Supporting Information

Halogen Bonds in Ligand-Protein Systems: Molecular Orbital Theory for Drug Design.

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SI 1| Cartesian coordinates of optimized monomers

Cartesian coordinates (Å) and total bonding energies (kcal mol^{-1}) of all the optimized monomers used in this work, computed at BLYP-D3(BJ)/TZ2P level of theory. All minima have been verified by frequency analysis and have only positive frequencies.

Bromobenzene (PhBr)

-1630.83 kcal mol^{-1}

1.C	-1.644834	12.973234	-0.207388
2.C	-2.229974	13.808331	0.745763
3.C	-1.862348	15.158728	0.774854
4.C	-0.925588	15.658887	-0.135937
5.C	-0.351309	14.803440	-1.082289
6.C	-0.707741	13.450426	-1.125210
7.H	-2.956399	13.414161	1.449774
8.H	-2.313421	15.816981	1.514052
9.H	-0.644780	16.708812	-0.108317
10.H	0.378032	15.184128	-1.793842
11.H	-0.265777	12.781522	-1.857273
12.Br	-2.147126	11.103576	-0.258742

1

-494.37 kcal mol^{-1}

1.O	-2.938983	2.338927	0.000000
2.C	-3.047249	1.131940	0.000000
3.H	-2.158661	0.459103	0.000000
4.H	-4.041387	0.627970	0.000000

2

-869.65 kcal mol^{-1}

1.O	-3.417619	8.079859	0.399669
2.C	-2.582484	7.797901	1.237590
3.H	-1.787102	8.535527	1.511808
4.C	-2.512562	6.484084	1.980192

5.H	-1.532075	6.018608	1.803769
6.H	-3.314192	5.810768	1.664713
7.H	-2.577862	6.674126	3.061305

3

-1242.55 kcal mol^{-1}

1.O	-3.232260	8.027787	0.253322
2.C	-2.497296	7.826131	1.208291
3.C	-1.494257	8.870356	1.686844
4.C	-2.531687	6.516234	1.988260
5.H	-1.572516	5.992906	1.872330
6.H	-3.341310	5.880991	1.621774
7.H	-2.659670	6.709675	3.061436
8.H	-0.487952	8.436295	1.753510
9.H	-1.763602	9.203949	2.698495
10.H	-1.489891	9.726670	1.008585

4

-783.11 kcal mol^{-1}

1.O	-3.200747	8.012303	0.185688
2.C	-2.617436	7.829342	1.244491
3.H	-1.909849	8.568066	1.681315
4.N	-2.747147	6.715324	2.027799
5.H	-3.366616	5.967058	1.734956
6.H	-2.235880	6.622348	2.896376

5

-1143.79 kcal mol^{-1}

1.O	-3.452186	8.122509	0.349198
2.C	-2.774724	7.923936	1.350911
3.H	-2.260657	8.741274	1.904765
4.N	-2.555277	6.701370	1.922244
5.H	-2.999096	5.910368	1.462667
6.C	-1.748038	6.469254	3.116559
7.H	-0.897152	5.810208	2.902733
8.H	-2.345391	6.025689	3.923115

9.H	-1.357933	7.430086	3.467467

5'

-1154.29 kcal mol^{-1}

1.O	-3.655404	8.258692	0.661205
2.C	-2.743250	7.948833	1.423245
3.C	-1.729666	8.968800	1.940467
4.N	-2.568991	6.659110	1.868582
5.H	-3.221278	5.948934	1.556701
6.H	-1.823294	6.397394	2.498460
7.H	-0.958664	8.536771	2.587199
8.H	-2.270343	9.744012	2.493955
9.H	-1.252082	9.449322	1.080355

6

-1513.90 kcal mol^{-1}

1.O	-3.286655	8.149615	0.351742
2.C	-2.583707	7.957459	1.345590
3.C	-1.545718	8.968004	1.827589
4.N	-2.702973	6.808989	2.095209
5.H	-3.375365	6.142477	1.729029
6.C	-1.885754	6.421000	3.244422
7.H	-0.839669	6.229082	2.966684
8.H	-2.299138	5.503068	3.670250
9.H	-1.901477	7.191328	4.024601
10.H	-0.542893	8.523737	1.857850
11.H	-1.780461	9.320331	2.839968
12.H	-1.548244	9.814924	1.140127

6'

-1520.15 kcal mol^{-1}

1.O	-3.306048	8.416815	0.716093
2.C	-2.671539	7.765240	1.542368
3.C	-1.728199	8.409651	2.568299
4.N	-2.739666	6.392494	1.594152
5.H	-3.296271	5.908444	0.899247

6.H	-2.209741	5.849816	2.262523
7.H	-1.588598	7.741958	3.429100
8.C	-2.213901	9.794267	3.020749
9.H	-0.747829	8.498530	2.077139
10.H	-1.473336	10.266760	3.675384
11.H	-3.159570	9.717007	3.569527
12.H	-2.382631	10.438126	2.152877

7

-1847.91 kcal mol^{-1}

1.O	-2.801208	8.530670	0.791521
2.C	-2.371930	7.846538	1.717728
3.C	-0.882885	7.685819	2.009321
4.N	-3.239331	7.184475	2.570527
5.H	-4.220652	7.310540	2.342212
6.C	-2.875565	6.304220	3.671016
7.H	-2.134790	6.758498	4.340097
8.C	-2.348470	4.933011	3.220246
9.H	-3.774099	6.117097	4.274704
10.H	-0.569356	6.636642	1.945104
11.H	-0.637138	8.040022	3.018247
12.H	-0.328981	8.271572	1.274673
13.O	-1.612685	4.241564	3.891539
14.H	-2.701646	4.614191	2.208521

8

-2135.54 kcal mol^{-1}

1.O	-3.406540	8.329306	0.604244
2.C	-2.753331	7.841351	1.525423
3.C	-1.235823	7.957025	1.617089
4.N	-3.380859	7.143478	2.544268
5.H	-4.394845	7.141469	2.478540
6.C	-2.752098	6.507657	3.696558
7.H	-1.921234	7.110244	4.076392
8.C	-2.196287	5.076830	3.487401
9.H	-3.485110	6.441871	4.507737
10.H	-0.759158	6.976738	1.732212

11.H	-0.947172	8.569675	2.480567
12.H	-0.876715	8.435211	0.704804
13.O	-1.544965	4.532304	4.373970
14.N	-2.491848	4.495871	2.287628
15.H	-3.028481	4.987054	1.584138
16.H	-2.161480	3.556036	2.105198

9

-2497.68 kcal mol^{-1}

1.O	-3.277247	8.156124	0.321490
2.C	-2.672032	7.762954	1.317998
3.C	-1.156775	7.860101	1.458052
4.N	-3.353502	7.195286	2.381675
5.H	-4.364104	7.208340	2.276804
6.C	-2.784301	6.695548	3.629699
7.H	-1.959610	7.330633	3.967984
8.C	-2.244471	5.243476	3.620977
9.H	-3.552013	6.740509	4.409452
10.H	-0.708933	6.894193	1.718238
11.H	-0.888685	8.573079	2.248052
12.H	-0.750334	8.211434	0.508698
13.O	-1.648246	4.809592	4.607115
14.N	-2.488491	4.531677	2.484085
15.H	-2.989558	5.001693	1.737948
16.C	2.059142	3.146390	2.303205
17.H	-1.375621	3.058260	1.450175
18.H	-2.921291	2.489260	2.137936
19.H	-1.541015	2.838156	3.214118

HOH

-317.9 kcal mol^{-1}

1.O	3.317721	0.110963	0.000000
2.H	2.346557	0.058733	0.000000
3.H	3.610511	-0.816464	0.000000

NC_5H_5

-1573.88 kcal mol^{-1}

1.C	-0.000000	0.175426	-2.258196
2.C	0.000000	-1.041899	-0.184253
3.C	-0.000000	-1.048323	-1.583687
4.H	-0.000000	2.328407	-1.982966
5.H	0.000000	2.152609	0.507691
6.C	0.000000	1.252725	-0.108190
7.H	0.000000	-1.980670	0.370587
8.C	-0.000000	1.351832	-1.504121
9.H	-0.000000	-1.991088	-2.126153
10.H	-0.000000	0.211506	-3.345290
11.N	0.000000	0.082142	0.555338

SI 2 | Cartesian coordinates of optimized complexes

Cartesian coordinates (Å) and total bonding energies (kcal mol^{-1}) of all the optimized complexes, computed at BLYP-D3(BJ)/TZ2P level of theory. Single-point energy calculated using QZ4P basis set is reported.

1

-2127.29 kcal mol^{-1}
-2132.16 kcal mol^{-1} (QZ4P)

1.C	-1.849889	12.908509	-0.147206
2.C	-2.386471	13.848941	0.734908
3.C	-1.847083	15.140328	0.759126
4.C	-0.787184	15.482289	-0.087701
5.C	-0.263774	14.526466	-0.965139
6.C	-0.792593	13.230959	-1.000806
7.H	-3.210210	13.578735	1.388790
8.H	-2.261042	15.877713	1.443429
9.H	-0.372697	16.487139	-0.064826
10.H	0.559307	14.784257	-1.628063
11.H	-0.391175	12.485726	-1.680965
12.Br	-2.587214	11.119174	-0.187468
13.O	-3.308612	8.079435	0.313624
14.C	-2.567011	7.858742	1.247753
15.H	-1.898642	8.645529	1.663061
16.H	-2.519504	6.858090	1.734230

2

-2502.76 kcal mol^{-1}

-2508.53 kcal mol^{-1} (QZ4P)

1.C	-1.867830	12.909646	-0.086207
2.C	-2.397764	13.892020	0.753708
3.C	-1.847934	15.178873	0.724985
4.C	-0.783252	15.476312	-0.132683
5.C	-0.266024	14.479739	-0.967496
6.C	-0.805724	13.188395	-0.949655
7.H	-3.225098	13.656465	1.416482
8.H	-2.257271	15.947874	1.376558
9.H	-0.360378	16.477786	-0.151120
10.H	0.560712	14.702529	-1.638569
11.H	-0.408869	12.411943	-1.596836
12.Br	-2.619713	11.126674	-0.051347
13.O	-3.401463	8.153668	0.442359
14.C	-2.578747	7.830689	1.279913
15.H	-1.818182	8.569671	1.629620
16.C	-2.490950	6.464622	1.914698
17.H	-1.493406	6.041448	1.727722
18.H	-3.264949	5.797645	1.525528
19.H	-2.587077	6.565112	3.005466

3

-2875.86 kcal mol^{-1}

-2882.54 kcal mol^{-1} (QZ4P)

1.C	-1.730514	13.170704	-0.123550
2.C	-2.345879	14.150982	0.659069
3.C	-1.972624	15.489407	0.490773
4.C	-0.996828	15.840862	-0.448390
5.C	-0.391570	14.846251	-1.224368

6.C	-0.755100	13.503836	-1.066733
7.H	-3.103638	13.873487	1.385789
8.H	-2.449533	16.256173	1.097565
9.H	-0.710766	16.882163	-0.575137
10.H	0.367153	15.110434	-1.957904
11.H	-0.289028	12.728621	-1.667696
12.Br	-2.236062	11.316631	0.106936
13.O	-2.967937	8.361851	0.625794
14.C	-2.380581	7.700296	1.470744
15.C	-1.185132	8.246680	2.239465
16.C	-2.811747	6.278704	1.809850
17.H	-2.011468	5.576361	1.538859
18.H	-3.724131	6.021488	1.267018
19.H	-2.972948	6.173869	2.890813
20.H	-0.335926	7.554558	2.168051
21.H	-1.441018	8.325311	3.305140
22.H	-0.904312	9.230582	1.858578

4

-2416.41 kcal mol^{-1}

-2422.21 kcal mol^{-1} (QZ4P)

1.C	-1.849612	12.892958	-0.111067
2.C	-2.424942	13.874395	0.700015
3.C	-1.886198	15.166173	0.690992
4.C	-0.786855	15.470530	-0.119262
5.C	-0.223785	14.475581	-0.925952
6.C	-0.752188	13.179504	-0.926945
7.H	-3.279318	13.633774	1.325726
8.H	-2.331493	15.933827	1.320277

9.H	-0.372763	16.475856	-0.122857
10.H	0.630139	14.703556	-1.560305
11.H	-0.319703	12.404348	-1.552607
12.Br	-2.585634	11.103498	-0.103670
13.O	-3.405271	8.169769	0.350159
14.C	-2.697904	7.902973	1.313842
15.H	-2.006624	8.641238	1.771869
16.N	-2.663709	6.690751	1.941294
17.H	-3.255033	5.936547	1.608206
18.H	-2.056808	6.529403	2.734988

5

-2777.22 kcal mol^{-1}

-2783.82 kcal mol^{-1} (QZ4P)

1.C	-1.852055	12.908197	-0.107045
2.C	-2.461898	13.893343	0.674020
3.C	-1.944877	15.193888	0.655628
4.C	-0.832541	15.503899	-0.134539
5.C	-0.234710	14.505604	-0.911593
6.C	-0.741272	13.200881	-0.902672
7.H	-3.326261	13.648511	1.284241
8.H	-2.417288	15.964023	1.261724
9.H	-0.435327	16.515981	-0.145568
10.H	0.629510	14.737788	-1.530334
11.H	-0.281671	12.423170	-1.505475
12.Br	-2.556329	11.106115	-0.085688
13.O	-3.328520	8.179865	0.356924
14.C	-2.640451	7.920503	1.340450
15.H	-1.985144	8.674348	1.826837

16.N	-2.585612	6.704649	1.956376
17.H	-3.165755	5.973522	1.552777
18.C	-1.767238	6.399048	3.126889
19.H	-1.036994	5.609825	2.908439
20.H	-2.387211	6.083424	3.975297
21.H	-1.221164	7.302110	3.417314

5'

-2787.92 kcal mol^{-1}

-2794.58 kcal mol^{-1} (QZ4P)

1.C	-1.739839	13.111750	-0.110818
2.C	-2.337159	14.094994	0.682619
3.C	-1.939124	15.428274	0.531328
4.C	-0.955881	15.773248	-0.402532
5.C	-0.368381	14.776798	-1.189828
6.C	-0.757058	13.439674	-1.048679
7.H	-3.101468	13.823163	1.404746
8.H	-2.402643	16.196387	1.146834
9.H	-0.650591	16.810581	-0.516544
10.H	0.395919	15.035714	-1.919526
11.H	-0.304931	12.663314	-1.658882
12.Br	-2.281523	11.265279	0.093037
13.O	-3.059548	8.359732	0.515556
14.C	-2.555066	7.765366	1.467958
15.C	-1.565349	8.431467	2.418490
16.N	-2.855078	6.453295	1.740758
17.H	-3.510578	5.971809	1.136010
18.H	-2.446137	5.953944	2.518385
19.H	-1.188030	7.761157	3.197589

20.H	-2.056744	9.291100	2.885715
21.H	-0.726112	8.818820	1.832297

6

-3147.53 kcal mol^{-1}

-3155.00 kcal mol^{-1} (QZ4P)

1.C	-1.759393	13.245236	-0.161213
2.C	-2.454788	14.249723	0.517468
3.C	-2.108885	15.587783	0.296287
4.C	-1.079840	15.916666	-0.592968
5.C	-0.394001	14.899155	-1.265412
6.C	-0.729930	13.557028	-1.053513
7.H	-3.253696	13.989977	1.205805
8.H	-2.648710	16.372211	0.822565
9.H	-0.815146	16.957764	-0.761377
10.H	0.406581	15.145355	-1.959822
11.H	-0.201192	12.764241	-1.574517
12.Br	-2.227262	11.392560	0.143172
13.O	-2.887759	8.501883	0.765091
14.C	-2.324932	7.911050	1.692031
15.C	-1.109458	8.476808	2.417813
16.N	-2.775534	6.687945	2.126980
17.H	-3.579619	6.334128	1.618538
18.C	-2.199693	5.868445	3.192891
19.H	-1.172091	5.557473	2.962177
20.H	-2.809675	4.968683	3.305252
21.H	-2.194556	6.397652	4.154263
22.H	-0.249731	7.801122	2.327106
23.H	-1.315978	8.604643	3.487769

24.H	-0.861487	9.443883	1.979376

6’

-3154.19 kcal mol^{-1}

-3161.63 kcal mol^{-1} (QZ4P)

1.C	-1.817703	13.183216	-0.122024
2.C	-2.284889	14.272598	0.617888
3.C	-1.756222	15.543815	0.366068
4.C	-0.772818	15.721741	-0.613235
5.C	-0.316647	14.620093	-1.345412
6.C	-0.836724	13.343246	-1.104102
7.H	-3.049326	14.129885	1.375947
8.H	-2.118036	16.394790	0.939263
9.H	-0.365863	16.711575	-0.805175
10.H	0.446593	14.749220	-2.109874
11.H	-0.487257	12.485617	-1.671374
12.Br	-2.541139	11.422425	0.222731
13.O	-3.450711	8.565657	0.847639
14.C	-2.613346	7.932244	1.491489
15.C	-1.747729	8.577633	2.576703
16.N	-2.395186	6.595029	1.270683
17.H	-2.926671	6.130285	0.543355
18.H	-1.711894	6.065839	1.794599
19.H	-1.136324	7.824427	3.090235
20.C	-2.596070	9.372630	3.585712
21.H	-1.060641	9.260339	2.059173
22.H	-1.950191	9.894925	4.299929
23.H	-3.264036	8.708652	4.147221
24.H	-3.207180	10.112402	3.061773

7

-3481.39 kcal mol^{-1}

-3490.17 kcal mol^{-1} (QZ4P)

1.C	-1.748618	13.048176	-0.160449
2.C	-2.416800	14.041627	0.559695
3.C	-1.996799	15.370966	0.435382
4.C	-0.922580	15.700251	-0.398439
5.C	-0.265207	14.692580	-1.112637
6.C	-0.674539	13.358981	-0.998094
7.H	-3.251423	13.781387	1.203910
8.H	-2.514847	16.148095	0.993257
9.H	-0.600900	16.734633	-0.491952
10.H	0.570009	14.939600	-1.764498
11.H	-0.168821	12.573906	-1.552349
12.Br	-2.324836	11.208258	0.004129
13.O	-3.238068	8.305733	0.540718
14.C	-2.666545	7.839594	1.526224
15.C	-1.178226	8.031694	1.791180
16.N	-3.371805	7.114142	2.468592
17.H	-4.359485	7.009623	2.257134
18.C	-2.828000	6.466655	3.653183
19.H	-2.190103	7.139895	4.238250
20.C	-2.036122	5.184731	3.350898
21.H	-3.664590	6.178482	4.304141
22.H	-0.653887	7.071121	1.863565
23.H	-1.015065	8.568850	2.733679
24.H	-0.757715	8.614585	0.971574
25.O	-1.181864	4.734156	4.083759

26.H	-2.313062	4.688767	2.387982

8

-3769.06 kcal mol^{-1}

-3778.72 kcal mol^{-1} (QZ4P)

1.C	-1.800076	12.979156	-0.131148
2.C	-2.460504	13.956389	0.617527
3.C	-2.013319	15.281044	0.551153
4.C	-0.920540	15.621241	-0.253632
5.C	-0.271390	14.629378	-0.996852
6.C	-0.707572	13.300573	-0.940295
7.H	-3.309773	13.687808	1.238718
8.H	-2.524993	16.045971	1.131289
9.H	-0.577985	16.651981	-0.302109
10.H	0.578265	14.885062	-1.626294
11.H	-0.208474	12.527754	-1.517267
12.Br	-2.413654	11.145767	-0.049152
13.O	-3.347857	8.208678	0.374054
14.C	-2.701244	7.800415	1.340218
15.C	-1.183995	7.899953	1.422683
16.N	-3.343885	7.219145	2.417942
17.H	-4.357718	7.235091	2.350601
18.C	-2.730338	6.690935	3.631380
19.H	-1.881528	7.306790	3.943905
20.C	-2.217403	5.230324	3.574293
21.H	-3.462314	6.733045	4.444983
22.H	-0.724105	6.938649	1.677715
23.H	-0.892979	8.627196	2.190841
24.H	-0.812415	8.244691	0.457351

25.O	-1.588687	4.760337	4.517934
26.N	-2.522731	4.538889	2.437243
27.H	-3.037321	4.971818	1.681018
28.H	-2.217150	3.576962	2.353495

9

-4131.22 kcal mol^{-1}

-4141.64 kcal mol^{-1} (QZ4P)

1.C	-1.802932	12.933339	-0.129191
2.C	-2.478297	13.894924	0.626319
3.C	-2.030573	15.220743	0.595631
4.C	-0.922616	15.577492	-0.180755
5.C	-0.258719	14.601121	-0.931429
6.C	-0.695225	13.271387	-0.910462
7.H	-3.339189	13.613605	1.225470
8.H	-2.553728	15.973583	1.181308
9.H	-0.579702	16.609054	-0.201435
10.H	0.602818	14.869701	-1.538969
11.H	-0.184613	12.510533	-1.493234
12.Br	-2.415224	11.098035	-0.095915
13.O	-3.317305	8.135432	0.267336
14.C	-2.686944	7.762645	1.258550
15.C	-1.170908	7.863857	1.360628
16.N	-3.346095	7.221009	2.346519
17.H	-4.358808	7.239625	2.264769
18.C	-2.751764	6.756455	3.596649
19.H	-1.915770	7.396562	3.895024
20.C	-2.222452	5.300856	3.620273
21.H	-3.501250	6.831392	4.391586

22.H	-0.717474	6.917879	1.676703
23.H	-0.892238	8.632449	2.092190
24.H	-0.782618	8.155337	0.384308
25.O	-1.614402	4.890274	4.609135
26.N	-2.488217	4.559598	2.507333
27.H	-2.996779	5.012267	1.755608
28.C	-2.068961	3.167525	2.358038
29.H	-1.398260	3.052408	1.498070
30.H	-2.936930	2.511131	2.222955
31.H	-1.539447	2.881129	3.269535

PhBr-NC_5H_5

-3208.04 kcal mol^{-1}

-3216.02 kcal mol^{-1} (QZ4P)

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	0.032368	5.562166	2.502472
14.C	-0.365558	6.488866	2.095260
15.C	-0.407420	6.701372	0.714619

16.C	-0.927958	7.909348	0.238825
17.N	-1.392159	8.880224	1.044383
18.C	-1.347375	8.666269	2.370745
19.C	-0.845299	7.492086	2.941708
20.H	-0.045200	5.949559	0.017269
21.H	-0.976737	8.111587	-0.831112
22.H	-1.729906	9.471024	2.998493
23.H	-0.832500	7.371544	4.022450

HOH-NC_5H_5

-1899.65 kcal mol^{-1}

-1905.34 kcal mol^{-1} (QZ4P)

1.C	-0.037353	0.097683	-2.110854
2.C	-0.019116	-1.142664	-0.051770
3.C	-0.033850	-1.133289	-1.449392
4.H	-0.031462	2.248628	-1.820330
5.H	-0.007717	2.050151	0.674658
6.C	-0.012497	1.161408	0.044747
7.H	-0.019689	-2.080751	0.502002
8.C	-0.026948	1.269020	-1.348794
9.H	-0.043888	-2.070056	-2.001146
10.H	-0.049337	0.143232	-3.197365
11.N	-0.006902	-0.019666	0.689483
12.O	-0.247244	-0.195973	3.557831
13.H	-0.113094	-0.126327	2.578894
14.H	0.649097	-0.201396	3.932036

HOH-HCHO

-817.5 kcal mol^{-1}

-820.08 kcal mol^{-1} (QZ4P)

1.C	1.406343	-0.096092	0.000000
2.H	2.506111	-0.254353	0.000000
3.H	1.047328	0.954231	0.000000
4.O	-1.785601	0.531928	0.000000
5.H	-2.660858	0.111249	0.000000
6.O	0.633036	-1.035359	0.000000
7.H	-1.146360	-0.211604	0.000000

SI 3 | Basis superposition error (BSSE) for optimized complexes

The basis superposition error (BSSE) related to the monomers and complex is reported.

set	Complex	$BSSE_{DONOR}$ (kcal mol^{-1})	$BSSE_{ACCEPTOR}$ (kcal mol^{-1})	$BSSE_{TOT}$ (kcal mol^{-1})
1-3	1	0.17	0.08	0.25
	2	0.19	0.08	0.27
	3	0.23	0.07	0.30
1-9	1	0.17	0.08	0.25
	4	0.19	0.12	0.31
	5	0.20	0.10	0.30
	6	0.24	0.08	0.32
	7	0.23	0.07	0.30
	8	0.24	0.07	0.31
	9	0.24	0.08	0.32
1-6'	1	0.17	0.08	0.25
	4	0.19	0.12	0.31
	5'	0.24	0.09	0.33
	6'	0.28	0.08	0.36
	$HOH\bullet\bullet\bullet O{=}CH_2$	0.22	0.11	0.33
	$HOH\bullet\bullet\bullet NC_5H_5$	0.32	0.08	0.40
	$PhBr\bullet\bullet\bullet NC_5H_5$	0.27	0.07	0.34

SI 4 | Energy Decomposition Analysis of XB complexes.

Energy decomposition analysis of the halogen bond complexes is reported. Each energetic term is given in kcal mol^{-1} as a contribution to the overall interaction energy.

set	Complex	ΔV_{Elstat}	ΔE_{Pauli}	ΔE_{Oi}	ΔE_{Disp}	ΔE_{int}
1-3	1	-2.54	3.70	-1.41	-1.86	-2.11
	2	-2.86	4.25	-1.69	-1.99	-2.29
	3	-3.55	5.63	-2.20	-2.38	-2.50
1-9	1	-2.54	3.70	-1.41	-1.86	-2.11
	4	-3.24	4.81	-2.03	-2.03	-2.49
	5	-3.44	5.15	-2.22	-2.12	-2.63
	6	-4.09	6.47	-2.71	-2.49	-2.82
	7	-3.29	5.17	-1.94	-2.62	-2.68
	8	-3.09	4.91	-1.75	-2.78	-2.72
	9	-3.04	4.87	-1.73	-2.83	-2.73
1-6'	1	-2.54	3.70	-1.41	-1.86	-2.11
	4	-3.24	4.81	-2.03	-2.03	-2.49
	5'	-3.97	6.23	-2.46	-2.64	-2.83
	6'	-4.03	6.59	-2.46	-3.40	-3.29

SI 5| Analysis of intramolecular and intermolecular hydrogen bonds.

The C-H bond length in Å is reported, as referring to the hydrogen atom closest to the bromine, for both monomers and dimers. H•••O distances before and after complexation are also reported. Finally, the H•••Br distance in the dimer is described.

	C-H monomer	**C-H dimer**	**Δ (C-H)**	**H•••O monomer**	**H•••O dimer**	**H•••Br**
1	1.115	1.113	-0.002	2.035	2.032	3.165
2	1.119	1.117	-0.002	2.026	2.022	3.163
3	1.092	1.092	0.000	2.548	2.556	3.032
4	1.112	1.110	-0.002	2.052	2.049	3.149
5	1.113	1.111	-0.002	2.055	2.052	3.146
6	1.091	1.090	-0.001	2.533	2.543	3.006
7	1.091	1.090	-0.001	2.532	2.536	3.182
8	1.091	1.090	-0.001	2.534	2.537	3.352
9	1.091	1.090	-0.001	2.534	2.537	3.398
5'	1.095	1.095	0.000	2.715	2.718	3.381
6'	1.094	1.093	-0.001	2.646	2.712	3.197

SI 6 | Cartesian coordinates of constrained complexes

Cartesian coordinates (Å) and total bonding energies (kcal mol^{-1}) of complexes obtained by letting the monomers approach each other as blocks, computed at the BLYP-D3(BJ)/TZ2P level of theory. The coordinates of PhBr-NC_5H_5 and HOH-NC_5H_5 at each step are reported.

PhBr-NC_5H_5 (1)
-3208.02 kcal mol^{-1}

1.C	-3.031528	13.124814	-0.868580
2.C	-3.559284	14.099907	-0.017762
3.C	-4.041525	15.294974	-0.563890
4.C	-3.996508	15.512158	-1.945452
5.C	-3.465204	14.526291	-2.784313
6.C	-2.979719	13.326946	-2.250472
7.H	-3.592542	13.927807	1.054182
8.H	-4.452903	16.055767	0.096237
9.H	-4.372399	16.442218	-2.364984
10.H	-3.425973	14.686310	-3.859789
11.H	-2.566358	12.559540	-2.898539
12.Br	-2.360288	11.467160	-0.119574
13.H	-0.011262	5.538484	2.529573
14.C	-0.376077	6.475319	2.114622
15.C	-0.381793	6.689593	0.733649
16.C	-0.860858	7.910671	0.247689
17.N	-1.317852	8.892852	1.043636
18.C	-1.307886	8.676949	2.370417
19.C	-0.848861	7.490044	2.951202
20.H	-0.023551	5.929099	0.043690
21.H	-0.881050	8.114108	-0.822956
22.H	-1.684014	9.490632	2.990487
23.H	-0.863475	7.368645	4.031830

PhBr-NC_5H_5 (2)

-3208.01 kcal mol^{-1}

1.C	-0.022552	2.413526	0.000000
2.C	-0.010742	3.102296	1.216128
3.C	0.013435	4.501766	1.209666
4.C	0.025765	5.205002	0.000000
5.C	0.013435	4.501766	-1.209666
6.C	-0.010742	3.102296	-1.216128
7.H	-0.020058	2.553315	2.153400
8.H	0.022746	5.039960	2.155251
9.H	0.044790	6.292199	0.000000
10.H	0.022746	5.039960	-2.155251
11.H	-0.020058	2.553315	-2.153400
12.Br	-0.053238	0.473294	0.000000
13.H	0.088899	-6.354245	0.000000
14.C	0.046349	-5.267458	0.000000
15.C	0.018446	-4.554763	-1.201816
16.C	-0.036239	-3.158032	-1.150601-
17.N	-0.063431	-2.463515	0.000000
18.C	-0.036239	-3.158032	1.150601
19.C	0.018446	-4.554763	1.201816
20.H	0.038481	-5.066475	-2.161223
21.H	-0.059360	-2.567470	-2.066417
22.H	-0.059360	-2.567470	2.066417
23.H	0.038481	-5.066475	2.161223

PhBr-NC_5H_5 (3)

-3207.92 kcal mol^{-1}

1.C	-0.024444	2.383492	0.000000
2.C	-0.012188	3.072852	1.215881
3.C	0.012900	4.472326	1.209653
4.C	0.025706	5.175618	0.000000
5.C	0.012900	4.472326	-1.209653
6.C	-0.012188	3.072852	-1.215881
7.H	-0.021851	2.524035	2.153326
8.H	0.022571	5.010579	2.155231
9.H	0.045484	6.262819	0.000000
10.H	0.022571	5.010579	-2.155231
11.H	-0.021851	2.524035	-2.153326
12.Br	-0.056127	0.441652	0.000000
13.H	0.097790	-6.321501	0.000000
14.C	0.051260	-5.234893	0.000000
15.C	0.020844	-4.522412	-1.201904
16.C	-0.038308	-3.125948	-1.150829
17.N	-0.067892	-2.432008	0.000000
18.C	-0.038308	-3.125948	1.150829
19.C	0.020844	-4.522412	1.201904
20.H	0.042803	-5.034100	-2.161260
21.H	-0.062660	-2.534921	-2.066291
22.H	-0.062660	-2.534921	2.066291
23.H	0.042803	-5.034100	2.161260

PhBr-NC_5H_5 (4)

-3207.73 kcal mol^{-1}

1.C	-0.025003	2.353675	0.000000
2.C	-0.012610	3.043682	1.215607

3.C	0.012762	4.443177	1.209642
4.C	0.025735	5.146533	0.000000
5.C	0.012762	4.443177	-1.209642
6.C	-0.012610	3.043682	-1.215607
7.H	-0.022387	2.495045	2.153248
8.H	0.022542	4.981502	2.155212
9.H	0.045764	6.233749	0.000000
10.H	0.022542	4.981502	-2.155212
11.H	-0.022387	2.495045	-2.153248
12.Br	-0.056898	0.409898	0.000000
13.H	0.099733	-6.289287	0.000000
14.C	0.052376	-5.202731	0.000000
15.C	0.021436	-4.490383	-1.201996
16.C	-0.038671	-3.094055	-1.151074
17.N	-0.068663	-2.400604	0.000000
18.C	-0.038671	-3.094055	1.151074
19.C	0.021436	-4.490383	1.201996
20.H	0.043781	-5.002106	-2.161300
21.H	-0.063375	-2.502479	-2.066154
22.H	-0.063375	-2.502479	2.066154
23.H	0.043781	-5.002106	2.161300

PhBr-NC_5H_5 (5)

-3207.42 kcal mol^{-1}

1.C	-0.023479	2.324193	0.000000
2.C	-0.011884	3.014918	1.215304
3.C	0.011834	4.414470	1.209636
4.C	0.023943	5.117909	0.000000
5.C	0.011834	4.414470	-1.209636

6.C	-0.011884	3.014918	-1.215304
7.H	-0.021003	2.466459	2.153164
8.H	0.020964	4.952891	2.155195
9.H	0.042634	6.205169	0.000000
10.H	0.020964	4.952891	-2.155195
11.H	-0.021003	2.466459	-2.153164
12.Br	-0.053083	0.378082	0.000000
13.H	0.089466	-6.257997	0.000000
14.C	0.047017	-5.171254	0.000000
15.C	0.019299	-4.458879	-1.202089
16.C	-0.034503	-3.062401	-1.151336
17.N	-0.061305	-2.369275	0.000000
18.C	-0.034503	-3.062401	1.151336
19.C	0.019299	-4.458879	1.202089
20.H	0.039294	-4.970748	-2.161341
21.H	-0.056599	-2.470123	-2.066010
22.H	-0.056599	-2.470123	2.066010
23.H	0.039294	-4.970748	2.161341

PhBr-NC_5H_5 (6)

-3206.94 kcal mol^{-1}

1.C	-0.021590	2.294923	0.000000
2.C	-0.010747	2.986420	1.214969
3.C	0.011433	4.386038	1.209632
4.C	0.022764	5.089559	0.000000
5.C	0.011433	4.386038	-1.209632
6.C	-0.010747	2.986420	-1.214969
7.H	-0.019283	2.438172	2.153078
8.H	0.019975	4.924573	2.155176

9.H	0.040242	6.176865	0.000000
10.H	0.019975	4.924573	-2.155176
11.H	-0.019283	2.438172	-2.153078
12.Br	-0.049125	0.345971	0.000000
13.H	0.078363	-6.226928	0.000000
14.C	0.041003	-5.140017	0.000000
15.C	0.016608	-4.427628	-1.202189
16.C	-0.030720	-3.031029	-1.151622
17.N	-0.054263	-2.338235	0.000000
18.C	-0.030720	-3.031029	1.151622
19.C	0.016608	-4.427628	1.202189
20.H	0.034170	-4.939615	-2.161396
21.H	-0.050132	-2.437999	-2.065857
22.H	-0.050132	-2.437999	2.065857
23.H	0.034170	-4.939615	2.161396

PhBr-NC_5H_5 (7)

-3206.26 kcal mol^{-1}

1.C	-0.016226	2.265891	0.000000
2.C	-0.005221	2.958233	1.214590
3.C	0.017211	4.357896	1.209628
4.C	0.028639	5.061493	0.000000
5.C	0.017211	4.357896	-1.209628
6.C	-0.005221	2.958233	-1.214590
7.H	-0.013864	2.410260	2.153002
8.H	0.025821	4.896543	2.155156
9.H	0.046253	6.148824	0.000000
10.H	0.025821	4.896543	-2.155156
11.H	-0.013864	2.410260	-2.153002

12.Br	-0.044204	0.313607	0.000000
13.H	0.057064	-6.196219	0.000000
14.C	0.026991	-5.109104	0.000000
15.C	0.007348	-4.396682	-1.202304
16.C	-0.030796	-2.999933	-1.151943
17.N	-0.049768	-2.307440	0.000000
18.C	-0.030796	-2.999933	1.151943
19.C	0.007348	-4.396682	1.202304
20.H	0.021479	-4.908839	-2.161446
21.H	-0.046353	-2.406004	-2.065658
22.H	-0.046353	-2.406004	2.065658
23.H	0.021479	-4.908839	2.161446

PhBr-NC_5H_5 (8)

-3205.31 kcal mol^{-1}

1.C	-0.016840	2.236824	0.000000
2.C	-0.003445	2.930025	1.214175
3.C	0.023847	4.329657	1.209632
4.C	0.037790	5.033279	0.000000
5.C	0.023847	4.329657	-1.209632
6.C	-0.003445	2.930025	-1.214175
7.H	-0.013930	2.382367	2.152917
8.H	0.034374	4.868399	2.155141
9.H	0.059316	6.120568	0.000000
10.H	0.034374	4.868399	-2.155141
11.H	-0.013930	2.382367	-2.152917
12.Br	-0.050736	0.280722	0.000000
13.H	0.066701	-6.164502	0.000000
14.C	0.029774	-5.077628	0.000000

15.C	0.005690	-4.365437	-1.202404
16.C	-0.040839	-2.969112	-1.152289
17.N	-0.063813	-2.277139	0.000000
18.C	-0.040839	-2.969112	1.152289
19.C	0.005690	-4.365437	1.202404
20.H	0.022989	-4.877512	-2.161508
21.H	-0.059782	-2.374449	-2.065454
22.H	-0.059782	-2.374449	2.065454
23.H	0.022989	-4.877512	2.161508

PhBr- NC_5H_5 (9)

-3204.06 kcal mol^{-1}

1.C	-0.017745	2.208292	0.000000
2.C	-0.005499	2.902504	1.213713
3.C	0.019417	4.302251	1.209642
4.C	0.032141	5.005968	0.000000
5.C	0.019417	4.302251	-1.209642
6.C	-0.005499	2.902504	-1.213713
7.H	-0.015046	2.355160	2.152838
8.H	0.029034	4.841160	2.155128
9.H	0.051797	6.093327	0.000000
10.H	0.029034	4.841160	-2.155128
11.H	-0.015046	2.355160	-2.152838
12.Br	-0.048307	0.247411	0.000000
13.H	0.064979	-6.134122	0.000000
14.C	0.030522	-5.047198	0.000000
15.C	0.008030	-4.335045	-1.202504
16.C	-0.035371	-2.938850	-1.152691
17.N	-0.056727	-2.247311	0.000000

18.C	-0.035371	-2.938850	1.152691
19.C	0.008030	-4.335045	1.202504
20.H	0.024133	-4.847199	-2.161557
21.H	-0.053029	-2.343164	-2.065199
22.H	-0.053029	-2.343164	2.065199
23.H	0.024133	-4.847199	2.161557

PhBr- NC_5H_5 (10)

-3202.46 kcal mol^{-1}

1.C	-0.015347	2.180085	0.000000
2.C	-0.002248	2.875371	1.213197
3.C	0.024371	4.275172	1.209657
4.C	0.037978	4.978945	0.000000
5.C	0.024371	4.275172	-1.209657
6.C	-0.002248	2.875371	-1.213197
7.H	-0.012426	2.328426	2.152768
8.H	0.034630	4.814243	2.155115
9.H	0.058975	6.066318	0.000000
10.H	0.034630	4.814243	-2.155115
11.H	-0.012426	2.328426	-2.152768
12.Br	-0.047946	0.213582	0.000000
13.H	0.057095	-6.103967	0.000000
14.C	0.024259	-5.017031	0.000000
15.C	0.002836	-4.304925	-1.202595
16.C	-0.038389	-2.908985	-1.153156
17.N	-0.058567	-2.217974	0.000000
18.C	-0.038389	-2.908985	1.153156
19.C	0.002836	-4.304925	1.202595
20.H	0.018123	-4.817162	-2.161589

21.H	-0.055120	-2.312118	-2.064887
22.H	-0.055120	-2.312118	2.064887
23.H	0.018123	-4.817162	2.161589

PhBr- NC_5H_5 (11)

-3200.47 kcal mol^{-1}

1.C	-0.014614	2.152411	0.000000
2.C	-0.001839	2.848894	1.212625
3.C	0.024060	4.248810	1.209682
4.C	0.037281	4.952662	0.000000
5.C	0.024060	4.248810	-1.209682
6.C	-0.001839	2.848894	-1.212625
7.H	-0.011726	2.302386	2.152709
8.H	0.034048	4.788085	2.155107
9.H	0.057695	6.040090	0.000000
10.H	0.034048	4.788085	-2.155107
11.H	-0.011726	2.302386	-2.152709
12.Br	-0.046032	0.179168	0.000000
13.H	0.051643	-6.074532	0.000000
14.C	0.021362	-4.987569	0.000000
15.C	0.001623	-4.275463	-1.202676
16.C	-0.036350	-2.879809	-1.153678
17.N	-0.054837	-2.189237	0.000000
18.C	-0.036350	-2.879809	1.153678
19.C	0.001623	-4.275463	1.202676
20.H	0.015663	-4.787772	-2.161621
21.H	-0.051727	-2.281628	-2.064545
22.H	-0.051727	-2.281628	2.064545
23.H	0.015663	-4.787772	2.161621

PhBr- NC_5H_5 (12)

-3198.00 kcal mol^{-1}

1.C	-0.010323	2.125415	0.000000
2.C	0.003551	2.823188	1.211990
3.C	0.031596	4.223182	1.209717
4.C	0.045901	4.927080	0.000000
5.C	0.031596	4.223182	-1.209717
6.C	0.003551	2.823188	-1.211990
7.H	-0.007159	2.277204	2.152667
8.H	0.042390	4.762670	2.155104
9.H	0.067978	6.014525	0.000000
10.H	0.042390	4.762670	-2.155104
11.H	-0.007159	2.277204	-2.152667
12.Br	-0.044583	0.144198	0.000000
13.H	0.037093	-6.045895	0.000000
14.C	0.010446	-4.958890	0.000000
15.C	-0.006933	-4.246722	-1.202742
16.C	-0.040242	-2.851375	-1.154261
17.N	-0.056320	-2.161035	0.000000
18.C	-0.040242	-2.851375	1.154261
19.C	-0.006933	-4.246722	1.202742
20.H	0.005357	-4.759074	-2.161655
21.H	-0.053656	-2.251772	-2.064192
22.H	-0.053656	-2.251772	2.064192
23.H	0.005357	-4.759074	2.161655

PhBr- NC_5H_5 (13)

-3194.93 kcal mol^{-1}

1.C	-0.004944	2.099218	0.000000
2.C	0.010472	2.798426	1.211281
3.C	0.041512	4.198500	1.209761
4.C	0.057335	4.902436	0.000000
5.C	0.041512	4.198500	-1.209761
6.C	0.010472	2.798426	-1.211281
7.H	-0.001415	2.253071	2.152655
8.H	0.053453	4.738226	2.155104
9.H	0.081734	5.989886	0.000000
10.H	0.053453	4.738226	-2.155104
11.H	-0.001415	2.253071	-2.152655
12.Br	-0.043456	0.108505	0.000000
13.H	0.019986	-6.018203	0.000000
14.C	-0.002801	-4.931173	0.000000
15.C	-0.017660	-4.218878	-1.202780
16.C	-0.045995	-2.823910	-1.154918
17.N	-0.059481	-2.133543	0.000000
18.C	-0.045995	-2.823910	1.154918
19.C	-0.017660	-4.218878	1.202780
20.H	-0.007245	-4.731196	-2.161700
21.H	-0.057308	-2.222803	-2.063843
22.H	-0.057308	-2.222803	2.063843
23.H	-0.007245	-4.731196	2.161700

PhBr- NC_5H_5 (14)

-3191.16 kcal mol^{-1}

1.C	0.006170	2.074008	0.000000

2.C	0.025473	2.774757	1.210495
3.C	0.064179	4.174802	1.209816
4.C	0.083877	4.878708	0.000000
5.C	0.064179	4.174802	-1.209816
6.C	0.025473	2.774757	-1.210495
7.H	0.010645	2.230181	2.152681
8.H	0.079076	4.714754	2.155108
9.H	0.114246	5.966069	0.000000
10.H	0.079076	4.714754	-2.155108
11.H	0.010645	2.230181	-2.152681
12.Br	-0.043017	0.072084	0.000000
13.H	-0.013618	-5.991620	0.000000
14.C	-0.029989	-4.904551	0.000000
15.C	-0.040653	-4.192009	-1.202773
16.C	-0.060742	-2.797472	-1.155662
17.N	-0.069971	-2.106697	0.000000
18.C	-0.060742	-2.797472	1.155662
19.C	-0.040653	-4.192009	1.202773
20.H	-0.033331	-4.704228	-2.161741
21.H	-0.068496	-2.194786	-2.063522
22.H	-0.068496	-2.194786	2.063522
23.H	-0.033331	-4.704228	2.161741

PhBr- NC_5H_5 (15)

-3186.54 kcal mol^{-1}

1.C	0.018612	2.049964	0.000000
2.C	0.041582	2.752448	1.209625
3.C	0.087379	4.152469	1.209885
4.C	0.110606	4.856336	0.000000

5.C	0.087379	4.152469	-1.209885
6.C	0.041582	2.752448	-1.209625
7.H	0.023998	2.208793	2.152762
8.H	0.105007	4.692677	2.155123
9.H	0.146425	5.943599	0.000000
10.H	0.105007	4.692677	-2.155123
11.H	0.023998	2.208793	-2.152762
12.Br	-0.041164	0.034687	0.000000
13.H	-0.052715	-5.966400	0.000000
14.C	-0.060408	-4.879326	0.000000
15.C	-0.065396	-4.166412	-1.202700
16.C	-0.074450	-2.772439	-1.156520
17.N	-0.078116	-2.080780	0.000000
18.C	-0.074450	-2.772439	1.156520
19.C	-0.065396	-4.166412	1.202700
20.H	-0.062196	-4.678424	-2.161770
21.H	-0.077544	-2.168152	-2.063263
22.H	-0.077544	-2.168152	2.063263
23.H	-0.062196	-4.678424	2.161770

PhBr- NC_5H_5 (16)

-3180.93 kcal mol^{-1}

1.C	0.027022	2.027387	0.000000
2.C	0.052497	2.731888	1.208665
3.C	0.103058	4.131963	1.209968
4.C	0.128663	4.835822	0.000000
5.C	0.103058	4.131963	-1.209968
6.C	0.052497	2.731888	-1.208665
7.H	0.033056	2.189295	2.152919

8.H	0.122495	4.672486	2.155147
9.H	0.168130	5.923037	0.000000
10.H	0.122495	4.672486	-2.155147
11.H	0.033056	2.189295	-2.152919
12.Br	-0.040305	-0.003957	0.000000
13.H	-0.079342	-5.942873	0.000000
14.C	-0.081041	-4.855886	0.000000
15.C	-0.082126	-4.142471	-1.202540
16.C	-0.083583	-2.749290	-1.157521
17.N	-0.083308	-2.056138	0.000000
18.C	-0.083583	-2.749290	1.157521
19.C	-0.082126	-4.142471	1.202540
20.H	-0.081833	-4.654122	-2.161783
21.H	-0.083475	-2.143444	-2.063116
22.H	-0.083475	-2.143444	2.063116
23.H	-0.081833	-4.654122	2.161783

PhBr- NC_5H_5 (17)

-3174.16 kcal mol^{-1}

1.C	0.051301	2.006215	0.000000
2.C	0.084291	2.712826	1.207607
3.C	0.149250	4.112554	1.210062
4.C	0.182009	4.816199	0.000000
5.C	0.149250	4.112554	-1.210062
6.C	0.084291	2.712826	-1.207607
7.H	0.059220	2.171664	2.153173
8.H	0.174238	4.653266	2.155181
9.H	0.232500	5.903043	0.000000
10.H	0.174238	4.653266	-2.155181

11.H	0.059220	2.171664	-2.153173
12.Br	-0.039191	-0.043634	0.000000
13.H	-0.151830	-5.920465	0.000000
14.C	-0.138652	-4.833686	0.000000
15.C	-0.129977	-4.119620	-1.202268
16.C	-0.112574	-2.727520	-1.158699
17.N	-0.102739	-2.032092	0.000000
18.C	-0.112574	-2.727520	1.158699
19.C	-0.129977	-4.119620	1.202268
20.H	-0.136727	-4.630705	-2.161769
21.H	-0.104420	-2.120255	-2.063151
22.H	-0.104420	-2.120255	2.063151
23.H	-0.136727	-4.630705	2.161769

PhBr- NC_5H_5 (18)

-3166.05 kcal mol^{-1}

1.C	0.086576	1.986436	0.000000
2.C	0.131450	2.695195	1.206456
3.C	0.219158	4.093932	1.210170
4.C	0.263258	4.797060	0.000000
5.C	0.219158	4.093932	-1.210170
6.C	0.131450	2.695195	-1.206456
7.H	0.097565	2.155942	2.153555
8.H	0.253000	4.634612	2.155235
9.H	0.331259	5.883041	0.000000
10.H	0.253000	4.634612	-2.155235
11.H	0.097565	2.155942	-2.153555
12.Br	-0.040633	-0.084508	0.000000
13.H	-0.255362	-5.898472	0.000000

14.C	-0.222414	-4.812270	0.000000
15.C	-0.200743	-4.097505	-1.201850
16.C	-0.158148	-2.707097	-1.160089
17.N	-0.135337	-2.008495	0.000000
18.C	-0.158148	-2.707097	1.160089
19.C	-0.200743	-4.097505	1.201850
20.H	-0.216909	-4.607689	-2.161710
21.H	-0.139047	-2.098786	-2.063466
22.H	-0.139047	-2.098786	2.063466
23.H	-0.216909	-4.607689	2.161710

PhBr- NC_5H_5 (19)

-3156.35 kcal mol^{-1}

1.C	0.118760	1.968665	0.000000
2.C	0.176347	2.679783	1.205211
3.C	0.288388	4.077041	1.210285
4.C	0.344740	4.779436	0.000000
5.C	0.288388	4.077041	-1.210285
6.C	0.176347	2.679783	-1.205211
7.H	0.133320	2.142892	2.154089
8.H	0.331768	4.617510	2.155311
9.H	0.431745	5.864152	0.000000
10.H	0.331768	4.617510	-2.155311
11.H	0.133320	2.142892	-2.154089
12.Br	-0.046989	-0.126729	0.000000
13.H	-0.349251	-5.878149	0.000000
14.C	-0.300552	-4.792713	0.000000
15.C	-0.268492	-4.077070	-1.201269
16.C	-0.205381	-2.688763	-1.161749

17.N	-0.171269	-1.985737	0.000000
18.C	-0.205381	-2.688763	1.161749
19.C	-0.268492	-4.077070	1.201269
20.H	-0.292446	-4.586073	-2.161602
21.H	-0.177096	-2.079782	-2.064163
22.H	-0.177096	-2.079782	2.064163
23.H	-0.292446	-4.586073	2.161602

PhBr- NC_5H_5 (20)

-3144.76 kcal mol^{-1}

1.C	0.085928	1.957125	0.000000
2.C	0.130184	2.673000	1.203890
3.C	0.215140	4.072432	1.210404
4.C	0.257866	4.775967	0.000000
5.C	0.215140	4.072432	-1.210404
6.C	0.130184	2.673000	-1.203890
7.H	0.097560	2.137376	2.154792
8.H	0.247988	4.614140	2.155400
9.H	0.323784	5.862274	0.000000
10.H	0.247988	4.614140	-2.155400
11.H	0.097560	2.137376	-2.154792
12.Br	-0.045667	-0.172352	0.000000
13.H	-0.245068	-5.871594	0.000000
14.C	-0.215370	-4.785657	0.000000
15.C	-0.195913	-4.067970	-1.200501
16.C	-0.157219	-2.680261	-1.163716
17.N	-0.134780	-1.970145	0.000000
18.C	-0.157219	-2.680261	1.163716
19.C	-0.195913	-4.067970	1.200501

20.H	-0.211271	-4.576256	-2.161410
21.H	-0.139814	-2.070271	-2.065371
22.H	-0.139814	-2.070271	2.065371
23.H	-0.211271	-4.576256	2.161410

HOH- NC_5H_5 (1)

-1894.85 kcal mol^{-1}

1.C	-0.121597	2.346124	0.000000
2.C	0.014774	0.238579	-1.149544
3.C	-0.075723	1.633588	-1.201042
4.H	-0.109870	2.143604	2.160938
5.H	0.050962	-0.346450	2.068567
6.C	0.014774	0.238579	1.149544
7.H	0.050962	-0.346450	-2.068567
8.C	-0.075723	1.633588	1.201042
9.H	-0.109870	2.143604	-2.160938
10.H	-0.192070	3.431451	0.000000
11.N	0.061237	-0.459799	0.000000
12.O	-0.177327	-4.424291	0.000000
13.H	-0.060052	-3.457346	0.000000
14.H	0.729522	-4.774779	0.000000

HOH- NC_5H_5 (2)

-1895.08 kcal mol^{-1}

1.C	-0.167098	2.329208	0.000000
2.C	0.025268	0.226101	-1.149664
3.C	-0.102181	1.618197	-1.201074
4.H	-0.149972	2.127136	2.160946

5.H	0.076906	-0.357874	2.068577
6.C	0.025268	0.226101	1.149664
7.H	0.076906	-0.357874	-2.068577
8.C	-0.102181	1.618197	1.201074
9.H	-0.149972	2.127136	-2.160946
10.H	-0.266717	3.412237	0.000000
11.N	0.090085	-0.470610	0.000000
12.O	-0.125749	-4.373308	0.000000
13.H	-0.013462	-3.405626	0.000000
14.H	0.782900	-4.719023	0.000000

HOH- NC_5H_5 (3)

-1895.32 kcal mol^{-1}

1.C	-0.161213	2.316248	0.000000
2.C	0.020094	0.212248	-1.149791
3.C	-0.100062	1.604963	-1.201108
4.H	-0.145199	2.114173	2.160954
5.H	0.068599	-0.372154	2.068564
6.C	0.020094	0.212248	1.149791
7.H	0.068599	-0.372154	-2.068564
8.C	-0.100062	1.604963	1.201108
9.H	-0.145199	2.114173	-2.160954
10.H	-0.255101	3.399789	0.000000
11.N	0.081322	-0.484551	0.000000
12.O	-0.123805	-4.324781	0.000000
13.H	-0.013639	-3.356666	0.000000
14.H	0.785574	-4.668500	0.000000

HOH- NC_5H_5 (4)

-1895.58 kcal mol^{-1}

1.C	-0.155889	2.303186	0.000000
2.C	0.015707	0.198459	-1.149918
3.C	-0.098044	1.591675	-1.201140
4.H	-0.140893	2.101114	2.160958
5.H	0.061444	-0.386326	2.068552
6.C	0.015707	0.198459	1.149918
7.H	0.061444	-0.386326	-2.068552
8.C	-0.098044	1.591675	1.201140
9.H	-0.140893	2.101114	-2.160958
10.H	-0.244758	3.387148	0.000000
11.N	0.073768	-0.498389	0.000000
12.O	-0.122661	-4.276053	0.000000
13.H	-0.014172	-3.307539	0.000000
14.H	0.787285	-4.618198	0.000000

HOH- NC_5H_5 (5)

-1895.85 kcal mol^{-1}

1.C	-0.152958	2.289881	0.000000
2.C	0.012988	0.184795	-1.150052
3.C	-0.097045	1.578273	-1.201178
4.H	-0.138572	2.087847	2.160969
5.H	0.057080	-0.400288	2.068539
6.C	0.012988	0.184795	1.150052
7.H	0.057080	-0.400288	-2.068539
8.C	-0.097045	1.578273	1.201178
9.H	-0.138572	2.087847	-2.160969
10.H	-0.238924	3.374075	0.000000
11.N	0.069220	-0.511962	0.000000

12.O	-0.121319	-4.226943	0.000000
13.H	-0.013831	-3.258074	0.000000
14.H	0.788912	-4.568232	0.000000

HOH- NC_5H_5 (6)

-1896.14 kcal mol^{-1}

1.C	-0.147661	2.276693	0.000000
2.C	0.010711	0.171135	-1.150204
3.C	-0.094319	1.564958	-1.201223
4.H	-0.134057	2.074716	2.160977
5.H	0.052612	-0.414331	2.068507
6.C	0.010711	0.171135	1.150204
7.H	0.052612	-0.414331	-2.068507
8.C	-0.094319	1.564958	1.201223
9.H	-0.134057	2.074716	-2.160977
10.H	-0.229753	3.361184	0.000000
11.N	0.064468	-0.525532	0.000000
12.O	-0.124925	-4.177637	0.000000
13.H	-0.017211	-3.208500	0.000000
14.H	0.785186	-4.519162	0.000000

HOH- NC_5H_5 (7)

-1896.46 kcal mol^{-1}

1.C	-0.082348	2.257673	0.000000
2.C	-0.029213	0.146959	-1.150398
3.C	-0.064403	1.544249	-1.201285
4.H	-0.078272	2.055404	2.160992
5.H	-0.016300	-0.440113	2.068507

6.C	-0.029213	0.146959	1.150398
7.H	-0.016300	-0.440113	-2.068507
8.C	-0.064403	1.544249	1.201285
9.H	-0.078272	2.055404	-2.160992
10.H	-0.110373	3.344908	0.000000
11.N	-0.010901	-0.551262	0.000000
12.O	-0.113495	-4.143983	0.000000
13.H	-0.142720	-3.168998	0.000000
14.H	0.836214	-4.351337	0.000000

HOH- NC_5H_5 (8)

-1896.77 kcal mol^{-1}

1.C	-0.158956	2.239784	0.000000
2.C	-0.040541	0.131841	-1.150558
3.C	-0.118990	1.527321	-1.201326
4.H	-0.148801	2.037839	2.161002
5.H	-0.009404	-0.454775	2.068477
6.C	-0.040541	0.131841	1.150558
7.H	-0.009404	-0.454775	-2.068477
8.C	-0.118990	1.527321	1.201326
9.H	-0.148801	2.037839	-2.161002
10.H	-0.220551	3.325626	0.000000
11.N	-0.000490	-0.565191	0.000000
12.O	0.042224	-4.096392	0.000000
13.H	-0.026235	-3.122956	0.000000
14.H	0.999480	-4.265323	0.000000

HOH- NC_5H_5 (9)

-1897.09 kcal mol^{-1}

1.C	-0.101345	2.229028	0.000000
2.C	-0.049891	0.118504	-1.150738
3.C	-0.084107	1.515732	-1.201386
4.H	-0.097602	2.026992	2.161012
5.H	-0.037490	-0.469097	2.068426
6.C	-0.049891	0.118504	1.150738
7.H	-0.037490	-0.469097	-2.068426
8.C	-0.084107	1.515732	1.201386
9.H	-0.097602	2.026992	-2.161012
10.H	-0.128256	3.316285	0.000000
11.N	-0.031861	-0.579121	0.000000
12.O	-0.033113	-4.047947	0.000000
13.H	-0.089067	-3.073202	0.000000
14.H	0.921822	-4.229306	0.000000

HOH- NC_5H_5 (10)

-1897.43 kcal mol^{-1}

1.C	-0.100040	2.215621	0.000000
2.C	-0.047642	0.105253	-1.150925
3.C	-0.082422	1.502414	-1.201443
4.H	-0.096191	2.013716	2.161027
5.H	-0.035068	-0.482636	2.068378
6.C	-0.047642	0.105253	1.150925
7.H	-0.035068	-0.482636	-2.068378
8.C	-0.082422	1.502414	1.201443
9.H	-0.096191	2.013716	-2.161027
10.H	-0.127592	3.302858	0.000000
11.N	-0.029402	-0.592037	0.000000

12.O	-0.040627	-3.998292	0.000000
13.H	-0.093330	-3.022776	0.000000
14.H	0.913638	-4.182869	0.000000

HOH- NC_5H_5 (11)

-1897.76 kcal mol^{-1}

1.C	-0.066881	2.203335	0.000000
2.C	-0.045600	0.092585	-1.151126
3.C	-0.059771	1.490047	-1.201512
4.H	-0.066101	2.001554	2.161044
5.H	-0.041767	-0.495771	2.068309
6.C	-0.045600	0.092585	1.151126
7.H	-0.041767	-0.495771	-2.068309
8.C	-0.059771	1.490047	1.201512
9.H	-0.066101	2.001554	-2.161044
10.H	-0.078538	3.290860	0.000000
11.N	-0.037713	-0.604533	0.000000
12.O	-0.101521	-3.947744	0.000000
13.H	-0.138401	-2.970812	0.000000
14.H	0.849532	-4.147937	0.000000

HOH- NC_5H_5 (12)

-1898.10 kcal mol^{-1}

1.C	-0.102697	2.188162	0.000000
2.C	-0.051982	0.078068	-1.151338
3.C	-0.085629	1.475137	-1.201582
4.H	-0.099065	1.986569	2.161062
5.H	-0.040013	-0.510552	2.068234

6.C	-0.051982	0.078068	1.151338
7.H	-0.040013	-0.510552	-2.068234
8.C	-0.085629	1.475137	1.201582
9.H	-0.099065	1.986569	-2.161062
10.H	-0.129475	3.275410	0.000000
11.N	-0.034321	-0.618499	0.000000
12.O	-0.025827	-3.900029	0.000000
13.H	-0.083458	-2.923238	0.000000
14.H	0.929156	-4.080251	0.000000

HOH- NC_5H_5 (13)

-1898.42 kcal mol^{-1}

1.C	-0.079238	2.175088	0.000000
2.C	-0.059653	0.064650	-1.151563
3.C	-0.072795	1.461999	-1.201661
4.H	-0.078732	1.973649	2.161080
5.H	-0.056311	-0.524498	2.068142
6.C	-0.059653	0.064650	1.151563
7.H	-0.056311	-0.524498	-2.068142
8.C	-0.072795	1.461999	1.201661
9.H	-0.078732	1.973649	-2.161080
10.H	-0.089860	3.262613	0.000000
11.N	-0.052132	-0.631688	0.000000
12.O	-0.047408	-3.851114	0.000000
13.H	-0.103522	-2.873205	0.000000
14.H	0.907141	-4.033295	0.000000

HOH- NC_5H_5 (14)

-1898.73 kcal mol^{-1}

1.C	-0.076244	2.161609	0.000000
2.C	-0.060859	0.051330	-1.151802
3.C	-0.071199	1.448623	-1.201746
4.H	-0.076189	1.960365	2.161100
5.H	-0.058752	-0.538289	2.068033
6.C	-0.060859	0.051330	1.151802
7.H	-0.058752	-0.538289	-2.068033
8.C	-0.071199	1.448623	1.201746
9.H	-0.076189	1.960365	-2.161100
10.H	-0.084811	3.249147	0.000000
11.N	-0.054754	-0.644613	0.000000
12.O	-0.049557	-3.802139	0.000000
13.H	-0.105410	-2.822971	0.000000
14.H	0.904774	-3.985091	0.000000

HOH- NC_5H_5 (15)

-1899.01 kcal mol^{-1}

1.C	-0.091594	2.147147	0.000000
2.C	-0.066488	0.037165	-1.152060
3.C	-0.083285	1.434315	-1.201841
4.H	-0.090633	1.946108	2.161130
5.H	-0.061715	-0.552962	2.067905
6.C	-0.066488	0.037165	1.152060
7.H	-0.061715	-0.552962	-2.067905
8.C	-0.083285	1.434315	1.201841
9.H	-0.090633	1.946108	-2.161130
10.H	-0.105100	3.234629	0.000000
11.N	-0.057144	-0.658292	0.000000
12.O	-0.009871	-3.753823	0.000000

13.H	-0.078632	-2.773973	0.000000
14.H	0.946582	-3.924942	0.000000

HOH- NC_5H_5 (16)

-1899.25 kcal mol^{-1}

1.C	-0.086175	2.133735	0.000000
2.C	-0.068937	0.023896	-1.152332
3.C	-0.080499	1.421008	-1.201941
4.H	-0.085990	1.932922	2.161155
5.H	-0.066403	-0.566818	2.067758
6.C	-0.068937	0.023896	1.152332
7.H	-0.066403	-0.566818	-2.067758
8.C	-0.080499	1.421008	1.201941
9.H	-0.085990	1.932922	-2.161155
10.H	-0.095693	3.221251	0.000000
11.N	-0.062222	-0.671124	0.000000
12.O	-0.013103	-3.705315	0.000000
13.H	-0.082331	-2.723657	0.000000
14.H	0.943181	-3.876906	0.000000

HOH- NC_5H_5 (17)

-1899.42 kcal mol^{-1}

1.C	-0.070060	2.120404	0.000000
2.C	-0.074927	0.010749	-1.152626
3.C	-0.071917	1.407811	-1.202059
4.H	-0.072082	1.919869	2.161186
5.H	-0.078516	-0.580612	2.067583
6.C	-0.074927	0.010749	1.152626

7.H	-0.078516	-0.580612	-2.067583
8.C	-0.071917	1.407811	1.202059
9.H	-0.072082	1.919869	-2.161186
10.H	-0.068098	3.207951	0.000000
11.N	-0.075413	-0.683776	0.000000
12.O	-0.026107	-3.657052	0.000000
13.H	-0.095287	-2.673151	0.000000
14.H	0.929850	-3.830008	0.000000

HOH- NC_5H_5 (18)

-1899.51 kcal mol^{-1}

1.C	-0.064463	2.106818	0.000000
2.C	-0.079526	-0.002514	-1.152945
3.C	-0.069769	1.394405	-1.202189
4.H	-0.067501	1.906586	2.161222
5.H	-0.085933	-0.594576	2.067385
6.C	-0.079526	-0.002514	1.152945
7.H	-0.085933	-0.594576	-2.067385
8.C	-0.069769	1.394405	1.202189
9.H	-0.067501	1.906586	-2.161222
10.H	-0.057265	3.194335	0.000000
11.N	-0.083342	-0.696473	0.000000
12.O	-0.024429	-3.609167	0.000000
13.H	-0.096764	-2.622742	0.000000
14.H	0.931720	-3.780574	0.000000

HOH- NC_5H_5 (19)

-1899.48 kcal mol^{-1}

1.C	-0.050389	2.093404	0.000000
2.C	-0.085092	-0.015400	-1.153287
3.C	-0.062347	1.381246	-1.202330
4.H	-0.055350	1.893524	2.161260
5.H	-0.096927	-0.608196	2.067150
6.C	-0.085092	-0.015400	1.153287
7.H	-0.096927	-0.608196	-2.067150
8.C	-0.062347	1.381246	1.202330
9.H	-0.055350	1.893524	-2.161260
10.H	-0.033037	3.180799	0.000000
11.N	-0.095379	-0.708699	0.000000
12.O	-0.034895	-3.561586	0.000000
13.H	-0.107769	-2.571816	0.000000
14.H	0.920903	-3.734449	0.000000

HOH- NC_5H_5 (20)

-1899.47 kcal mol^{-1}

1.C	-0.138898	2.088873	0.000000
2.C	-0.023328	-0.016713	-1.153631
3.C	-0.100254	1.377848	-1.202459
4.H	-0.130495	1.889402	2.161300
5.H	0.005214	-0.609797	2.066854
6.C	-0.023328	-0.016713	1.153631
7.H	0.005214	-0.609797	-2.066854
8.C	-0.100254	1.377848	1.202459
9.H	-0.130495	1.889402	-2.161300
10.H	-0.199196	3.174716	0.000000
11.N	0.016778	-0.708184	0.000000
12.O	-0.058027	-3.501598	0.000000

13.H	0.020075	-2.508181	0.000000
14.H	0.856995	-3.827106	0.000000

SI 7 | Cartesian coordinates of constrained angle complexes

Cartesian coordinates (Å), single point total bonding energies (kcal mol^{-1}) and overlap coefficients S^2 (a.u.) of the halogen bond complex Pyridine-Bromobenzene were computed at the BLYP-D3(BJ)/TZ2P level of theory, changing the N-Br-C_{Ar} angle θ from 180° to 90°. Zenith and azimuthal angle transits are considered, along with transverse and coplanar orientation of the pyridine towards the phenyl ring.

TRANSVERSE – zenith N-Br =2.986 Å

θ (deg)	S^2 (a.u.) <HOMO|HOMO>
180	0.00000961
170	0.00017956
160	0.00087025
150	0.00198025
140	0.00332929
130	0.00473344
120	0.00595984
110	0.00680625
100	0.00710649
90	0.00667489

θ = 180°

(-3.43 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275

4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	2.070212	-4.505878	4.013283
14.C	1.729570	-3.765611	3.292920
15.C	1.165625	-2.560638	3.720837
16.C	0.742366	-1.639951	2.756587
17.N	0.850603	-1.855476	1.434043
18.C	1.394370	-3.017477	1.032583
19.C	1.846707	-3.999599	1.920113
20.H	1.054096	-2.334688	4.778790
21.H	0.297725	-0.689347	3.051022
22.H	1.469122	-3.164243	-0.044869
23.H	2.278944	-4.922498	1.540414

θ = 170°

(-3.24 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058

8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	1.756846	-3.719688	4.862020
14.C	1.467340	-3.107122	4.011194
15.C	0.875650	-1.855453	4.201806
16.C	0.520726	-1.104459	3.076361
17.N	0.720325	-1.526517	1.815681
18.C	1.290072	-2.731769	1.642888
19.C	1.679295	-3.555313	2.704568
20.H	0.691121	-1.465238	5.200024
21.H	0.057189	-0.123879	3.184258
22.H	1.439301	-3.047306	0.610320
23.H	2.136385	-4.522240	2.507432

θ = 160°

(-2.55 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685

12.Br	-0.135362	0.288056	-0.395351
13.H	1.385745	-2.811830	5.551022
14.C	1.156238	-2.345549	4.595583
15.C	0.553351	-1.085833	4.543144
16.C	0.277697	-0.527285	3.290695
17.N	0.564050	-1.142424	2.130137
18.C	1.143833	-2.353712	2.191219
19.C	1.458092	-2.993665	3.394790
20.H	0.300221	-0.543734	5.451334
21.H	-0.191740	0.453006	3.208811
22.H	1.364168	-2.827929	1.234871
23.H	1.927292	-3.974745	3.386172

θ = 150°

(-1.45 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	0.968185	-1.809887	6.059355
14.C	0.805719	-1.504030	5.028331
15.C	0.208521	-0.275163	4.734479

16.C	0.020663	0.074033	3.393077
17.N	0.386525	-0.714865	2.367858
18.C	0.960097	-1.894793	2.660915
19.C	1.189818	-2.331721	3.969809
20.H	-0.106729	0.401826	5.525086
21.H	-0.441496	1.023779	3.123934
22.H	1.246003	-2.512779	1.809809
23.H	1.658018	-3.296649	4.149933

θ = 140°

(-0.12 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	0.516852	-0.744305	6.371573
14.C	0.426431	-0.608135	5.296289
15.C	-0.148361	0.551925	4.769998
16.C	-0.242566	0.681225	3.380395
17.N	0.193144	-0.256832	2.521620
18.C	0.744446	-1.368957	3.037705
19.C	0.882626	-1.589594	4.412152

20.H	-0.517362	1.342712	5.419038
21.H	-0.684491	1.571097	2.932206
22.H	1.088398	-2.111432	2.317663
23.H	1.336744	-2.508555	4.775510

θ = 130°

(1.23 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	0.045461	0.352541	6.478190
14.C	0.029901	0.314916	5.391314
15.C	-0.506452	1.370302	4.648622
16.C	-0.503991	1.275841	3.253036
17.N	-0.010217	0.217757	2.586752
18.C	0.503433	-0.792180	3.310139
19.C	0.545848	-0.789833	4.708380
20.H	-0.919202	2.250334	5.136412
21.H	-0.913343	2.078332	2.639452
22.H	0.896141	-1.636081	2.743004
23.H	0.973233	-1.634410	5.243893

θ = 120°

(2.35 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	-0.431666	1.447323	6.375965
14.C	-0.371825	1.237075	5.310521
15.C	-0.854872	2.155101	4.374039
16.C	-0.755670	1.839814	3.014869
17.N	-0.217379	0.694483	2.561274
18.C	0.244380	-0.181988	3.469941
19.C	0.189718	0.043261	4.849490
20.H	-1.300039	3.097115	4.685795
21.H	-1.121097	2.530070	2.254568
22.H	0.675075	-1.101171	3.072907
23.H	0.578530	-0.700772	5.540852

θ = 110°

(2.99 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842

2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	-0.900031	2.506777	6.068005
14.C	-0.766540	2.130324	5.056364
15.C	-1.183035	2.882477	3.954591
16.C	-0.989955	2.356009	2.673130
17.N	-0.422048	1.158861	2.445960
18.C	-0.024840	0.443080	3.512254
19.C	-0.174944	0.884376	4.831196
20.H	-1.648302	3.857327	4.080881
21.H	-1.301441	2.912585	1.789249
22.H	0.431915	-0.522954	3.297349
23.H	0.164627	0.263988	5.657364

θ = 100°

(2.99 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997

6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300
10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	-1.345403	3.498712	5.563668
14.C	-1.142250	2.967521	4.636565
15.C	-1.480968	3.530328	3.403023
16.C	-1.199727	2.808741	2.238204
17.N	-0.618004	1.596780	2.244315
18.C	-0.296049	1.064030	3.435794
19.C	-0.537057	1.707955	4.654054
20.H	-1.953409	4.507871	3.340048
21.H	-1.448895	3.214256	1.257633
22.H	0.174050	0.081000	3.409510
23.H	-0.255900	1.230559	5.589889

θ = 90°

(2.37 kcal mol^{-1})

1.C	-0.775880	1.680653	-1.583842
2.C	-2.106787	1.663188	-2.010121
3.C	-2.563379	2.671992	-2.866275
4.C	-1.698432	3.686525	-3.291230
5.C	-0.368541	3.690211	-2.855997
6.C	0.100189	2.687042	-1.999774
7.H	-2.775080	0.873955	-1.678058
8.H	-3.599009	2.660950	-3.199679
9.H	-2.057887	4.468068	-3.956300

10.H	0.311221	4.474990	-3.181331
11.H	1.131761	2.686441	-1.659685
12.Br	-0.135362	0.288056	-0.395351
13.H	-1.754251	4.392988	4.878277
14.C	-1.487540	3.723229	4.063879
15.C	-1.739620	4.078970	2.736095
16.C	-1.378614	3.184254	1.723304
17.N	-0.799294	1.994935	1.962465
18.C	-0.561005	1.661996	3.242883
19.C	-0.885618	2.488973	4.323445
20.H	-2.206089	5.028980	2.485806
21.H	-1.558979	3.425916	0.675872
22.H	-0.090684	0.692342	3.405982
23.H	-0.670273	2.169570	5.340476

TRANSVERSE – azimuth

θ (deg)	S^2 (a.u.) <HOMO|HOMO-2>
180	0.00000001
170	0.00051076
160	0.00197136
150	0.00418609
140	0.00687241
130	0.00968256
120	0.01225449
110	0.01425636
100	0.015376

90	0.015376

θ = 180°

(-3.42 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	2.019980	-4.378171	4.172279
14.C	1.687575	-3.658732	3.427382
15.C	1.117611	-2.442844	3.814503
16.C	0.705426	-1.549977	2.819776
17.N	0.829864	-1.802347	1.505199
18.C	1.379301	-2.974561	1.143075
19.C	1.821536	-3.930958	2.063190
20.H	0.993085	-2.187468	4.864281
21.H	0.256560	-0.591970	3.082050
22.H	1.467232	-3.151370	0.071143
23.H	2.259015	-4.863672	1.714765

θ = 170°

(-3.16 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	3.079265	-3.826931	4.078514
14.C	2.579487	-3.194464	3.348334
15.C	1.890934	-2.046933	3.751043
16.C	1.264014	-1.265359	2.774977
17.N	1.289885	-1.562498	1.464127
18.C	1.954757	-2.668280	1.086913
19.C	2.612495	-3.512410	1.987859
20.H	1.838158	-1.759651	4.798631
21.H	0.717445	-0.363253	3.049774
22.H	1.958566	-2.883665	0.018444
23.H	3.135807	-4.395145	1.627767

θ = 160°

(-2.40 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061

5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	4.039057	-3.146165	3.854680
14.C	3.387597	-2.621141	3.159766
15.C	2.593005	-1.556156	3.592821
16.C	1.771425	-0.912154	2.661771
17.N	1.706599	-1.266421	1.366556
18.C	2.474714	-2.291955	0.959887
19.C	3.327689	-2.997473	1.815200
20.H	2.606395	-1.227941	4.629572
21.H	1.137404	-0.077658	2.961238
22.H	2.401199	-2.556445	-0.094945
23.H	3.927644	-3.819983	1.432743

θ = 150°

(-1.25 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798

9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	4.870191	-2.356558	3.507579
14.C	4.087353	-1.956185	2.867406
15.C	3.202495	-0.985426	3.344647
16.C	2.212240	-0.501094	2.483597
17.N	2.067347	-0.923112	1.215451
18.C	2.923374	-1.857020	0.765858
19.C	3.945385	-2.401792	1.550458
20.H	3.274454	-0.608492	4.362241
21.H	1.503676	0.256137	2.819133
22.H	2.781681	-2.179654	-0.265578
23.H	4.610465	-3.155661	1.135618

θ = 140°

(0.11 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351

13.H	5.547416	-1.482102	3.047756
14.C	4.657493	-1.219800	2.480138
15.C	3.700882	-0.352084	3.014059
16.C	2.573066	-0.044668	2.245869
17.N	2.361167	-0.543002	1.015402
18.C	3.287104	-1.376690	0.510720
19.C	4.446817	-1.743467	1.201678
20.H	3.822036	0.079874	4.004761
21.H	1.805132	0.627991	2.627776
22.H	3.088450	-1.764741	-0.488271
23.H	5.163524	-2.422365	0.745420

θ = 130°

(1.43 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	6.050153	-0.549366	2.489184
14.C	5.080693	-0.434359	2.009730
15.C	4.073025	0.324627	2.611104
16.C	2.842940	0.443255	1.955810

17.N	2.579131	-0.137641	0.772488
18.C	3.554854	-0.865561	0.202227
19.C	4.816748	-1.042501	0.779457
20.H	4.232504	0.816241	3.567994
21.H	2.032613	1.026605	2.392982
22.H	3.312187	-1.324311	-0.756257
23.H	5.570015	-1.642375	0.274004

θ = 120°

(2.47 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	6.363127	0.413308	1.848834
14.C	5.344095	0.376270	1.470473
15.C	4.307615	1.024144	2.148024
16.C	3.013662	0.947850	1.622235
17.N	2.714616	0.280654	0.494090
18.C	3.718486	-0.339161	-0.150250
19.C	5.043939	-0.320192	0.296624
20.H	4.493384	1.578235	3.065210

21.H	2.179207	1.439866	2.121884
22.H	3.446093	-0.871747	-1.061394
23.H	5.817588	-0.839391	-0.264304

θ = 110°

(2.90 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	6.476828	1.376672	1.146164
14.C	5.439695	1.187460	0.878753
15.C	4.397525	1.725214	1.638890
16.C	3.080044	1.453785	1.255277
17.N	2.763507	0.699175	0.188667
18.C	3.773030	0.186514	-0.535999
19.C	5.121486	0.401513	-0.232149
20.H	4.596751	2.342703	2.511686
21.H	2.240459	1.855219	1.822721
22.H	3.486098	-0.420800	-1.394411
23.H	5.898721	-0.037812	-0.853149

θ = 100°

(2.90 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469
3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	6.387803	2.311452	0.402522
14.C	5.364588	1.974560	0.252549
15.C	4.340023	2.406535	1.099172
16.C	3.040069	1.945687	0.866087
17.N	2.724317	1.105204	-0.134501
18.C	3.716828	0.695492	-0.943301
19.C	5.047032	1.100685	-0.790798
20.H	4.539463	3.086418	1.924241
21.H	2.214508	2.260043	1.504582
22.H	3.430989	0.014828	-1.745188
23.H	5.810948	0.738008	-1.474640

θ = 90°

(3.07 kcal mol^{-1})

1.C	-0.762410	1.646131	-1.630075
2.C	-2.099016	1.640540	-2.038469

3.C	-2.545788	2.624367	-2.928212
4.C	-1.665499	3.602455	-3.404061
5.C	-0.330077	3.594656	-2.986161
6.C	0.128948	2.616200	-2.096726
7.H	-2.779225	0.879619	-1.666872
8.H	-3.585822	2.622496	-3.247798
9.H	-2.017369	4.364699	-4.095079
10.H	0.361594	4.351147	-3.351001
11.H	1.164771	2.606792	-1.769946
12.Br	-0.135362	0.288056	-0.395351
13.H	6.098755	3.189247	-0.359496
14.C	5.121058	2.713657	-0.389112
15.C	4.136856	3.047406	0.545268
16.C	2.894953	2.408611	0.466490
17.N	2.598237	1.486404	-0.465595
18.C	3.551588	1.172308	-1.359779
19.C	4.822841	1.756081	-1.362347
20.H	4.323263	3.786782	1.320724
21.H	2.102144	2.642038	1.177133
22.H	3.282439	0.421900	-2.103068
23.H	5.556937	1.464496	-2.109893

COPLANAR – zenith N-Br =2.983 Å

θ (deg)	S^2 (a.u.) <HOMO|HOMO>
180	0.00000036
170	0.00023409
160	0.00094249
150	0.00200704

140	0.003249
130	0.003249
120	0.00544644
110	0.00594441
100	0.00585225
90	0.00505521

θ = 180°

(-3.38 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	-0.043535	5.535973	2.512974
14.C	-0.429372	6.467018	2.104043
15.C	-0.462412	6.680119	0.723255
16.C	-0.967683	7.893672	0.245202
17.N	-1.424984	8.869497	1.048725
18.C	-1.388944	8.654851	2.375241
19.C	-0.902436	7.475183	2.948371
20.H	-0.105137	5.924475	0.027497
21.H	-1.009567	8.096396	-0.824936

22.H	-1.766161	9.463431	3.001288
23.H	-0.896434	7.354221	4.029125

θ = 170°

(-3.14 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	1.042263	6.005706	2.320651
14.C	0.485722	6.860464	1.943038
15.C	0.322389	7.054606	0.568734
16.C	-0.401489	8.168788	0.131531
17.N	-0.950385	9.066088	0.968532
18.C	-0.787663	8.870463	2.288483
19.C	-0.080969	7.787519	2.821961
20.H	0.745380	6.359682	-0.152988
21.H	-0.550070	8.353759	-0.932309
22.H	-1.243595	9.613931	2.942249
23.H	0.020038	7.677663	3.899192

θ = 160°

(-2.43 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	2.023469	6.640188	2.053703
14.C	1.313131	7.392796	1.719130
15.C	1.024949	7.547604	0.360429
16.C	0.104435	8.529322	-0.020921
17.N	-0.519845	9.334833	0.855683
18.C	-0.235846	9.178031	2.160205
19.C	0.669545	8.225194	2.638905
20.H	1.501194	6.922848	-0.391630
21.H	-0.145963	8.679891	-1.071004
22.H	-0.757011	9.844947	2.846964
23.H	0.862103	8.141348	3.705952

θ = 150°

(-1.33 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694

4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	2.870271	7.420139	1.720242
14.C	2.027715	8.047841	1.439122
15.C	1.623924	8.144132	0.104670
16.C	0.534716	8.964321	-0.207521
17.N	-0.146445	9.667564	0.713607
18.C	0.249739	9.568208	1.994304
19.C	1.326302	8.774912	2.404764
20.H	2.139339	7.596859	-0.681180
21.H	0.190478	9.064883	-1.236808
22.H	-0.321194	10.149460	2.718327
23.H	1.604175	8.731185	3.455274

θ = 140°

(-0.02 kcal mol^{-1})

1.C	-3.03446500	13.11265400	-0.85730200
2.C	-3.56160000	14.09141100	-0.01025500
3.C	-4.01581300	15.29683500	-0.55769400
4.C	-3.94378000	15.52073300	-1.93705400
5.C	-3.41361700	14.53117800	-2.77230100
6.C	-2.95601000	13.32159900	-2.23695800
7.H	-3.61593100	13.91414400	1.06001100

8.H	-4.42656000	16.06043300	0.09959600
9.H	-4.29791000	16.45881200	-2.35767000
10.H	-3.35352600	14.69637300	-3.84603600
11.H	-2.54353000	12.55134800	-2.88224700
12.Br	-2.40042600	11.44072200	-0.10629900
13.H	2.86978135	7.41958886	1.72044542
14.C	2.02730084	8.04737903	1.43929255
15.C	1.62357844	8.14372011	0.10482371
16.C	0.53446822	8.96402239	-0.20740911
17.N	-0.14666149	9.66732805	0.71369239
18.C	0.24945620	9.56792360	1.99440657
19.C	1.32592120	8.77451436	2.40490883
20.H	2.13897206	7.59639971	-0.68100841
21.H	0.19028523	9.06462681	-1.23671150
22.H	-0.32144933	10.14922861	2.71840819
23.H	1.60374249	8.73075289	3.45543114

θ = 130°

(1.25 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247

12.Br	-2.400426	11.440722	-0.106299
13.H	3.556939	8.321862	1.330401
14.C	2.607761	8.805695	1.111523
15.C	2.101112	8.826066	-0.190772
16.C	0.876281	9.460567	-0.422599
17.N	0.158469	10.054172	0.546619
18.C	0.654339	10.029140	1.795821
19.C	1.869348	9.419968	2.126653
20.H	2.640426	8.361236	-1.012840
21.H	0.449029	9.497036	-1.424683
22.H	0.050613	10.518217	2.560246
23.H	2.223706	9.429255	3.154778

θ = 120°

(2.39 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	4.371916	10.378163	0.430307
14.C	3.298369	10.535298	0.354508
15.C	2.636274	10.361306	-0.863868

16.C	1.254759	10.575085	-0.911386
17.N	0.528143	10.940753	0.158811
18.C	1.174243	11.105522	1.326040
19.C	2.552257	10.915397	1.473399
20.H	3.175152	10.066150	-1.761206
21.H	0.703644	10.449269	-1.843313
22.H	0.559299	11.402033	2.175718
23.H	3.024147	11.062601	2.442083

θ = 110°

(3.08 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	4.475462	11.470260	-0.052596
14.C	3.387946	11.454494	-0.051906
15.C	2.677988	11.167963	-1.221069
16.C	1.280172	11.159493	-1.170243
17.N	0.581670	11.413787	-0.050227
18.C	1.273750	11.688267	1.069016
19.C	2.671372	11.720332	1.118106

20.H	3.192544	10.954883	-2.155174
21.H	0.691971	10.940417	-2.061349
22.H	0.680722	11.890238	1.960954
23.H	3.180736	11.948251	2.051540

θ = 100°

(3.24kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	4.370101	12.561069	-0.538014
14.C	3.301656	12.372990	-0.460608
15.C	2.565889	11.968149	-1.577671
16.C	1.194219	11.738450	-1.428326
17.N	0.544588	11.887641	-0.260966
18.C	1.261158	12.277349	0.807525
19.C	2.635906	12.531110	0.757937
20.H	3.040877	11.831951	-2.546464
21.H	0.587171	11.421739	-2.276402
22.H	0.707693	12.389795	1.739759

23.H	3.166881	12.844382	1.653829

θ = 90°

(2.87 kcal mol^{-1})

1.C	-3.034465	13.112654	-0.857302
2.C	-3.561600	14.091411	-0.010255
3.C	-4.015813	15.296835	-0.557694
4.C	-3.943780	15.520733	-1.937054
5.C	-3.413617	14.531178	-2.772301
6.C	-2.956010	13.321599	-2.236958
7.H	-3.615931	13.914144	1.060011
8.H	-4.426560	16.060433	0.099596
9.H	-4.297910	16.458812	-2.357670
10.H	-3.353526	14.696373	-3.846036
11.H	-2.543530	12.551348	-2.882247
12.Br	-2.400426	11.440722	-0.106299
13.H	4.059035	13.617444	-1.011197
14.C	3.042121	13.262879	-0.859179
15.C	2.303383	12.737550	-1.922840
16.C	0.999510	12.294363	-1.677795
17.N	0.418024	12.347915	-0.467005
18.C	1.136849	12.854871	0.549511
19.C	2.446935	13.323097	0.403835
20.H	2.724758	12.670704	-2.923189
21.H	0.392429	11.878610	-2.481938
22.H	0.639392	12.885524	1.518854
23.H	2.983004	13.723769	1.261034

COPLANAR – azimuth

θ (deg)	S^2 (a.u.) <HOMO|HOMO-2>
180	0.00000049
170	0.000484
160	0.00192721
150	0.00414736
140	0.00685584
130	0.00972196
120	0.01238769
110	0.01456849
100	0.01600225
90	0.01646089

θ = 180°

(-3.38 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-0.072295	5.203333	1.613113
14.C	-0.453420	6.186529	1.346635
15.C	-0.536795	6.580565	0.008403
16.C	-1.033729	7.854877	-0.284398

17.N	-1.436877	8.723590	0.658902
18.C	-1.352705	8.335136	1.943050
19.C	-0.869971	7.082171	2.335263
20.H	-0.224390	5.917519	-0.795025
21.H	-1.113774	8.197767	-1.315933
22.H	-1.686639	9.060182	2.685226
23.H	-0.823535	6.819513	3.389565

θ = 170°

(-3.11 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-0.168804	4.960052	0.443581
14.C	-0.534468	5.981128	0.362142
15.C	-0.672531	6.591821	-0.887287
16.C	-1.146829	7.906627	-0.940886
17.N	-1.478038	8.615956	0.151891
18.C	-1.341689	8.019662	1.348912
19.C	-0.876055	6.709813	1.504689
20.H	-0.419161	6.064079	-1.803810

21.H	-1.267887	8.416293	-1.896726
22.H	-1.617812	8.619065	2.216380
23.H	-0.785143	6.276189	2.497867

θ = 160°

(-2.30 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-0.329793	4.914733	-0.743114
14.C	-0.669813	5.942374	-0.636908
15.C	-0.851923	6.753177	-1.760525
16.C	-1.290664	8.068060	-1.573080
17.N	-1.547214	8.594158	-0.362952
18.C	-1.368991	7.806222	0.711484
19.C	-0.933717	6.479569	0.625966
20.H	-0.659218	6.378669	-2.763187
21.H	-1.444185	8.730534	-2.424904
22.H	-1.584793	8.259933	1.678750
23.H	-0.806286	5.886534	1.528611

θ = 150°

(-1.07 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-0.550373	5.068742	-1.910951
14.C	-0.855343	6.071434	-1.620190
15.C	-1.069523	7.059728	-2.584806
16.C	-1.460867	8.334269	-2.161791
17.N	-1.642305	8.658855	-0.869998
18.C	-1.433782	7.701290	0.050114
19.C	-1.041204	6.398421	-0.274229
20.H	-0.937273	6.851731	-3.644036
21.H	-1.637315	9.130947	-2.884436
22.H	-1.588583	7.993685	1.088657
23.H	-0.886319	5.662369	0.511223

θ = 140°

(0.40 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893

3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-0.823841	5.417402	-3.024446
14.C	-1.085421	6.364388	-2.557828
15.C	-1.318720	7.502161	-3.335083
16.C	-1.652267	8.697167	-2.689133
17.N	-1.760421	8.808080	-1.353840
18.C	-1.534092	7.708055	-0.615100
19.C	-1.195250	6.468834	-1.168546
20.H	-1.244877	7.468892	-4.419594
21.H	-1.841409	9.605366	-3.261361
22.H	-1.629067	7.828410	0.464031
23.H	-1.022810	5.610505	-0.523386

θ = 130°

(1.84 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614

7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-1.141887	5.950116	-4.049764
14.C	-1.353056	6.812334	-3.421331
15.C	-1.591941	8.067031	-3.988561
16.C	-1.859048	9.145726	-3.139082
17.N	-1.897975	9.037300	-1.799778
18.C	-1.666875	7.826310	-1.263946
19.C	-1.391174	6.688670	-2.029811
20.H	-1.572684	8.211400	-5.066295
21.H	-2.050266	10.139376	-3.544225
22.H	-1.705016	7.769129	-0.176149
23.H	-1.211613	5.732518	-1.543778

θ = 120°

(3.00 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579

11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-1.494849	6.650700	-4.955754
14.C	-1.650116	7.401661	-4.184463
15.C	-1.880884	8.737176	-4.525385
16.C	-2.074928	9.666318	-3.497967
17.N	-2.050785	9.339549	-2.194262
18.C	-1.828094	8.052464	-1.876711
19.C	-1.623023	7.051248	-2.831854
20.H	-1.910733	9.056694	-5.564490
21.H	-2.257540	10.716752	-3.724433
22.H	-1.814120	7.817644	-0.812431
23.H	-1.446990	6.024700	-2.518950

θ = 110°

(4.20 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-1.872002	7.497867	-5.714886
14.C	-1.967576	8.114464	-4.824037

15.C	-2.176771	9.492234	-4.929241
16.C	-2.293347	10.243125	-3.754883
17.N	-2.214210	9.705644	-2.525306
18.C	-2.012852	8.379644	-2.434775
19.C	-1.883754	7.545552	-3.550306
20.H	-2.248754	9.979090	-5.899042
21.H	-2.456932	11.319950	-3.796511
22.H	-1.953065	7.972481	-1.425482
23.H	-1.721790	6.478174	-3.419273

θ = 100°

(8.97 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-2.261887	8.465875	-6.304096
14.C	-2.295788	8.929084	-5.320618
15.C	-2.470612	10.309262	-5.187861
16.C	-2.507667	10.858620	-3.902023
17.N	-2.383283	10.124462	-2.782851
18.C	-2.215536	8.797908	-2.921182

19.C	-2.165442	8.156563	-4.163338
20.H	-2.576475	10.950562	-6.059785
21.H	-2.642385	11.930642	-3.758268
22.H	-2.117630	8.228935	-1.996676
23.H	-2.027663	7.079162	-4.217389

θ = 90°

(33.75 kcal mol^{-1})

1.C	-3.026734	13.207519	-0.603826
2.C	-3.185054	14.184579	0.382893
3.C	-3.635488	15.458446	0.017627
4.C	-3.924561	15.751735	-1.319673
5.C	-3.761285	14.762978	-2.296213
6.C	-3.311435	13.485329	-1.943614
7.H	-2.959666	13.953338	1.419991
8.H	-3.759506	16.220870	0.783887
9.H	-4.274218	16.742836	-1.598556
10.H	-3.983492	14.981847	-3.338579
11.H	-3.183178	12.715443	-2.699028
12.Br	-2.400426	11.440722	-0.106299
13.H	-2.652655	9.525313	-6.705479
14.C	-2.624782	9.820769	-5.659120
15.C	-2.753477	11.163437	-5.293386
16.C	-2.711379	11.494102	-3.934918
17.N	-2.552868	10.583276	-2.959072
18.C	-2.429985	9.294549	-3.321153
19.C	-2.459531	8.865715	-4.652323
20.H	-2.883939	11.941593	-6.041835
21.H	-2.808264	12.530273	-3.610867
22.H	-2.302814	8.579215	-2.508656

23.H -2.355315 7.809402 -4.889049