0	-2.813636	-1.287276	0.028033
5	1	0	1.341862	-0.098459	0.042992
6	1	0	-2.319750	0.363116	-1.156242
7	1	0	-2.670879	-1.020516	-2.096914
8	1	0	-2.715904	-0.914086	2.139761
9	1	0	-2.343340	0.420308	1.138092
10	1	0	-2.648610	-2.366016	0.057286
11	1	0	-3.883587	-1.090842	0.011316
12	1	0	-0.006452	0.971160	0.001793
13	1	0	-0.388477	0.383167	2.325669
14	1	0	-0.339393	0.269494	-2.297171
15	33	0	-0.410371	-0.784698	1.630050
16	33	0	-0.376606	-0.862879	-1.545802

1.7 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.039589	-0.507445	-1.269063
2	6	0	-0.142687	-0.040939	-0.016404
3	6	0	-2.066744	-0.479407	1.204667
4	6	0	-2.705433	-1.094146	-0.032612
5	1	0	0.932999	-0.192715	-0.002372
6	1	0	-2.300293	0.555736	-1.371541
7	1	0	-2.343478	-1.021687	-2.178320
8	1	0	-2.391013	-0.973235	2.118174
9	1	0	-2.329881	0.585659	1.277384
10	1	0	-2.555130	-2.174262	-0.018439
11	1	0	-3.778417	-0.896362	-0.046922
12	1	0	-0.380763	1.037084	-0.031788
13	8	0	-0.657997	-0.612336	1.148486
14	8	0	-0.632426	-0.639238	-1.178761

1.8 Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.189689	-0.632777	-1.228243
2	6	0	0.155318	0.034706	0.033314
3	6	0	-2.203085	-0.541889	1.320441
4	6	0	-2.717681	-1.237889	0.066491
5	1	0	1.241400	-0.012345	0.040863
6	1	0	-2.443219	0.428274	-1.285343
7	1	0	-2.639624	-1.122349	-2.090163
8	1	0	-2.657846	-0.974342	2.209944
9	1	0	-2.462069	0.519131	1.301507
10	1	0	-2.468531	-2.299012	0.105860
11	1	0	-3.808234	-1.155086	0.058064
12	1	0	-0.143939	1.082077	-0.008704
13	16	0	-0.414165	-0.699039	1.584496
14	16	0	-0.398973	-0.814352	-1.463623

1.9 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.174709	-0.590256	-1.184850
2	6	0	0.062677	-0.047191	0.005052
3	6	0	-2.158691	-0.553790	1.242567
4	6	0	-2.688009	-1.189667	0.041454
5	1	0	1.141416	-0.115877	-0.001229
6	1	0	-2.502667	0.423561	-1.237623
7	1	0	-2.718051	-1.068124	-1.971734
8	1	0	-2.689667	-1.010550	2.050178
9	1	0	-2.488700	0.460290	1.271986
10	1	0	-2.160626	-2.130318	0.053305
11	1	0	-3.762215	-1.272630	0.050360
12	1	0	0.052319	1.029543	-0.012307
13	34	0	-0.547096	-0.842010	-1.482387
14	34	0	-0.526412	-0.795122	1.524506

1.10 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.136543	-0.692642	-1.344162
2	6	0	0.001000	-0.037354	0.157343
3	6	0	-2.024748	-0.611486	1.180355
4	6	0	-2.634781	-1.294189	-0.036573
5	1	0	1.075249	-0.079311	0.315607
6	1	0	-2.438103	0.353749	-1.427962
7	1	0	-2.536838	-1.224427	-2.204674
8	1	0	-2.378016	-1.078159	2.097843
9	1	0	-2.322172	0.447029	1.200943
10	1	0	-2.398217	-2.358615	-0.008149
11	1	0	-3.721128	-1.190851	0.023037
12	1	0	-0.322229	1.009926	0.120659
13	8	0	-0.614213	-0.700064	1.218086
14	16	0	-0.324921	-0.795180	-1.466041

1.11 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.192019	-0.464668	-1.243681
2	6	0	-0.066132	-0.021459	0.061166
3	6	0	-2.098252	-0.343554	1.212979
4	6	0	-2.744555	-1.000132	0.017784
5	1	0	0.973610	-0.207886	0.291451
6	1	0	-2.401910	0.581654	-1.315490
7	1	0	-2.783892	-0.825359	-2.060871
8	1	0	-2.453612	-0.837340	2.110874
9	1	0	-2.338134	0.730255	1.272860
10	1	0	-2.383472	-2.020350	0.084052
11	1	0	-3.822340	-0.965379	0.125115
12	1	0	-0.194793	1.056486	0.005348
13	8	0	-0.699232	-0.499328	1.227656
14	34	0	-0.559895	-0.883919	-1.405748

1.12 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.130130	-0.491953	-1.248025
2	6	0	0.102453	-0.018451	-0.081514
3	6	0	-2.317181	-0.434164	1.221152
4	6	0	-2.731974	-1.125962	-0.061715
5	1	0	1.172659	-0.158241	-0.005722
6	1	0	-2.268719	0.553343	-1.105598
7	1	0	-2.768501	-0.711507	-2.080120
8	1	0	-2.742028	-0.975219	2.055226
9	1	0	-2.633101	0.607534	1.281039
10	1	0	-2.261916	-2.090526	0.089351
11	1	0	-3.812442	-1.214601	-0.071094
12	1	0	-0.032752	1.048712	-0.243284
13	34	0	-0.557283	-0.952835	-1.519114
14	16	0	-0.526972	-0.535067	1.527122

2.1 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.079781	-0.540507	-1.339438
2	6	0	-0.553873	-0.615380	-1.312184
3	6	0	-0.006854	-0.084191	-0.005181
4	6	0	-0.618064	-0.727423	1.220637
5	6	0	-2.143563	-0.651322	1.178468
6	6	0	-2.691981	-1.232327	-0.123035
7	1	0	-0.224715	-1.652169	-1.406021
8	1	0	-0.106639	-0.048694	-2.128440
9	1	0	-2.386768	0.507632	-1.354107
10	1	0	-2.449235	-0.991468	-2.260491
11	1	0	-0.292146	-1.769401	1.237729
12	1	0	-0.212097	-0.236539	2.104687
13	1	0	-2.557056	-1.179142	2.037892
14	1	0	-2.452159	0.392432	1.269600
15	1	0	-2.467918	-2.302995	-0.165136
16	1	0	-3.778023	-1.136501	-0.146976
17	9	0	-0.216311	1.273519	0.049682
18	9	0	1.352379	-0.245757	0.022136

2.2 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.344965	-0.639185	-1.132366
2	6	0	0.370302	0.092344	-0.006844
3	6	0	-2.220570	-0.500273	1.442941
4	6	0	-2.754992	-1.256557	0.214948
5	1	0	-0.050988	-2.142588	-1.561269
6	1	0	-0.137141	-0.021935	-2.759137
7	1	0	-2.647065	0.411478	-1.163105
8	1	0	-2.883451	-1.133980	-1.943762
9	1	0	0.109433	-1.965050	1.807057
10	1	0	0.130621	0.270418	2.778028
11	1	0	-2.678026	-0.902490	2.349548
12	1	0	-2.522668	0.549386	1.388542
13	1	0	-2.429183	-2.300083	0.256148
14	1	0	-3.845204	-1.282153	0.270082
15	14	0	-0.351495	-0.561803	1.650713
16	14	0	-0.503552	-0.729188	-1.509446
17	9	0	0.117183	1.461402	-0.067211
18	9	0	1.739494	-0.047579	-0.066107

2.3 orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.240913	-0.757498	-1.186946
2	6	0	0.317039	0.006978	0.034502
3	6	0	-2.221224	-0.659515	1.349354
4	6	0	-2.740552	-1.363160	0.110346
5	1	0	-2.489358	0.301427	-1.172966
6	1	0	-2.813619	-1.177068	-2.006757
7	1	0	-2.781845	-1.013235	2.207588
8	1	0	-2.467784	0.395744	1.256773
9	1	0	-2.455037	-2.416948	0.149544
10	1	0	-3.831744	-1.345567	0.118089
11	1	0	0.024711	-2.151165	1.740311
12	1	0	0.002807	-2.269761	-1.504992
13	32	0	-0.386041	-0.741823	1.654770
14	32	0	-0.410637	-0.858740	-1.515242
15	1	0	-0.017891	0.131131	2.765551
16	1	0	-0.063960	-0.067201	-2.691976
17	9	0	1.690921	0.067254	0.021397
18	9	0	-0.125948	1.328156	-0.010275

2.4aa orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.970410	-0.541294	-1.352926
2	6	0	-0.026578	-0.080502	-0.001867
3	6	0	-2.085071	-0.610938	1.137481
4	6	0	-2.632134	-1.216267	-0.153444
5	1	0	-2.298572	0.497523	-1.421710
6	1	0	-2.249130	-1.024745	-2.287328
7	1	0	-2.448210	-1.143035	2.014668
8	1	0	-2.420134	0.423650	1.232354
9	1	0	-2.423796	-2.290358	-0.174317
10	1	0	-3.714850	-1.091407	-0.200675
11	7	0	-0.621979	-0.610042	1.187115
12	7	0	-0.509250	-0.541549	-1.267702
13	1	0	-0.256446	-1.540022	1.339514
14	1	0	-0.129464	-1.462853	-1.436888
15	9	0	1.297410	-0.349657	0.051302
16	9	0	-0.188218	1.266842	0.028348

2.4ae orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.064176	-0.276885	-1.375918
2	6	0	-0.072282	0.014951	-0.036467
3	6	0	-2.133296	-0.447871	1.105707
4	6	0	-2.733941	-0.967116	-0.197130
5	1	0	-0.125970	0.009006	-2.037355
6	1	0	-2.359990	0.779514	-1.398175
7	1	0	-2.377975	-0.729393	-2.315106
8	1	0	-2.514506	-0.991841	1.967797
9	1	0	-2.393582	0.602288	1.248103
10	1	0	-2.575240	-2.045257	-0.272253
11	1	0	-3.808503	-0.783267	-0.222354
12	7	0	-0.673324	-0.549708	1.119628
13	7	0	-0.612556	-0.430081	-1.268212
14	1	0	-0.377138	-1.514526	1.178721
15	9	0	1.249846	-0.267822	-0.028441
16	9	0	-0.158303	1.388780	0.072595

2.4ee orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.096175	-0.474601	-1.237363
2	6	0	-0.068063	-0.049835	0.006199
3	6	0	-2.099855	-0.464545	1.246917
4	6	0	-2.696920	-1.108423	0.006472
5	1	0	-0.184358	-0.167697	-1.969674
6	1	0	-2.430463	0.567283	-1.319697
7	1	0	-2.422176	-1.000682	-2.133007
8	1	0	-0.190201	-0.152198	1.982592
9	1	0	-2.428785	-0.983208	2.145798
10	1	0	-2.434171	0.578051	1.319657
11	1	0	-2.479208	-2.176965	0.011227
12	1	0	-3.778577	-0.976286	0.004265
13	7	0	-0.643895	-0.564874	1.180735
14	7	0	-0.640407	-0.574100	-1.165947
15	9	0	1.262205	-0.288695	0.009135
16	9	0	-0.131486	1.364004	0.000526

2.5aa orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.235095	-0.568783	-1.271247
2	6	0	0.228916	0.045092	0.014015
3	6	0	-2.237253	-0.570240	1.294428
4	6	0	-2.735734	-1.226607	0.010801
5	1	0	-2.516474	0.486984	-1.294352
6	1	0	-2.713536	-1.025326	-2.139098
7	1	0	-2.717156	-1.027739	2.160969
8	1	0	-2.518649	0.485507	1.318244
9	1	0	-2.460141	-2.284072	0.010426
10	1	0	-3.828333	-1.190575	0.009876
11	15	0	-0.418194	-0.624321	1.649782
12	1	0	-0.198221	-1.982259	1.309897
13	15	0	-0.415451	-0.622432	-1.623607
14	1	0	-0.196028	-1.980762	-1.284928
15	9	0	1.586184	-0.111228	0.015072
16	9	0	-0.017723	1.396588	0.014597

2.5ae orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.266850	-0.457461	-1.298595
2	6	0	0.206988	0.045852	0.010433
3	6	0	-2.234500	-0.533718	1.262047
4	6	0	-2.793471	-1.127347	-0.030566
5	1	0	-2.512021	0.607178	-1.295578
6	1	0	-2.757969	-0.878402	-2.177285
7	1	0	-2.747239	-0.968356	2.120574
8	1	0	-2.405336	0.542810	1.289057
9	1	0	-2.582554	-2.199047	-0.070050
10	1	0	-3.880985	-1.024566	-0.014161
11	15	0	-0.428903	-0.911898	1.489805
12	15	0	-0.446604	-0.557155	-1.652178
13	1	0	-0.268090	-1.931747	-1.354994
14	1	0	-0.130815	0.095116	2.440662
15	9	0	1.570144	-0.040077	-0.008330
16	9	0	-0.090284	1.383315	0.097191

2.5ee Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.206083	-0.518677	-1.307292
2	6	0	0.219980	-0.011668	0.006120
3	6	0	-2.226825	-0.586992	1.252399
4	6	0	-2.759351	-1.192311	-0.048865
5	1	0	-2.390698	0.554861	-1.268282
6	1	0	-2.714572	-0.909936	-2.188789
7	1	0	-2.748696	-1.025007	2.103606
8	1	0	-2.412541	0.486982	1.268939
9	1	0	-2.548788	-2.264798	-0.076275
10	1	0	-3.846031	-1.089378	-0.055117
11	15	0	-0.416935	-0.934763	1.515911
12	15	0	-0.392521	-0.854828	-1.559366
13	1	0	-0.136115	0.116717	2.421539
14	1	0	-0.096336	0.240993	-2.405631
15	9	0	1.586432	-0.031929	0.016697
16	9	0	-0.125807	1.316505	0.038152

2.6aa orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.230019	-0.570765	-1.173294
2	6	0	0.245580	-0.016447	-0.006695
3	6	0	-2.169586	-0.510020	1.301715
4	6	0	-2.774049	-1.142906	0.093001
5	1	0	-2.492206	0.482806	-1.201153
6	1	0	-2.793609	-0.939252	-2.022205
7	1	0	-2.692148	-0.834158	2.193827
8	1	0	-2.429440	0.544428	1.289109
9	1	0	-2.483502	-2.190512	0.111632
10	1	0	-3.856485	-1.054540	0.117730
11	33	0	-0.411697	-0.615589	1.676624
12	33	0	-0.491577	-0.694050	-1.626114
13	1	0	-0.178426	-1.949758	1.480447
14	1	0	-0.246265	-2.017475	-1.379115
15	9	0	1.605588	-0.141935	-0.036913
16	9	0	-0.011951	1.340038	-0.032503

2.6ae orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.087679	-0.569914	-1.317400
2	6	0	0.261221	-0.015423	-0.053935
3	6	0	-2.259135	-0.549339	1.101099
4	6	0	-2.819902	-1.133547	-0.156064
5	1	0	-2.200991	0.506226	-1.280877
6	1	0	-2.590845	-0.814353	-2.249358
7	1	0	-2.839283	-0.858217	1.964927
8	1	0	-2.456391	0.518208	1.086593
9	1	0	-2.647489	-2.208428	-0.118014
10	1	0	-3.879699	-0.921137	-0.263749
11	1	0	-0.261539	0.399076	-2.406932
12	33	0	-0.520119	-0.753965	1.530413
13	33	0	-0.323256	-0.763701	-1.708104
14	1	0	-0.331936	-2.079382	1.238444
15	9	0	1.617642	-0.018805	0.053958
16	9	0	-0.107014	1.323154	-0.010467

2.6ee orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.133126	-0.619013	-1.216538
2	6	0	0.220989	-0.001608	0.024006
3	6	0	-2.165899	-0.595565	1.213590
4	6	0	-2.842695	-1.114363	-0.005920
5	1	0	-2.209110	0.463012	-1.192383
6	1	0	-2.668155	-0.894030	-2.121905
7	1	0	-2.724583	-0.854104	2.109470
8	1	0	-2.240789	0.485738	1.166618
9	1	0	-2.870246	-2.204210	0.004545
10	1	0	-3.860399	-0.735151	-0.023708
11	1	0	-0.312237	0.302931	2.368462
12	1	0	-0.249966	0.258780	-2.339042
13	33	0	-0.411684	-0.834196	1.634979
14	33	0	-0.368583	-0.864579	-1.587438
15	9	0	1.575355	0.148465	0.041018
16	9	0	-0.272210	1.307884	0.004983

2.7 Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.156066	-0.552592	-1.081440
2	6	0	-0.143999	-0.101205	0.021987
3	6	0	-2.002261	-0.525305	1.378051
4	6	0	-2.700282	-1.168498	0.194257
5	1	0	-2.463732	0.492013	-1.178466
6	1	0	-2.474435	-1.092629	-1.968328
7	1	0	-2.205012	-1.046242	2.309258
8	1	0	-2.297448	0.521177	1.491269
9	1	0	-2.513221	-2.242493	0.194214
10	1	0	-3.775875	-1.004911	0.261008
11	8	0	-0.585026	-0.597291	1.207228
12	8	0	-0.728392	-0.623861	-1.087783
13	9	0	1.157145	-0.347528	-0.056535
14	9	0	-0.294409	1.260391	0.015511

2.8 Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.237123	-0.357199	-1.347238
2	6	0	0.122742	0.057359	0.016917
3	6	0	-2.325632	-0.404807	1.194313
4	6	0	-2.837992	-1.001622	-0.107467
5	1	0	-2.420396	0.717096	-1.359899
6	1	0	-2.677605	-0.777640	-2.249543
7	1	0	-2.828017	-0.856116	2.048059
8	1	0	-2.508516	0.668914	1.233492
9	1	0	-2.654700	-2.076503	-0.121494
10	1	0	-3.920125	-0.850442	-0.143351
11	16	0	-0.560552	-0.705540	1.516602
12	16	0	-0.453155	-0.645342	-1.555743
13	9	0	1.456255	-0.119716	0.060073
14	9	0	-0.103377	1.396669	0.035377

2.9 Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.161337	-0.457025	-1.330763
2	6	0	0.042576	-0.076101	-0.015817
3	6	0	-2.251859	-0.580408	1.082563
4	6	0	-2.711436	-1.156034	-0.175471
5	1	0	-2.461984	0.561353	-1.297612
6	1	0	-2.687054	-0.850871	-2.173832
7	1	0	-2.839730	-1.052713	1.839959
8	1	0	-2.550776	0.437955	1.129551
9	1	0	-2.185678	-2.096398	-0.204952
10	1	0	-3.782700	-1.251000	-0.221590
11	34	0	-0.540322	-0.742245	-1.616365
12	34	0	-0.656622	-0.901052	1.459320
13	9	0	1.393907	-0.168279	0.030409
14	9	0	-0.215625	1.275234	0.044479

2.10 Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.217792	-0.609043	-1.334020
2	6	0	0.002717	-0.049325	0.127331
3	6	0	-2.056213	-0.528822	1.175959
4	6	0	-2.687850	-1.214793	-0.021333
5	1	0	-2.512859	0.437066	-1.414659
6	1	0	-2.628823	-1.141321	-2.188916
7	1	0	-2.360952	-1.002774	2.104813
8	1	0	-2.338918	0.525995	1.216970
9	1	0	-2.454431	-2.279771	0.001810
10	1	0	-3.771278	-1.106110	0.062003
11	8	0	-0.630242	-0.630750	1.171702
12	16	0	-0.409253	-0.728447	-1.515525
13	9	0	1.313357	-0.224466	0.316021
14	9	0	-0.224092	1.296279	0.143093

2.11 Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.140971	-0.547973	-1.341162
2	6	0	-0.064542	-0.122840	0.048163
3	6	0	-2.150054	-0.544020	1.112407
4	6	0	-2.703518	-1.179566	-0.133160
5	1	0	-2.375130	0.488703	-1.340662
6	1	0	-2.701057	-0.875149	-2.191663
7	1	0	-2.449449	-1.128231	1.972574
8	1	0	-2.488402	0.489048	1.247508
9	1	0	-2.282847	-2.177928	-0.099367
10	1	0	-3.782299	-1.218153	-0.059042
11	8	0	-0.722997	-0.550908	1.146038
12	34	0	-0.511800	-0.928187	-1.511158
13	9	0	1.237698	-0.316698	0.311120
14	9	0	-0.221720	1.239379	-0.061956

2.12 Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.170396	-0.258065	-1.279616
2	6	0	0.091812	0.014951	-0.080554
3	6	0	-2.377396	-0.356175	1.175558
4	6	0	-2.801789	-0.954604	-0.146474
5	1	0	-2.260867	0.780145	-1.095140
6	1	0	-2.800790	-0.398077	-2.134850
7	1	0	-2.819625	-0.926222	1.980711
8	1	0	-2.644259	0.692881	1.293465
9	1	0	-2.371195	-1.946132	-0.061763
10	1	0	-3.884055	-1.002269	-0.174080
11	34	0	-0.630768	-0.798264	-1.587885
12	16	0	-0.587355	-0.525992	1.508094
13	9	0	1.418362	-0.215851	-0.020991
14	9	0	-0.042430	1.369564	-0.221651

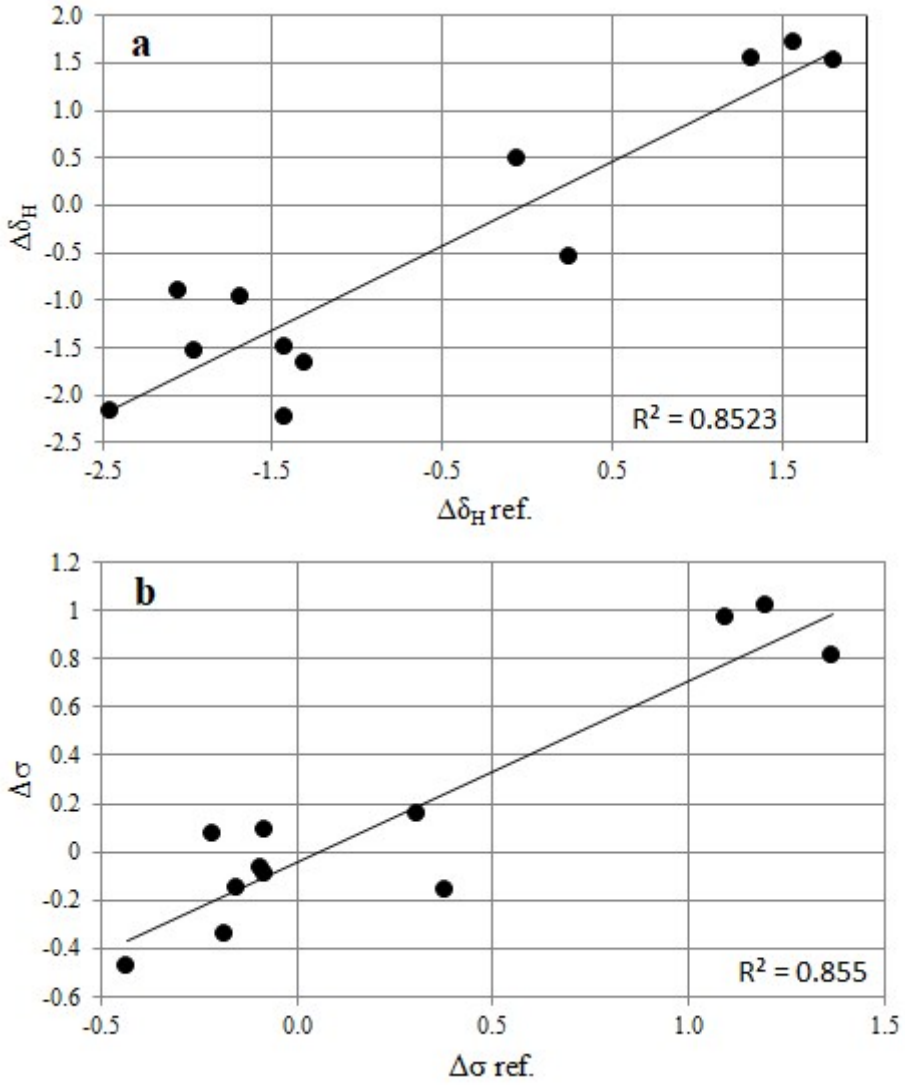

Figure S3. Validation of the calculated data obtained in this work by comparison with the literature (ref. 22): a) $\Delta\delta_{ref} \times \Delta\delta$; b) $\Delta\sigma_{ref} \times \Delta\sigma$

Table S1. Total delocalization[a] (kcal mol^{-1}) and orbital occupancies for the studied compounds.

Periodic family	Compound	Δdelocalization[a]	Δoccupancy(σ)	Δoccupancy(σ*)
4A	**1**.1	3.05	-0.00152	0.00509
	1.2	0.17	-0.00228	0.00020
	1.3	-0.69	-0.00252	-0.00054
5A	**1**.4aa	4.63	-0.00175	0.01278
	1.4ae	7.60	0.00435	0.02336
	1.4ee	11.88	0.01113	0.03804
	1.5aa	2.20	0.00019	0.00395
	1.5ae	2.49	0.00415	0.00635
	1.5ee	2.96	0.01015	0.01127
	1.6aa	1.45	0.00016	0.00402
	1.6ae	1.57	0.00086	0.00300
	1.6ee	2.06	0.00560	0.00547
6A	**1**.7	7.74	0.00801	0.02417
	1.8	7.04	0.00739	0.02088
	1.9	14.03	0.00849	0.02831
	1.10	6.67	0.00668	0.02046
	1.11	9.35	0.00795	0.02487
	1.12	8.14	0.00718	0.02290
4A	**2**.1	4.73	-0.00008	0.00610
	2.2	2.10	-0.00046	0.00241
	2.3	1.49	-0.00054	0.00212
5A	**2**.4aa	13.61	0.00054	0.02694
	2.4ae	19.53	0.00162	0.04992
	2.4ee	34.09	0.00282	0.08757
	2.5aa	3.75	-0.00025	0.00537
	2.5ae	4.04	-0.00005	0.01157
	2.5ee	5.26	0.00020	0.02294
	2.6aa	4.10	-0.00054	0.00780
	2.6ae	4.98	-0.00074	0.01476
	2.6ee	7.40	-0.00077	0.03000
6A	**2**.7	27.75	0.00242	0.05615
	2.8	16.61	0.00058	0.04438
	2.9	21.35	0.00013	0.05805
	2.10	22.14	0.00149	0.04704
	2.11	25.90	0.00151	0.05594
	2.12	18.68	-0.00004	0.05199

[a] Total delocalization to σ^*_{CHeq} (or σ^*_{CFeq}) and σ^*_{CHax} (or σ^*_{CFax}).

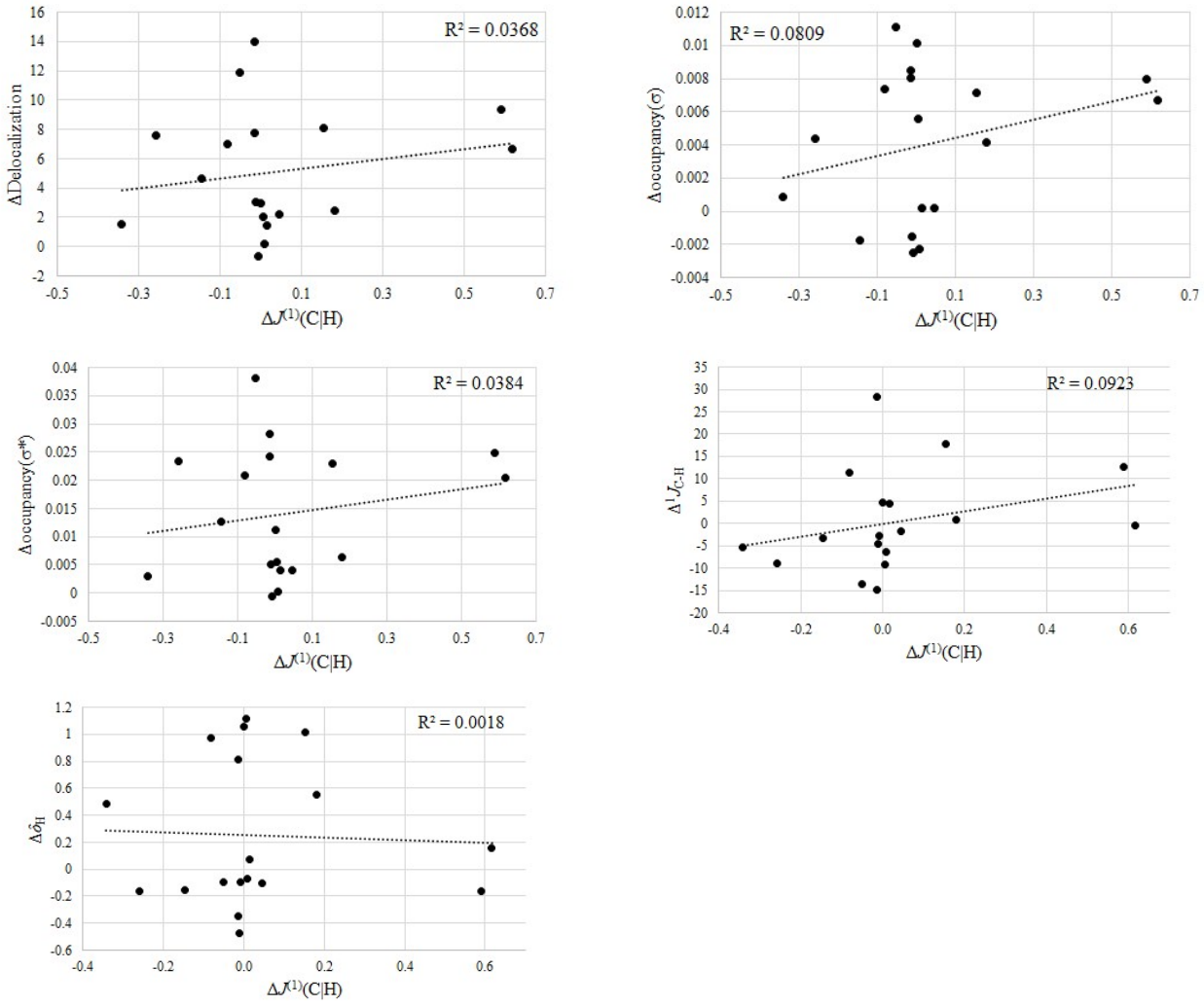

Figure S4. Relationship between $\Delta J^{(1)}$(C|H) ($\times 10^{-3}$, in a.u.) as described elsewhere[22] and delocalization, occupancy at $\sigma_{C\text{-}H}$ and $\sigma^*_{C\text{-}H}$, $\Delta^1 J_{C\text{-}H}$ and $\Delta\delta_H$ for hydrogenated molecules **1**.

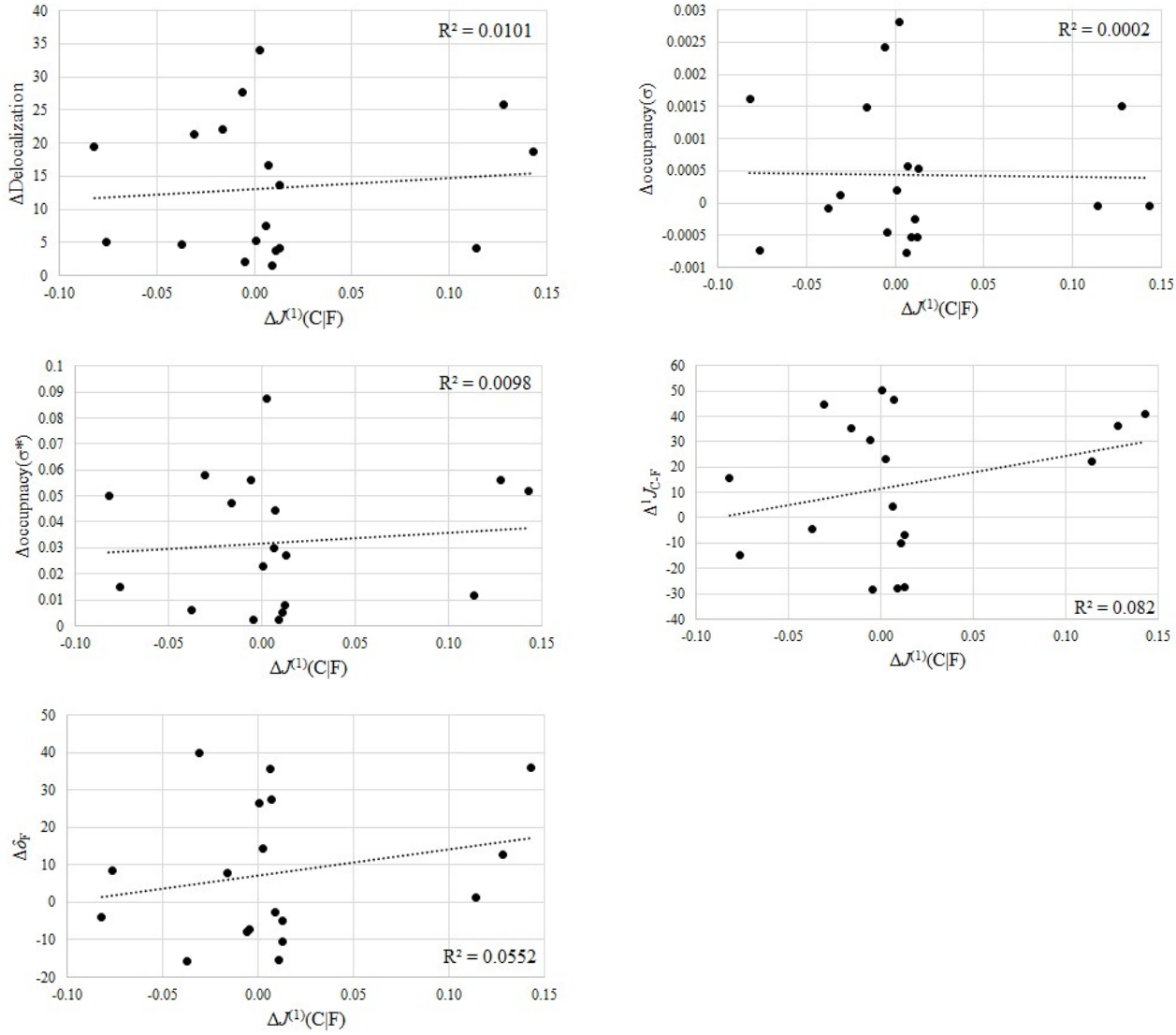

Figure S5. Relationship between $\Delta J^{(1)}$(C|F) ($\times 10^{-3}$, in a.u.) as described elsewhere[22] and delocalization, occupancy at $\sigma_{C\text{-}F}$ and $\sigma^*_{C\text{-}F}$, $\Delta^1 J_{C\text{-}F}$ and $\Delta\delta_F$ for fluorinated molecules **2**.

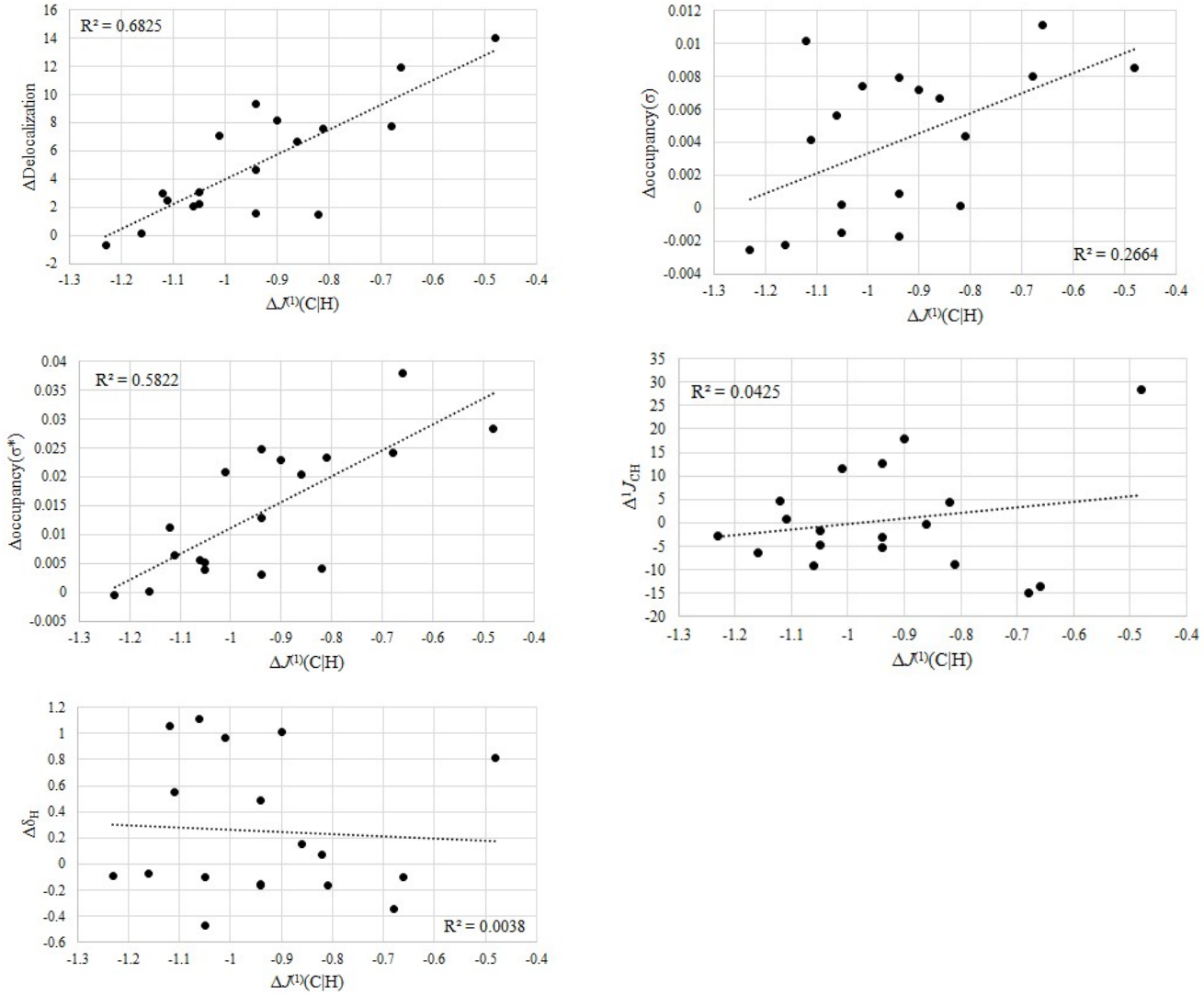

Figure S6. Relationship between $\Delta J^{(1)}$(C|H) ($\times 10^{-3}$, in a.u.) obtained with **B** perpendicular to both geminal atoms and delocalization, occupancy at $\sigma_{C\text{-}H}$ and $\sigma^*_{C\text{-}H}$, $\Delta^1 J_{C\text{-}H}$ and $\Delta\delta_H$ for hydrogenated molecules **1**.

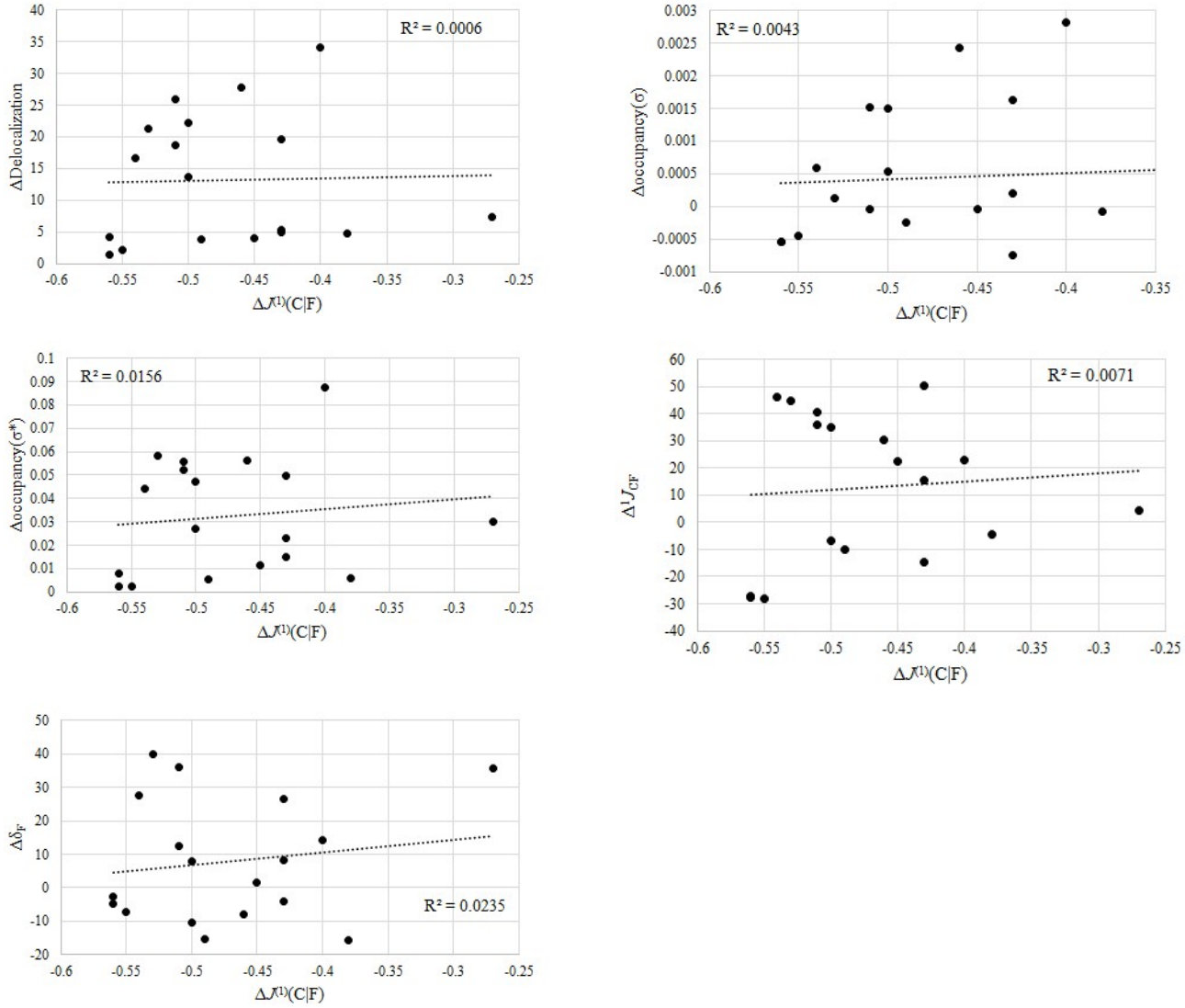

Figure S7. Relationship between $\Delta J^{(1)}$(C|F) ($\times 10^{-3}$, in a.u.) obtained with **B** perpendicular to both geminal atoms and delocalization, occupancy at $\sigma_{C\text{-}H}$ and $\sigma^*_{C\text{-}H}$, $\Delta^1J_{C\text{-}H}$ and $\Delta\delta_F$ for fluorinated molecules **2**.

Table S2. Angular dependence of delocalization (kcal mol^{-1}), σ^*_{CH} occupancy, SSCC (Hz), chemical shift (ppm), dipolar moment (debye) and ICD (a.u.) for ethane.

H–C–C–H	Delocal.	Occup.	Dip. Mom.	$^1J_{CH}$	δ_H	$J^{(1)}$(C|H)[a]	$J^{(1)}$(C|H)[b]
0	2.82	0.00570	0.0007	102.94	0.883	-0.000324969	-0.000638800
30	3.22	0.00673	0.0060	103.49	0.894	-0.000194865	-0.000659609
60	3.21	0.00794	0.0001	103.57	0.893	-0.000157725	-0.000760295
90	3.33	0.00696	0.0140	103.19	0.896	-0.000260992	-0.000736392
120	2.78	0.00564	0.0013	102.94	0.880	-0.000327990	-0.000809352
150	3.29	0.00693	0.0195	103.71	0.897	-0.000198082	-0.000717186
180	3.20	0.00794	0.0002	103.53	0.892	-0.000159727	-0.000681686
210	3.30	0.00693	0.0201	103.73	0.896	-0.000270516	-0.000766354
240	2.77	0.00564	0.0005	102.87	0.882	-0.000332368	-0.000693767
270	3.32	0.00696	0.0136	103.29	0.895	-0.000199750	-0.000618412
300	3.20	0.00793	0.0006	103.75	0.895	-0.000154044	-0.000716106
330	3.22	0.00673	0.0060	103.55	0.894	-0.000266579	-0.000769014
360	2.82	0.00570	0.0007	102.94	0.883	-0.000324969	-0.000638800

[a] First-order electronic current density over the analyzed hydrogen with magnetic field perpendicular to the hydrogen of interest and parallel to the geminal hydrogens, as described elsewhere[22] (J_XX(C|H) to hydrogen located along the Y-axis). [b] First-order electronic current density over the studied hydrogen with magnetic field perpendicular to both geminal hydrogens (J_YZ(C|H) and a hydrogen located along the Y-axis. This specific orientation is due to a better correlation with Δdelocalization.

Table S3. Angular dependence of delocalization (kcal mol^{-1}), σ^*_{CF} occupancy, SSCC (Hz), chemical shift (ppm), dipolar moment (debye) and ICD (a.u.) for 1,1-difluoroethane.

F–C–C–H	Delocal.	Occup.	Dip. Mom.	$\|^1J_{CF}\|$	δ_F	$J^{(1)}$(C|F)[a]	$J^{(1)}$(C|F)[b]
0	27.96	0.05709	2.2520	296.04	-110.20	0.000009579	-0.000430604
30	28.22	0.05698	2.2762	294.90	-116.04	0.000029851	-0.000323015
60	29.01	0.05907	2.2615	293.88	-119.83	0.000016102	-0.000384660
90	28.82	0.05938	2.2483	295.58	-114.45	0.000009186	-0.000365611
120	27.93	0.05703	2.2517	296.20	-110.29	0.000012438	-0.000376605
150	28.28	0.05721	2.2616	295.18	-115.91	0.000026148	-0.000395204
180	28.71	0.05902	2.2652	293.80	-119.69	0.000013161	-0.000418093
210	28.81	0.05940	2.2545	295.45	-113.53	0.000008645	-0.000407107
240	27.94	0.05706	2.2521	296.06	-110.34	0.000010683	-0.000424321
270	28.27	0.05706	2.2808	295.01	-116.87	0.000021766	-0.000376782
300	29.00	0.05899	2.2642	293.90	-119.69	0.000019961	-0.000365300
330	28.62	0.05878	2.2348	295.26	-114.62	0.000000664	-0.000395749
360	27.96	0.05709	2.2520	296.04	-110.20	0.000009579	-0.000430604

[a] First-order electronic current density over the analyzed fluorine with magnetic field perpendicular to the fluorine of interest and parallel to the geminal fluorines (J_XX(C|F) to fluorine located along the Y-axis). [b] First-order electronic current density over the studied fluorine with magnetic field perpendicular to both geminal fluorines (J_YZ(C|F) and a fluorine located along the Y-axis. This specific orientation is due to a better correlation with Δdelocalization found for the hydrogenated analog.

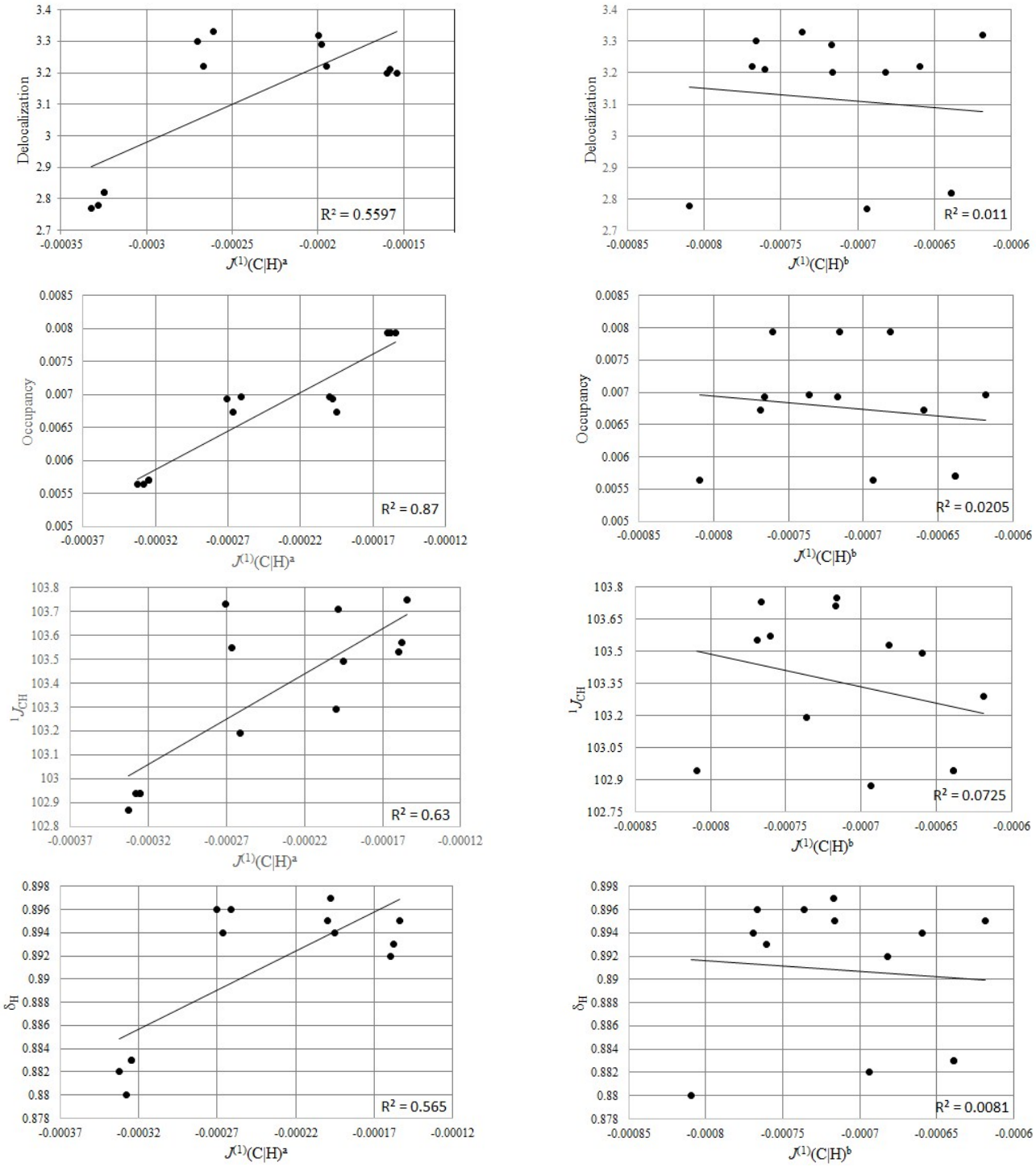

Figure S8. Relationship between ICD[a] and delocalization, occupancy, SSCC's and chemical shift (first column); and between ICD[b] and delocalization, occupancy, SSCC's and chemical shift (second column) to ethane.

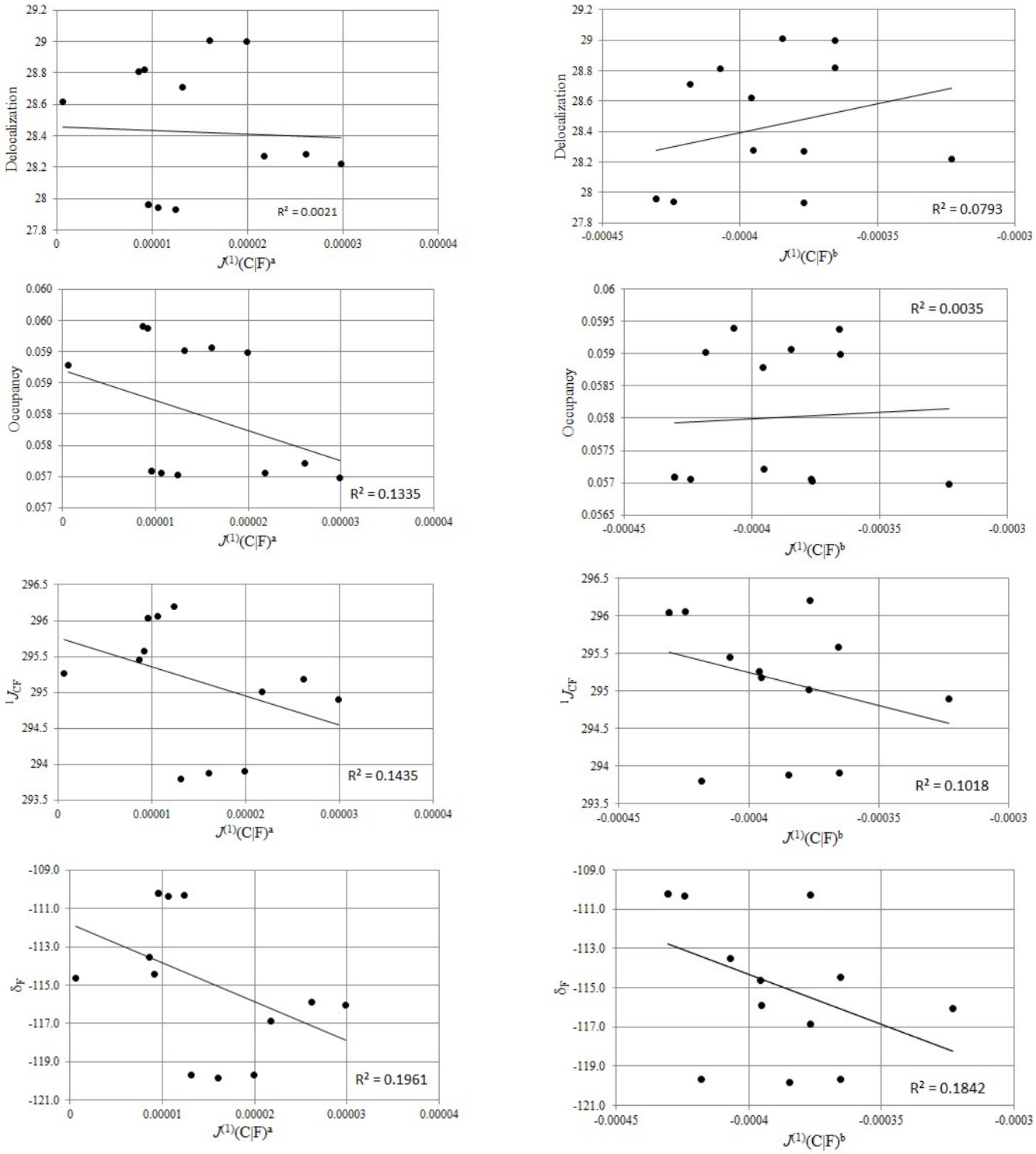

Figure S9. Relationship between ICD[a] and delocalization, occupancy, SSCC's and chemical shift (first column); and between ICD[b] and delocalization, occupancy, SSCC's and chemical shift (second column) to 1,1-difluoroethane.

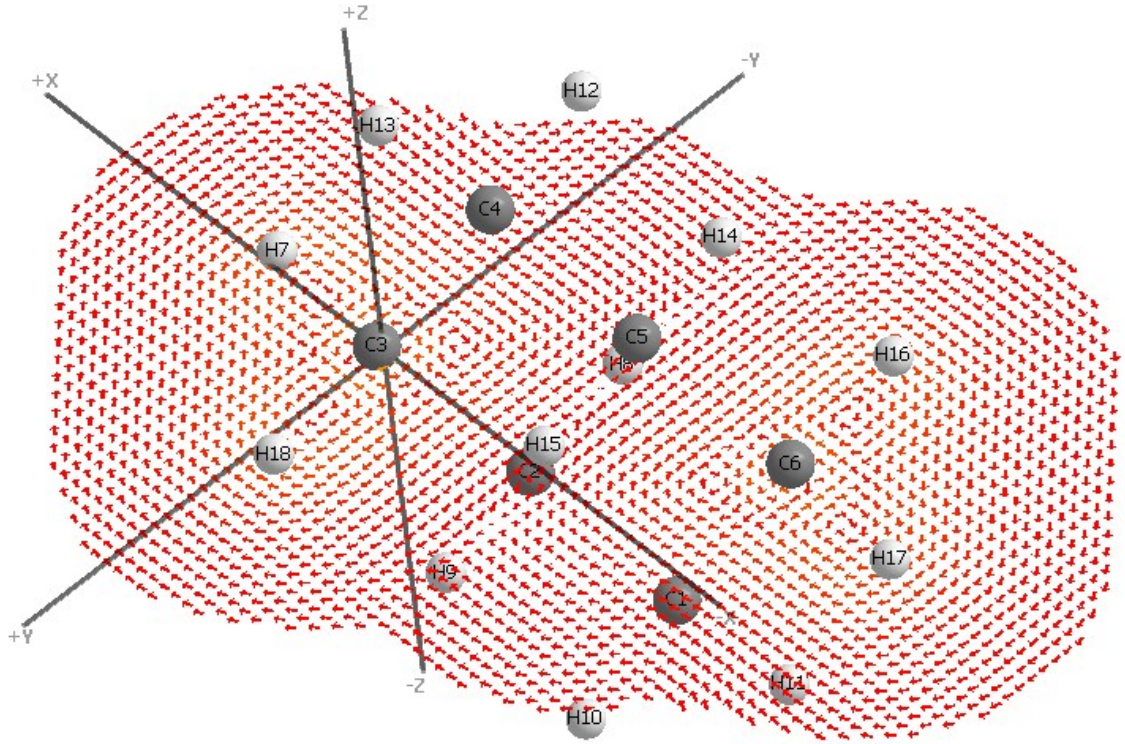

Figure S10. ICD behavior for molecule **1.1** with **B** applied along the z-axis (Perlin effect).

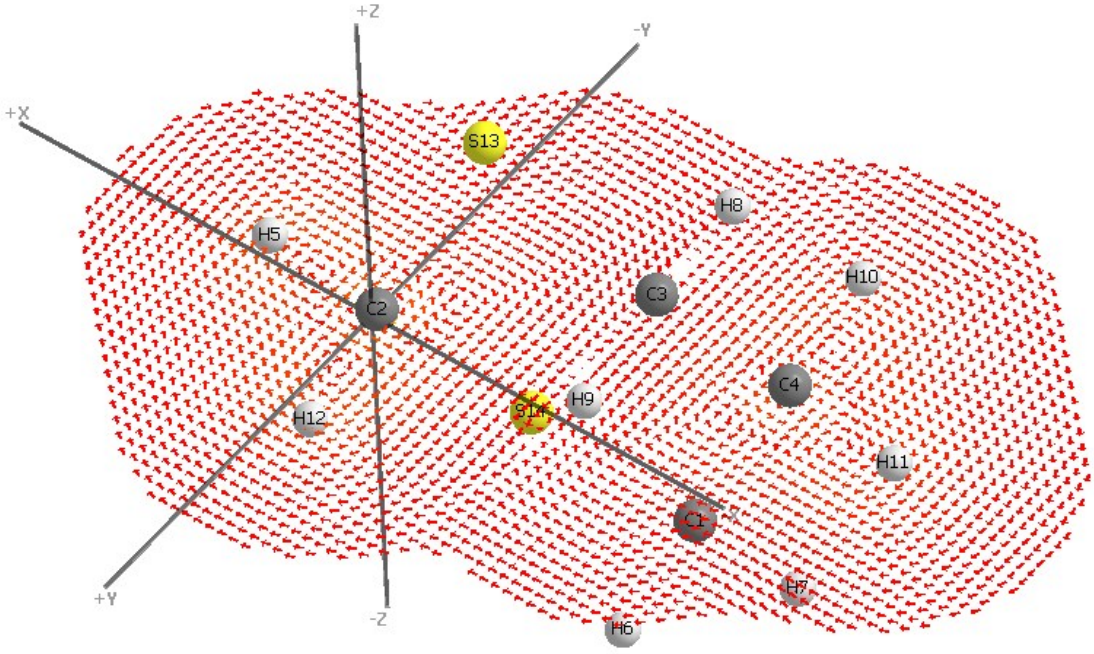

Figure S11. ICD behavior for molecule **1.8** with **B** applied along the z-axis (Reverse Perlin effect).

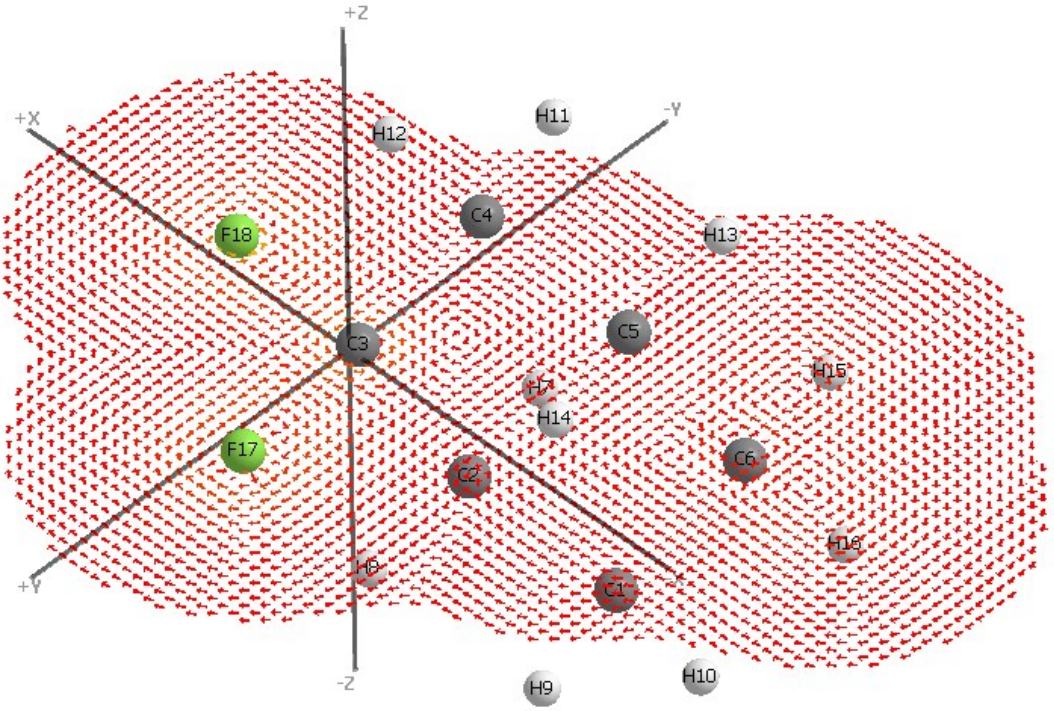

Figure S12. ICD behavior for molecule **2.1** with **B** applied along the z-axis (Fluorine Perlin effect).

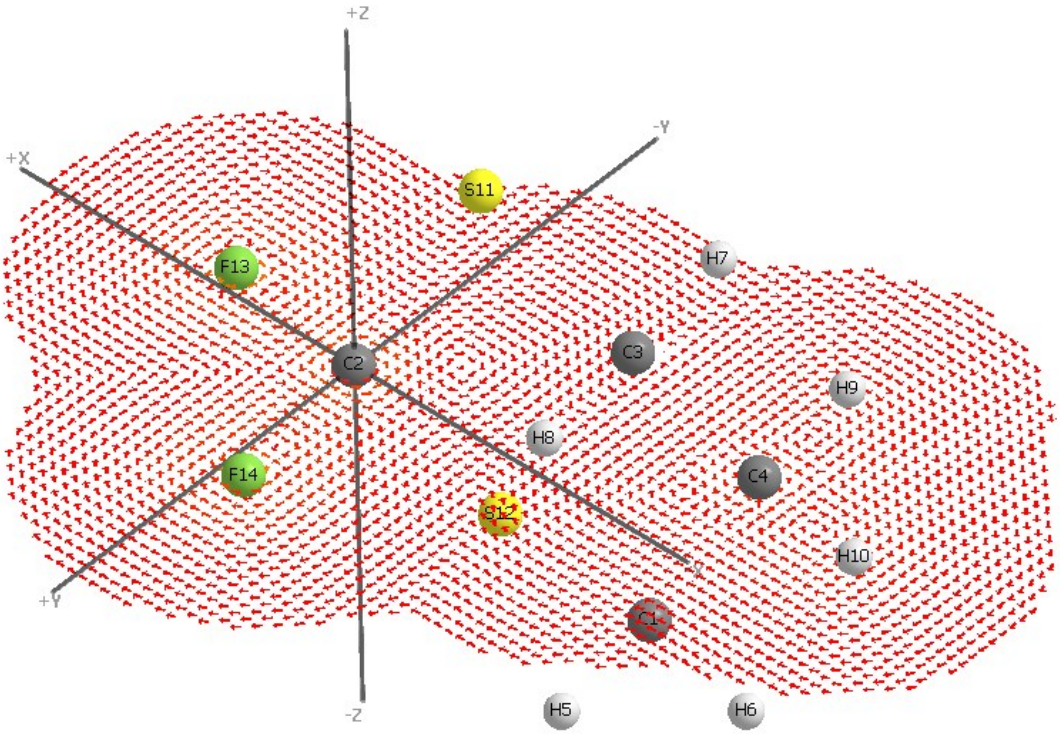

Figure S13. ICD behavior for molecule **2.8** with **B** applied along z-axis (Reverse Fluorine Perlin effect).

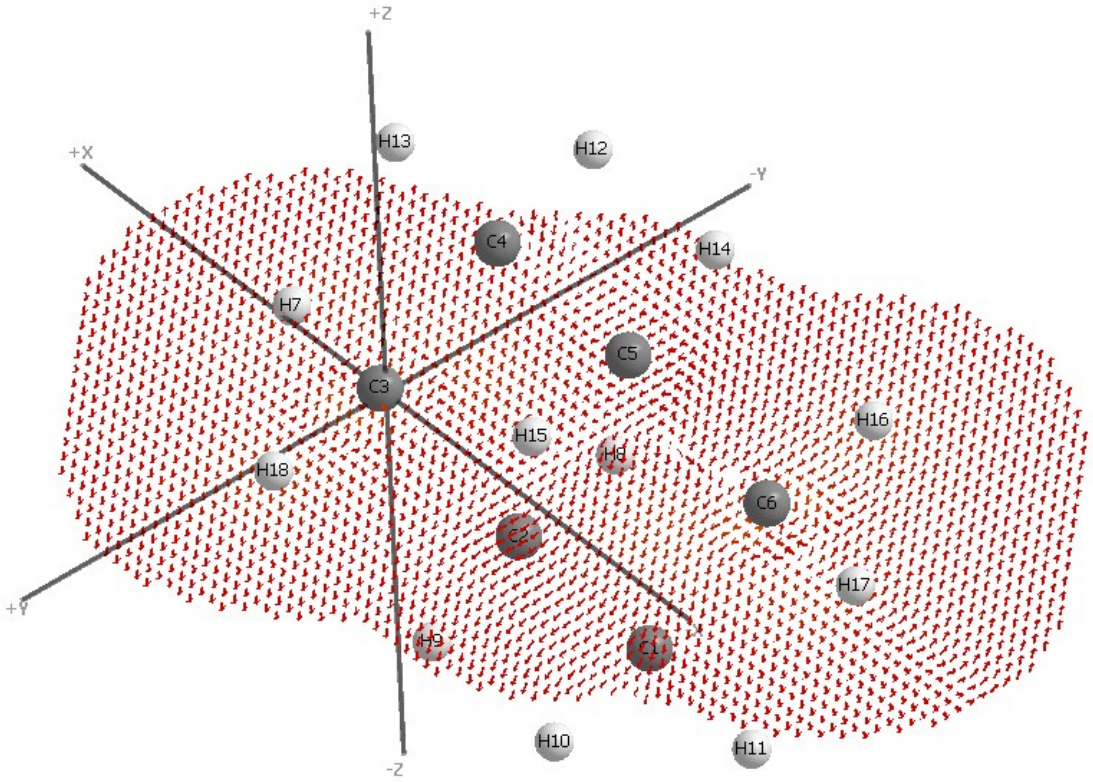

Figure S14. ICD behavior for molecule **1.1** with **B** applied along the x-axis (Perlin effect).

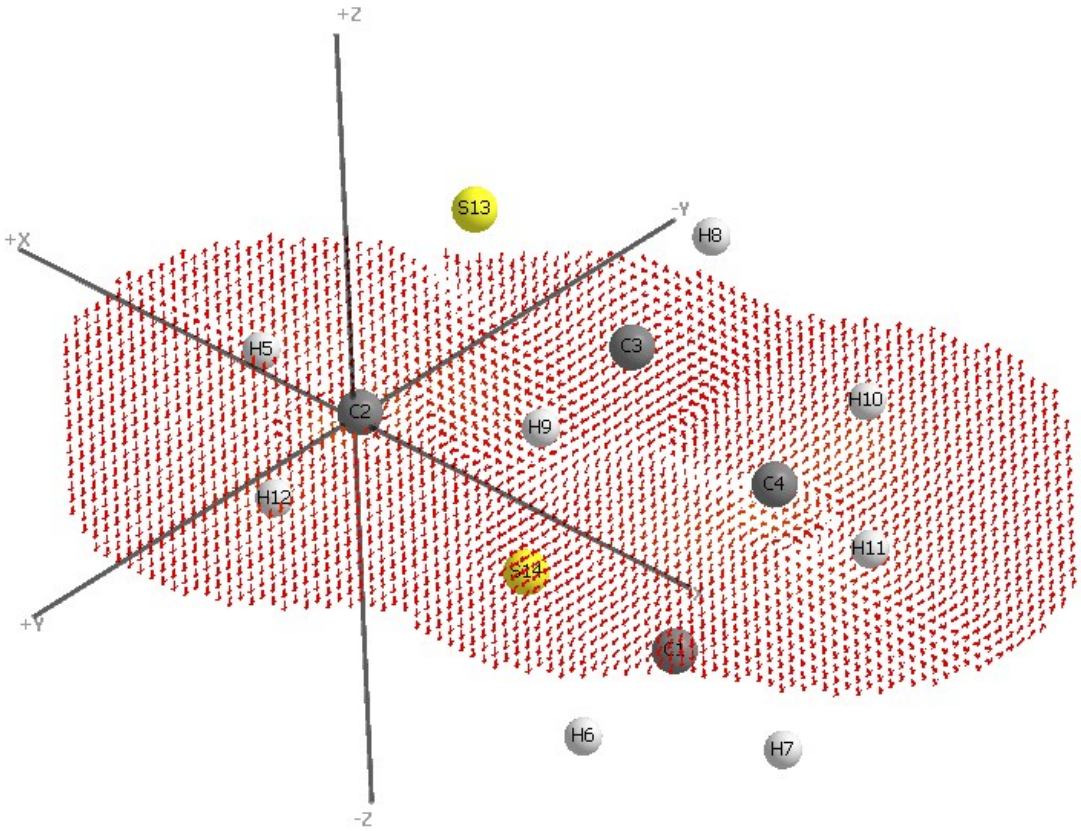

Figure S15. ICD behavior for molecule **1.8** with **B** applied along the x-axis (Reverse Perlin effect).

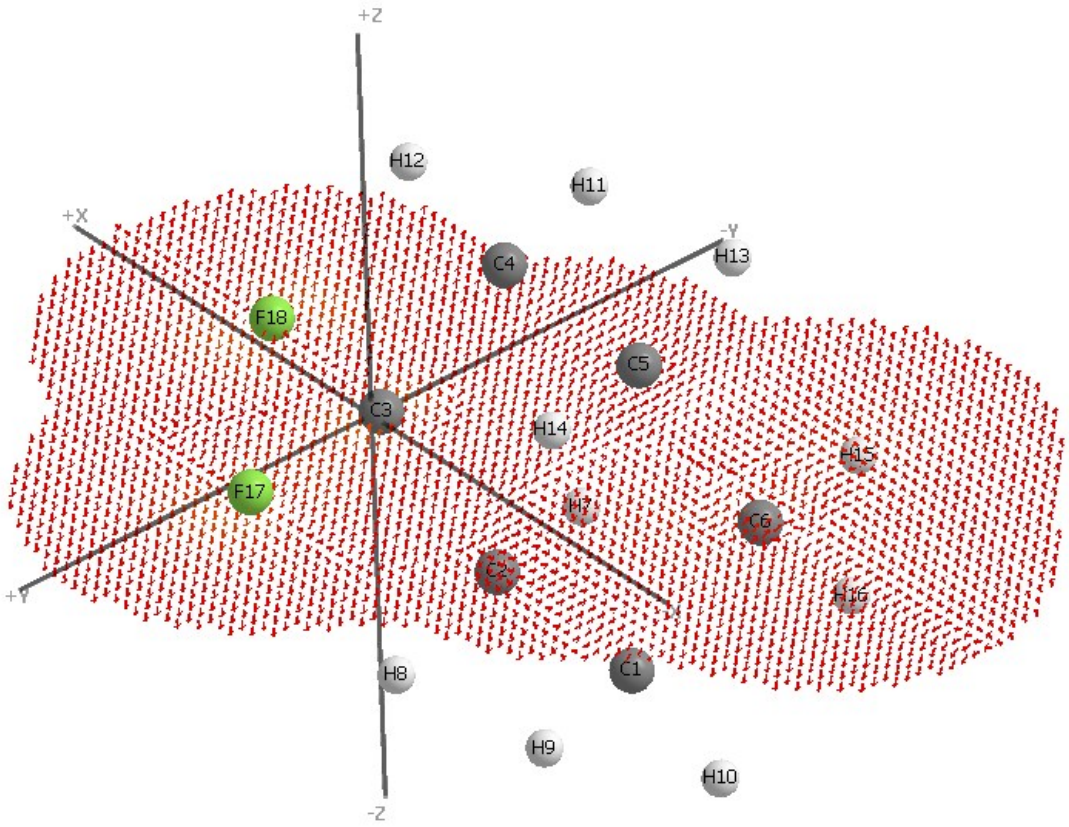

Figure S16. ICD behavior for molecule **2.1** with **B** applied along the x-axis (Fluorine Perlin effect).

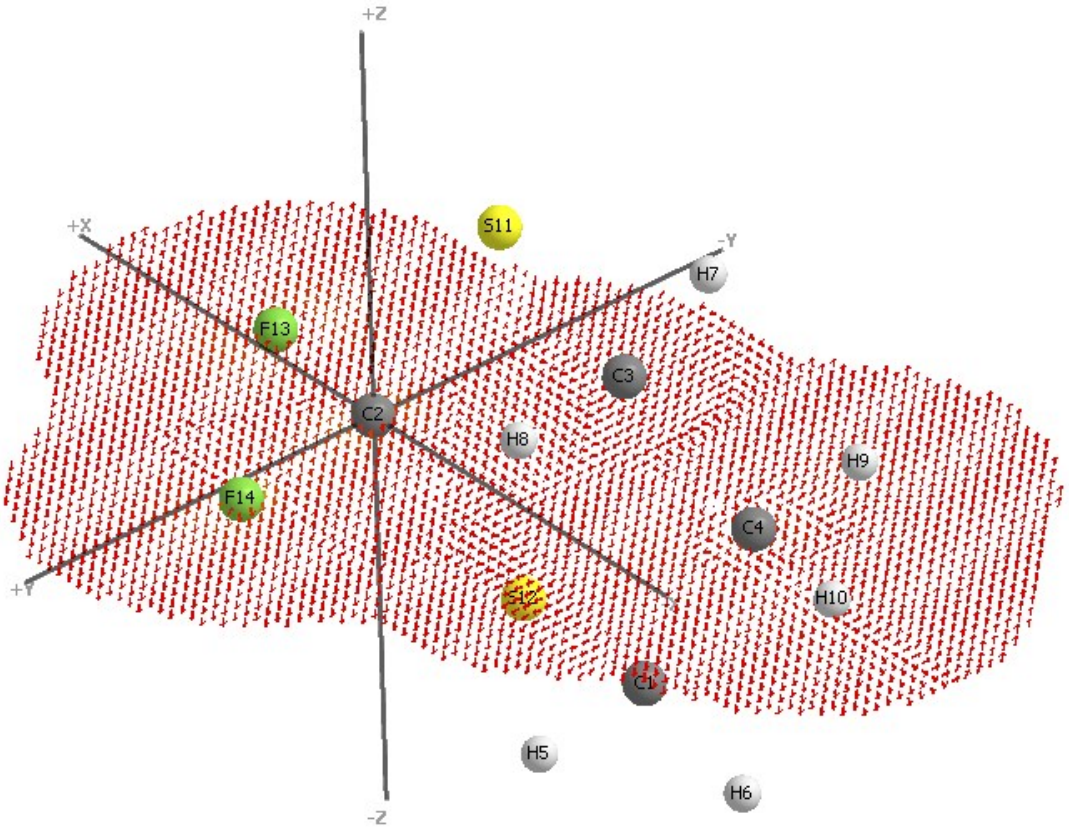

Figure S17. ICD behavior for molecule **2.8** with **B** applied along the x-axis (Reverse Fluorine Perlin effect).