

Selected geometric parameters of the obtained complexes.

Check the explanation in the paper to understand how the complexes are named.
The definition of some parameters of the following tables is:

Radius 1 is defined as the average distance between carbons 1 and 2 of the three pincers (see figure bellow) and their mass centre, CM1.

Radius 2 is like radius 1 but using carbons 3 and 4 (see figure bellow) and their mass centre, CM2.

Depth 1 is the distance from CM1 to the X atom.

Depth 2 is the same but with CM2.

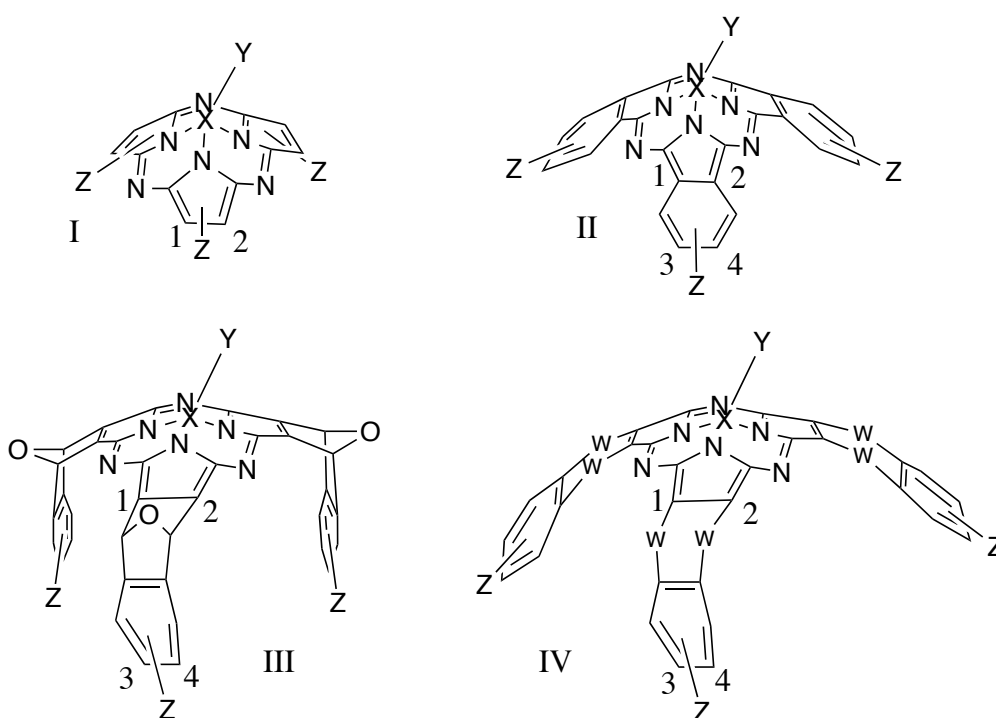


Table 1. Selected geometric parameters in Å for compound I.

	Distance X-ion	Radius 1	Depth 1
I-CN-B-CN			
Monomer	---	3.308	1.731
Cl ⁻	3.568	3.268	1.781
Br ⁻	3.756	3.268	1.782
I ⁻	4.000	3.272	1.762
BF ₄ ⁻	4.235 ^a	3.298	1.720
I-CN-P-CN			
Monomer	---	3.318	1.863
Br ⁻	3.680	3.324	1.819
I ⁻	3.963	3.327	1.813
BF ₄ ⁻	4.289 ^a	3.300	1.852
I-Cl-B-CN			
Monomer	---	3.315	1.698

Br ⁻	3.740	3.279	1.736
I ⁻	3.979	3.287	1.714
I-Cl-P-CN			
Monomer	---	3.317	1.876
Br ⁻	3.713	3.313	1.829
I ⁻	3.981	3.321	1.811
I-CN-B-F			
Monomer	---	3.300	1.703
Br ⁻	3.772	3.268	1.738
I-CN-P-F			
Monomer	---	3.307	1.833
Br ⁻	3.709	3.282	1.808
I-Cl-B-F			
Monomer	---	3.308	1.662
Br ⁻	3.744	3.278	1.681
I-Cl-P-F			
Monomer	---	3.299	1.850
Br ⁻	3.731	3.280	1.818

^a Distance to the central Boron atom.

Table 2. Selected geometric parameters in Å for compound **II**.

	Distance X-ion	Radius 1	Radius 2	Depth 1	Depth 2
II-CN-B-CN					
Monomer	---	3.348	5.597	1.624	2.686
Br ⁻	3.739	3.284	5.307	1.765	3.050
I ⁻	3.959	3.298	5.338	1.734	2.992
BF ₄ ⁻	4.179 ^a	3.321	5.353	1.671	2.943
II-CN-P-CN					
Monomer	---	3.347	5.407	1.836	3.082
Br ⁻	3.707	3.311	5.294	1.870	3.239
II-CN-B-F					
Monomer	---	3.353	5.475	1.598	2.678
Br ⁻	3.764	3.311	5.332	1.680	2.936
I ⁻	3.994	3.315	5.333	1.670	2.929
BF ₄ ⁻	4.187 ^a	3.334	5.344	1.625	2.899
II-CN-P-F					
Monomer	---	3.357	5.398	1.815	3.056
Br ⁻	3.780	3.329	5.275	1.836	3.222

^a Distance to the central Boron atom.

Table 3. Selected geometric parameters in Å for compounds **III** and **IV**.

	Distance X-ion	Radius 1	Radius 2	Depth 1	Depth 2
III-CN-B-CN					
Monomer	---	3.303	3.494	1.698	6.335
Br ⁻	3.929	3.300	3.542	1.671	6.372
I ⁻	4.098	3.290	3.430	1.697	6.337
BF ₄ ⁻	4.330 ^a	3.290	3.327	1.698	6.338
III-Cl-B-CN					
Monomer	---	3.341	3.946	1.566	6.213
Br ⁻	3.863	3.312	3.782	1.604	6.314
III-CN-P-CN					
Monomer	---	3.112	3.406	1.786	6.420
Br ⁻	3.866	3.307	3.378	1.790	6.432
I ⁻	4.063	3.312	3.406	1.785	6.411
BF ₄ ⁻	4.429 ^a	3.302	3.315	1.811	6.460
IV-CN-B-CN-O					
Monomer	---	3.275	6.652	1.753	5.062
Br ⁻	3.792	3.232	6.607	1.810	5.130
IV-CN-B-CN-S					
Monomer	---	3.283	4.920	1.784	6.614
Br ⁻	3.908	3.232	4.087	1.872	6.906
III-CN-B-F					
Monomer	---	3.303	2.921	1.702	6.318
Br ⁻	3.890	3.292	2.927	1.701	6.315
I ⁻	4.016	3.289	2.975	1.710	6.331
BF ₄ ⁻	4.282 ^a	3.294	2.953	1.689	6.292
III-Cl-B-F					
Monomer	---	3.309	2.934	1.663	6.272
Br ⁻	3.866	3.298	2.940	1.655	6.264
III-Cl-P-F					
Monomer	---	3.300	2.783	1.845	6.434
Br ⁻	3.790	3.300	2.835	1.801	6.396

^a Distance to the central Boron atom.

Wavelength (nm) and oscillator strength of the main electronic transitions. Orbital transitions with a coefficient larger than 0.1 for each electronic transition.

Only electronic transitions with oscillator strength bigger than 0.1 are presented. Check the explanation in the paper to understand how the complexes are named.

I-CN-B-CN Monomer

Wavelength	fosc	Main Transitions	Coefficients
417.3	0.342139718	104 -> 105	0.780385
417.3	0.342183640	104 -> 106	0.780388
310.5	0.353285208	103 -> 105	0.449419
310.5	0.352906340	103 -> 106	0.448083
293.0	0.802923408	100 -> 105;103 -> 105	0.182710; 0.283925
293.0	0.803689451	100 -> 106;103 -> 106	0.183877; 0.283653

I-CN-B-CN...Br⁻

Wavelength	fosc	Main Transitions	Coefficients
430.6	0.370163650	119 -> 123	0.813912
430.5	0.370053353	119 -> 124	0.813789

I-CN-B-CN...BF₄

Wavelength	fosc	Main Transitions	Coefficients
439.8	0.388593976	125 -> 126	0.839089
435.8	0.322890855	125 -> 127	0.832256
340.6	0.178919483	122 -> 127;123 -> 126	0.124969;0.242206
		124 -> 126;124 -> 127	0.265750;0.125660
328.0	0.433124254	123 -> 126;124 -> 126	0.189295;0.401423
316.2	0.508778757	121 -> 126	0.512728
308.2	0.573068974	122 -> 127;124 -> 127	0.280053;0.282682
311.7	0.436382591	121 -> 127;124 -> 127	0.407806;0.107927

II-CN-B-CN Monomer

Wavelength	fosc	Main Transitions	Coefficients
463.7	0.693422978	179 -> 180	0.888683
463.5	0.693861389	179 -> 181	0.888483

II-CN-B-CN...Br⁻

Wavelength	fosc	Main Transitions	Coefficients
486.0	0.577011301	194 -> 198	0.879180
486.0	0.576040630	194 -> 199	0.879086
404.8	0.113563465	194 -> 201	0.951063
404.7	0.113966652	194 -> 202	0.951078

III-CN-B-CN Monomer

Wavelength	fosc	Main Transitions	Coefficients
408.6	0.202665990	230 -> 231	0.797104
407.3	0.202163333	230 -> 232	0.793727
317.6	0.103713272	228 -> 233;229 -> 231	0.137232;0.153089
317.7	0.104507987	229 -> 231	0.153782
308.1	0.111360088	229 -> 231	0.234021
305.0	0.114928283	229 -> 232;230 -> 237	0.140021;0.109346

III-CN-B-CN...Br⁻

Wavelength	fosc	Main Transitions	Coefficients
414.6	0.225391642	245 -> 249	0.812004
414.0	0.227582128	245 -> 250	0.811078

Cartesian coordinates of the different grippers and obtained complexes.

Check the explanation in the paper to understand how the complexes are named.

5

BF4

B	-0.529152	0.155887	-2.186304
F	-1.545438	-0.841683	-2.060145
F	0.079274	0.054101	-3.476140
F	-1.110665	1.452982	-2.035436
F	0.460491	-0.042497	-1.173760

33

I-CN-B-CN

N	-1.192808	0.688575	0.829618
N	-0.000015	-1.377987	0.830786
N	1.192956	0.688686	0.830793
C	-1.144214	1.974617	0.348597
C	-2.282369	0.003344	0.348680
C	-1.138402	-1.979876	0.351910
C	1.137576	-1.978040	0.347802
C	2.282770	0.004174	0.350595
C	1.145071	1.975173	0.351123
N	0.000350	2.665084	0.197295
N	-2.308059	-1.333094	0.197245
N	2.307821	-1.332238	0.196634
C	-2.447283	2.225565	-0.262624
C	-3.150716	1.007203	-0.263312
C	-0.704010	-3.233095	-0.260850
C	0.702799	-3.232079	-0.263801
C	3.151376	1.006775	-0.261227
C	2.447874	2.225182	-0.261837
B	-0.000117	-0.000154	1.469112
C	2.845048	3.443239	-0.857822
N	3.175346	4.451565	-1.339567
C	4.405129	0.741929	-0.855872
N	5.442509	0.525441	-1.340469
C	1.559134	-4.185627	-0.858057
N	2.268941	-4.975503	-1.337668
C	-1.560727	-4.186069	-0.855503
N	-2.267951	-4.975229	-1.340304
C	-4.404626	0.742503	-0.857904
N	-5.443242	0.523293	-1.338680
C	-2.845184	3.444257	-0.855798
N	-3.175232	4.452046	-1.338852
C	-0.000135	0.000101	3.053376
N	0.000313	0.000164	4.216149

33

I-CN-P-CN

N	-1.307896	0.750872	1.353050
N	0.010165	-1.512677	1.371615
N	1.247560	0.726216	1.231550
C	-1.171944	2.053868	0.716054
C	-2.375664	-0.030211	0.717312
C	-1.192807	-2.055197	0.724967
C	1.215653	-2.032279	0.733835
C	2.370646	-0.001652	0.728362
C	1.165325	2.054355	0.707706
N	-0.051619	2.702701	0.561928
N	-2.272867	-1.328212	0.464133
N	2.336202	-1.380534	0.592947
C	-2.493067	2.237439	0.111067
C	-3.160571	0.987439	0.074098
C	-0.689138	-3.230739	0.072111
C	0.727836	-3.264601	0.114558
C	3.157401	0.973008	0.117236
C	2.404458	2.252799	0.100882
C	2.802572	3.415213	-0.596143
N	3.150208	4.369180	-1.168643
C	4.379993	0.746319	-0.552591
N	5.395926	0.583576	-1.100565
C	1.565022	-4.215407	-0.504185
N	2.264879	-5.008160	-0.996615
C	-1.510607	-4.133268	-0.646584
N	-2.186275	-4.881282	-1.230460
C	-4.361873	0.715519	-0.624683
N	-5.355424	0.488121	-1.188465
C	-2.917776	3.433688	-0.501252
N	-3.269231	4.429087	-0.997939
C	0.043934	0.049273	3.722366
N	0.083444	0.105070	4.887673
P	-0.006254	-0.001253	1.960776

32

I-Cl-B-CN

N	-0.694526	1.182894	0.353939
N	-0.677196	-1.192916	0.353977
N	1.372147	0.010046	0.353719
C	-0.020168	2.282845	-0.116540
C	-1.983553	1.129902	-0.117187
C	-1.966902	-1.158734	-0.117022
C	0.013092	-2.282887	-0.116558
C	1.986734	-1.123766	-0.118517
C	1.970182	1.152665	-0.118498
N	1.315427	2.317448	-0.273108
N	-2.664917	-0.019433	-0.271958

N	1.349051	-2.297960	-0.273115
C	-1.034161	3.150849	-0.712621
C	-2.247120	2.437735	-0.713947
C	-2.211419	-2.470218	-0.713813
C	-0.988163	-3.165563	-0.712663
C	3.244991	-0.679990	-0.715099
C	3.234759	0.727146	-0.715126
Cl	0.000116	-0.000006	2.839499
B	0.000233	0.000006	0.983834
C	4.192456	1.589289	-1.294459
N	4.988165	2.299834	-1.762874
C	4.215128	-1.528249	-1.294280
N	5.021039	-2.227297	-1.762538
C	-0.720545	-4.425274	-1.294352
N	-0.502673	-5.468778	-1.764956
C	-3.430497	-2.886373	-1.294772
N	-4.438390	-3.235740	-1.763895
C	-3.472074	2.836199	-1.295014
N	-4.484785	3.171010	-1.764286
C	-0.784787	4.414358	-1.294114
N	-0.581837	5.460955	-1.764523

32

I-Cl-P-CN

N	1.475146	0.001484	1.265939
N	-0.747251	1.238672	1.061981
N	-0.792208	-1.311196	1.254626
C	2.023598	-1.208526	0.637114
C	2.011799	1.196621	0.628352
C	-0.015068	2.357869	0.562322
C	-2.078265	1.170987	0.552238
C	-2.085126	-1.165666	0.594009
C	-0.005770	-2.378197	0.615562
N	1.294916	-2.283757	0.373366
N	1.366568	2.315400	0.449970
N	-2.731559	-0.045638	0.426044
C	3.217250	-0.718068	0.008082
C	3.257316	0.698880	0.041306
C	-0.982943	3.148783	-0.052264
C	-2.271968	2.408039	-0.057623
C	-2.262436	-2.476880	-0.029121
C	-1.013543	-3.148352	-0.054798
C	-0.734614	-4.332255	-0.780532
N	-0.509587	-5.309510	-1.373046
C	-3.443357	-2.882223	-0.684841
N	-4.425211	-3.223476	-1.214623
C	-3.442002	2.824582	-0.730575
N	-4.403283	3.193335	-1.277351
C	-0.746982	4.367527	-0.725900

N	-0.570898	5.380589	-1.274974
C	4.227374	1.526107	-0.560226
N	5.036553	2.217074	-1.038528
C	4.142400	-1.550256	-0.667769
N	4.915869	-2.233204	-1.208214
Cl	-0.127082	0.126436	3.858844
P	-0.042974	0.005411	1.851828

27

I-CN-B-F

N	-1.195375	0.690015	0.603456
N	0.000260	-1.381094	0.605417
N	1.195632	0.690196	0.605440
C	-1.145066	1.983608	0.124005
C	-2.290596	-0.000735	0.124684
C	-1.145584	-1.985309	0.128402
C	1.145365	-1.983151	0.123865
C	2.291179	0.000422	0.126745
C	1.145750	1.984346	0.127833
N	0.000274	2.671594	-0.036330
N	-2.313517	-1.336693	-0.035945
N	2.313684	-1.335288	-0.037216
C	-2.447651	2.213462	-0.478499
C	-3.140634	1.013096	-0.478538
C	-0.693046	-3.227494	-0.475646
C	0.693039	-3.226286	-0.478707
C	3.141274	1.013392	-0.475747
C	2.447979	2.213610	-0.475864
B	-0.000147	-0.000123	1.225925
F	1.484747	-4.128284	-1.060093
F	-1.484911	-4.129115	-1.057565
F	-4.318971	0.779449	-1.057540
F	-2.833816	3.350262	-1.059089
F	2.833006	3.349823	-1.058502
F	4.317411	0.779335	-1.059184
C	-0.000387	0.000329	2.822422
N	0.000621	0.000324	3.985694

27

I-CN-P-F

C	2.866496	-1.674687	-0.205333
C	2.319304	-0.471013	0.435419
N	1.140334	-1.037131	1.141230
C	0.690649	-2.263909	0.426701
C	1.940644	-2.684972	-0.217849
P	-0.006535	0.000878	1.655475
C	-0.040537	0.050878	3.419581
N	-0.536553	-2.602573	0.200520
C	-1.613693	-1.804528	0.516647

N	-1.402677	-0.444387	0.974614
C	-2.305327	0.527425	0.387527
C	-3.286328	-0.316744	-0.180648
C	-2.850011	-1.671360	-0.147892
N	-2.048602	1.848387	0.309867
C	-0.754372	2.240834	0.387395
N	0.297969	1.422339	0.948027
C	1.627141	1.773080	0.503401
C	1.381680	2.997435	-0.142393
C	-0.014619	3.303242	-0.168774
N	2.543439	0.781799	0.208928
F	2.293199	3.707139	-0.810617
F	-0.534207	4.358373	-0.819924
F	-4.376160	0.102479	-0.847336
F	-3.458984	-2.647267	-0.824136
F	2.065092	-3.851174	-0.856156
F	4.046782	-1.686001	-0.830811
N	-0.118665	0.141283	4.582590

26

I-Cl-B-F

N	-1.191367	0.687702	0.582282
N	0.000252	-1.376412	0.584066
N	1.191561	0.687850	0.583943
C	-1.145220	1.984451	0.111779
C	-2.291408	-0.001059	0.112570
C	-1.146214	-1.985820	0.116104
C	1.146069	-1.983737	0.111744
C	2.291926	0.000104	0.114357
C	1.145851	1.985207	0.115596
N	0.000242	2.671181	-0.051216
N	-2.313138	-1.336490	-0.050803
N	2.313350	-1.335109	-0.052026
C	-2.454644	2.217305	-0.475675
C	-3.147525	1.017131	-0.475595
C	-0.692856	-3.235487	-0.472821
C	0.693019	-3.234366	-0.475688
C	3.148061	1.017504	-0.473037
C	2.454947	2.217573	-0.472949
Cl	0.000035	0.000447	3.069422
B	-0.000067	-0.000136	1.187902
F	1.485087	-4.146019	-1.043055
F	-1.484954	-4.146586	-1.041201
F	-4.334308	0.788048	-1.040675
F	-2.849042	3.359072	-1.042513
F	2.848326	3.358948	-1.041434
F	4.332528	0.788079	-1.042977

26

I-Cl-P-F

N	0.302932	1.413629	0.938000
N	-1.396548	-0.449515	0.971630
N	1.155583	-1.049923	1.195183
C	1.634165	1.773927	0.504783
C	-0.746378	2.234155	0.382031
C	-2.298912	0.521348	0.385602
C	-1.612880	-1.813429	0.514978
C	0.691915	-2.272695	0.450967
C	2.325003	-0.470989	0.461332
N	2.552358	0.777068	0.225383
N	-2.046179	1.841460	0.323417
N	-0.532746	-2.602641	0.204614
C	1.387922	2.988085	-0.151186
C	-0.011909	3.291062	-0.180554
C	-3.279811	-0.321110	-0.186804
C	-2.843303	-1.673282	-0.159955
C	1.932202	-2.675523	-0.216152
C	2.860033	-1.667488	-0.198919
P	-0.008761	0.003313	1.667381
F	-4.376154	0.101786	-0.843687
F	-3.452513	-2.649836	-0.837463
F	2.040590	-3.819414	-0.897681
F	4.019098	-1.662525	-0.865332
F	2.299767	3.698951	-0.820613
F	-0.531382	4.349770	-0.829008
Cl	-0.084254	0.098687	3.702163

34

I-CN-B-CN...Cl

N	0.291286	1.351911	0.946800
N	-1.317986	-0.424104	0.948384
N	1.025175	-0.929410	0.948658
C	1.524168	1.680640	0.439412
C	-0.696039	2.162841	0.444244
C	-2.220231	0.479422	0.443535
C	-1.524994	-1.683881	0.442828
C	0.694655	-2.162372	0.443066
C	2.221574	-0.480011	0.447252
N	2.546514	0.817556	0.326237
N	-1.982511	1.795996	0.326028
N	-0.564413	-2.614765	0.325357
C	1.359422	2.969385	-0.218052
C	-0.014670	3.267950	-0.214463
C	-3.252983	-0.307737	-0.215621
C	-2.823062	-1.646422	-0.215130
C	1.892890	-2.662901	-0.215425
C	2.838733	-1.622266	-0.210955

B	-0.000561	-0.000177	1.566118
C	4.108215	-1.620284	-0.830580
N	5.168437	-1.633978	-1.315029
C	2.016723	-3.926428	-0.835271
N	2.135479	-4.981761	-1.315290
C	-3.457714	-2.746462	-0.833863
N	-4.001484	-3.657408	-1.315906
C	-4.409036	0.217807	-0.835159
N	-5.381383	0.644822	-1.315157
C	-0.650219	4.367736	-0.832340
N	-1.167036	5.294222	-1.315055
C	2.393104	3.709503	-0.833804
N	3.250130	4.340404	-1.309092
C	-0.000858	0.000607	3.168625
N	-0.001799	0.000455	4.332080
Cl	0.000081	-0.001569	-2.001463

34

I-CN-B-CN...Br

N	0.290704	1.350828	0.954185
N	-1.317131	-0.423545	0.954873
N	1.023653	-0.928421	0.954316
C	1.525464	1.681663	0.450447
C	-0.697514	2.164272	0.455167
C	-2.222973	0.480892	0.455904
C	-1.525750	-1.684748	0.451222
C	0.694436	-2.164312	0.452756
C	2.223237	-0.479675	0.457893
N	2.549061	0.818660	0.341333
N	-1.985375	1.798396	0.342284
N	-0.565284	-2.617127	0.337825
C	1.359592	2.968567	-0.209039
C	-0.015926	3.267287	-0.205659
C	-3.254523	-0.305903	-0.204382
C	-2.822736	-1.645543	-0.207605
C	1.892829	-2.663607	-0.205271
C	2.839471	-1.621672	-0.200376
B	-0.000853	-0.000456	1.575113
C	4.108763	-1.621059	-0.820108
N	5.168817	-1.636152	-1.304618
C	2.018921	-3.926019	-0.826303
N	2.140321	-4.980455	-1.308102
C	-3.455772	-2.743379	-0.831010
N	-3.997472	-3.653426	-1.317937
C	-4.411449	0.219246	-0.821946
N	-5.384800	0.646731	-1.299944
C	-0.650736	4.365474	-0.826577
N	-1.167670	5.290392	-1.312491
C	2.391975	3.707030	-0.828442

N	3.248605	4.335752	-1.307476
C	-0.000191	-0.000747	3.176466
N	0.000399	-0.001535	4.339958
Br	-0.001357	0.001855	-2.180691

34

I-CN-P-CN...Br

N	1.509328	0.001756	1.313885
N	-0.773349	1.324568	1.260725
N	-0.752432	-1.253766	1.142998
C	1.979883	-1.187561	0.594495
C	2.057576	1.218629	0.710780
C	0.021096	2.380016	0.637686
C	-2.064567	1.178083	0.599444
C	-2.066265	-1.156763	0.593527
C	-0.013851	-2.376713	0.652480
N	1.360463	-2.337250	0.532981
N	1.335218	2.302179	0.446927
N	-2.718046	0.054700	0.458489
C	3.216310	-0.687033	-0.003959
C	3.241204	0.729573	0.062774
C	-0.977309	3.154511	-0.032166
C	-2.238454	2.491853	-0.001986
C	-2.264798	-2.405958	0.004518
C	-0.990517	-3.164260	0.041237
C	-0.764208	-4.403570	-0.595429
N	-0.605547	-5.446060	-1.094407
C	-3.428802	-2.815156	-0.681254
N	-4.390453	-3.186747	-1.227330
C	-3.419870	2.930103	-0.631736
N	-4.407235	3.314538	-1.122289
C	-0.703389	4.354884	-0.731740
N	-0.496117	5.362309	-1.279149
C	4.191990	1.562443	-0.571141
N	5.004441	2.244242	-1.054374
C	4.166592	-1.506683	-0.646455
N	4.975664	-2.185123	-1.143273
C	-0.086636	-0.038423	3.606568
N	-0.145060	-0.082640	4.771104
P	-0.022355	0.012683	1.830792
Br	0.162957	-0.001101	-1.844463

33

I-Cl-B-CN...Br

N	-0.901492	-1.037436	1.163398
N	1.351827	-0.260437	1.156058
N	-0.447404	1.302897	1.159326
C	-2.148785	-0.737760	0.671844
C	-0.431549	-2.232584	0.676632

C	1.716356	-1.492028	0.670073
C	2.149161	0.742899	0.662515
C	0.434962	2.233937	0.668841
C	-1.718052	1.493159	0.674385
N	-2.627664	0.511735	0.556719
N	0.872656	-2.531124	0.557609
N	1.755848	2.022041	0.547606
C	-2.628400	-1.952684	0.029100
C	-1.566829	-2.878256	0.034074
C	3.006097	-1.301864	0.022419
C	3.273603	0.081099	0.017510
C	-0.378005	3.257150	0.027496
C	-1.709677	2.798304	0.029997
Cl	0.008721	0.006699	3.653640
B	0.002532	0.002515	1.762850
C	-2.824189	3.418458	-0.577434
N	-3.745756	3.952038	-1.051491
C	0.117020	4.434317	-0.576742
N	0.517036	5.425231	-1.042119
C	4.368038	0.733688	-0.591207
N	5.292666	1.263043	-1.064473
C	3.776311	-2.320578	-0.581237
N	4.434641	-3.161756	-1.047951
C	-1.546713	-4.155116	-0.569859
N	-1.545936	-5.222122	-1.038884
C	-3.894304	-2.111997	-0.577221
N	-4.950681	-2.262097	-1.045939
Br	-0.005241	-0.004938	-1.977045

33

I-Cl-P-CN...Br

N	1.484656	-0.005812	1.264242
N	-0.799477	1.306405	1.185971
N	-0.760191	-1.258210	1.021411
C	1.970703	-1.190949	0.548916
C	2.035575	1.215401	0.667778
C	-0.000853	2.365759	0.570296
C	-2.082594	1.157033	0.508664
C	-2.077621	-1.177447	0.481376
C	-0.020105	-2.386379	0.557703
N	1.356938	-2.342882	0.469377
N	1.314694	2.297369	0.400927
N	-2.732498	0.032789	0.354541
C	3.208463	-0.683582	-0.037932
C	3.223948	0.733898	0.027675
C	-0.992407	3.135073	-0.113210
C	-2.252849	2.469064	-0.095107
C	-2.269409	-2.429524	-0.100313
C	-0.988690	-3.182531	-0.052731

C	-0.759569	-4.429820	-0.671846
N	-0.599039	-5.478356	-1.157813
C	-3.432842	-2.854461	-0.776669
N	-4.394875	-3.235051	-1.316086
C	-3.429652	2.904064	-0.735325
N	-4.415494	3.290256	-1.227821
C	-0.712618	4.336011	-0.809305
N	-0.501239	5.344335	-1.353711
C	4.168502	1.575103	-0.604372
N	4.971232	2.268764	-1.086989
C	4.168688	-1.494912	-0.676127
N	4.990119	-2.161819	-1.168494
Cl	-0.174771	-0.107435	3.801946
P	-0.056729	-0.009380	1.766603
Br	0.198567	0.029246	-1.937452

34

I-CN-B-CN...I

N	-1.036669	-0.913351	1.382857
N	1.307132	-0.443644	1.386339
N	-0.272218	1.350925	1.387365
C	-2.230966	-0.446390	0.889139
C	-0.727285	-2.158626	0.891017
C	1.502158	-1.710790	0.892524
C	2.231594	0.447823	0.897279
C	0.728278	2.153303	0.894697
C	-1.506768	1.708754	0.901302
N	-2.540914	0.857405	0.786342
N	0.526847	-2.629366	0.780310
N	2.012178	1.769503	0.788133
C	-2.863750	-1.581507	0.234252
C	-1.934194	-2.642032	0.238226
C	2.802435	-1.689695	0.239635
C	3.254438	-0.353669	0.244191
C	0.060742	3.269799	0.242468
C	-1.322702	2.995563	0.248966
B	-0.001106	-0.002986	2.008401
C	-2.343684	3.756312	-0.362596
N	-3.185280	4.406336	-0.840423
C	0.708561	4.365967	-0.368991
N	1.236042	5.291879	-0.841556
C	4.426270	0.150630	-0.361349
N	5.413592	0.554815	-0.831030
C	3.428883	-2.798782	-0.370710
N	3.968238	-3.718469	-0.842064
C	-2.083413	-3.907426	-0.370225
N	-2.224416	-4.963654	-0.843229
C	-4.139559	-1.568748	-0.371722
N	-5.208275	-1.575572	-0.837221

C	-0.002527	-0.005482	3.610453
N	-0.003001	-0.007669	4.774017
I	0.001168	0.005121	-1.991566

34

I-CN-P-CN...I

N	1.454456	0.009886	1.484384
N	-0.793924	1.264613	1.278149
N	-0.823535	-1.301375	1.387986
C	2.015251	-1.210762	0.902079
C	1.943061	1.197903	0.775965
C	-0.045679	2.395993	0.819708
C	-2.104206	1.177991	0.716540
C	-2.113659	-1.157764	0.721949
C	-0.026017	-2.362472	0.784897
N	1.295315	-2.292214	0.625956
N	1.327709	2.351271	0.714092
N	-2.760349	-0.027168	0.573299
C	3.218564	-0.726923	0.286681
C	3.188675	0.690402	0.201293
C	-1.012564	3.188961	0.198407
C	-2.289006	2.435938	0.138356
C	-2.280967	-2.468342	0.121975
C	-1.015496	-3.133876	0.102919
C	-0.733927	-4.334456	-0.592871
N	-0.518970	-5.343451	-1.134758
C	-3.455683	-2.909490	-0.517232
N	-4.437480	-3.300159	-1.014106
C	-3.439079	2.855150	-0.563552
N	-4.386386	3.234024	-1.129269
C	-0.773163	4.430081	-0.429430
N	-0.599595	5.472832	-0.922626
C	4.154760	1.504874	-0.424632
N	4.975691	2.177633	-0.908915
C	4.179995	-1.564380	-0.323291
N	4.996224	-2.250589	-0.794554
C	-0.169368	0.051041	3.760266
N	-0.241842	0.097317	4.924330
P	-0.081408	0.000819	1.986821
I	0.217901	0.041041	-1.965119

33

I-Cl-B-CN...I

N	-0.381817	1.321006	1.208711
N	-0.953631	-0.988799	1.205191
N	1.332561	-0.329766	1.207764
C	0.548365	2.209945	0.727897
C	-1.643881	1.581710	0.732459
C	-2.187320	-0.627193	0.720899

C	-0.546873	-2.211213	0.728204
C	1.638368	-1.579755	0.727257
C	2.187675	0.633086	0.729201
N	1.858701	1.931343	0.615645
N	-2.602301	0.646683	0.612422
N	0.741949	-2.575118	0.613586
C	-0.212640	3.280016	0.098828
C	-1.568830	2.892282	0.103648
C	-2.732167	-1.821710	0.090954
C	-1.718581	-2.802545	0.098592
C	2.945393	-1.455070	0.097964
C	3.285911	-0.086204	0.100903
B	-0.001448	0.000211	1.812942
C	4.425914	0.507540	-0.483312
N	5.387071	0.986934	-0.936682
C	3.674858	-2.512996	-0.488174
N	4.298355	-3.388425	-0.939627
C	-1.771534	-4.086407	-0.487023
N	-1.831022	-5.158160	-0.941958
C	-4.013347	-1.926034	-0.494018
N	-5.083985	-2.030248	-0.943200
C	-2.651449	3.579923	-0.487712
N	-3.545590	4.168638	-0.949550
C	0.339777	4.439042	-0.489864
N	0.788043	5.414571	-0.943889
Cl	-0.003532	-0.002037	3.701812
I	0.001045	0.000734	-2.165941

33

I-Cl-P-CN...I

N	-1.448594	0.006964	1.446667
N	0.826898	-1.300133	1.316242
N	0.787375	1.253053	1.161820
C	-1.946257	1.191858	0.736552
C	-2.013319	-1.220254	0.871246
C	0.024852	-2.368864	0.730697
C	2.108252	-1.160690	0.637125
C	2.101634	1.175576	0.611607
C	0.043018	2.392081	0.726458
N	-1.333529	2.346353	0.655862
N	-1.297087	-2.303313	0.594049
N	2.755422	-0.032188	0.472444
C	-3.190710	0.678029	0.168730
C	-3.216889	-0.739908	0.259420
C	1.009041	-3.145253	0.048080
C	2.273895	-2.477478	0.050949
C	2.289884	2.438604	0.049721
C	1.009785	3.192348	0.117332
C	0.781487	4.453112	-0.473107

N	0.620782	5.512645	-0.933867
C	3.451969	2.870113	-0.624126
N	4.415112	3.249000	-1.162978
C	3.450065	-2.919759	-0.584212
N	4.440108	-3.300766	-1.072306
C	0.726573	-4.363524	-0.614676
N	0.514219	-5.388900	-1.126359
C	-4.173173	-1.584220	-0.349649
N	-4.981836	-2.282394	-0.816459
C	-4.158455	1.485870	-0.464903
N	-4.977302	2.155781	-0.957611
Cl	0.261823	0.100207	3.957250
P	0.099512	0.008663	1.925015
I	-0.264209	0.002168	-2.039699

38

I-CN-B-CN...BF₄

N	1.479379	-0.474853	1.258787
N	-0.134847	1.299557	1.319884
N	-0.866244	-0.963626	1.300779
C	1.657896	-1.721802	0.711181
C	2.361407	0.435909	0.729645
C	0.828155	2.126178	0.801232
C	-1.391955	1.653650	0.902009
C	-2.095415	-0.513692	0.892952
C	-0.574319	-2.196893	0.779627
N	0.677990	-2.634004	0.575319
N	2.101897	1.750083	0.606394
N	-2.413986	0.787239	0.797276
C	2.940625	-1.679401	0.022820
C	3.376315	-0.343032	0.034141
C	0.113885	3.270543	0.242782
C	-1.256725	2.979736	0.307562
C	-2.770281	-1.671009	0.311013
C	-1.830536	-2.709496	0.239650
B	0.177898	-0.056702	1.910256
C	-2.003512	-3.977559	-0.356734
N	-2.156717	-5.037992	-0.815014
C	-4.088994	-1.677491	-0.193242
N	-5.194294	-1.702842	-0.561035
C	-2.317369	3.753179	-0.213534
N	-3.190185	4.420439	-0.600751
C	0.718475	4.395474	-0.360780
N	1.214237	5.342086	-0.826096
C	4.520704	0.185442	-0.603533
N	5.484972	0.607170	-1.104053
C	3.556200	-2.773922	-0.624830
N	4.086037	-3.681687	-1.128018
C	0.216697	-0.081668	3.511072

N	0.250671	-0.100424	4.673945
B	-0.545477	0.155912	-2.257020
F	-1.548333	-0.838701	-2.072238
F	0.056692	0.046990	-3.511409
F	-1.108285	1.447736	-2.055397
F	0.450218	-0.046127	-1.217568

38

I-CN-P-CN...BF₄

N	1.365881	-0.267690	1.457166
N	-0.800103	1.232372	1.413407
N	-0.982045	-1.356890	1.212743
C	1.818492	-1.470984	0.781159
C	2.023006	0.918493	0.894052
C	0.100503	2.249801	0.852214
C	-2.061709	1.211094	0.688461
C	-2.244261	-1.111991	0.575922
C	-0.286634	-2.463905	0.622964
N	1.094529	-2.533287	0.564248
N	1.399880	2.063162	0.669600
N	-2.795732	0.152532	0.479206
C	3.119036	-1.055232	0.260498
C	3.193188	0.358359	0.285076
C	-0.808576	3.120910	0.171922
C	-2.106232	2.552798	0.117010
C	-2.488024	-2.279093	-0.142468
C	-1.267458	-3.121113	-0.113485
C	-1.079636	-4.305224	-0.859525
N	-0.957493	-5.302220	-1.452186
C	-3.639559	-2.546081	-0.914079
N	-4.597307	-2.808315	-1.525646
C	-3.222234	3.089686	-0.556323
N	-4.157587	3.552620	-1.078485
C	-0.411880	4.320088	-0.468684
N	-0.103674	5.337317	-0.944138
C	4.219588	1.136902	-0.301311
N	5.100194	1.772669	-0.721014
C	4.052970	-1.932755	-0.325537
N	4.847185	-2.667672	-0.762329
C	-0.279885	-0.273611	3.715369
N	-0.354879	-0.357765	4.876110
P	-0.171800	-0.159768	1.943556
B	0.426711	0.510177	-2.250340
F	-0.067760	-0.075629	-0.992059
F	-0.134238	-0.195793	-3.315500
F	0.033615	1.870204	-2.251183
F	1.839491	0.398557	-2.223922

28

I-CN-B-F...Br

N	1.059077	-0.897096	1.075763
N	0.244165	1.362803	1.075758
N	-1.306100	-0.472889	1.074592
C	0.771336	-2.149423	0.572776
C	2.247818	-0.403090	0.579137
C	1.473169	1.738641	0.572973
C	-0.777174	2.145608	0.577601
C	-2.246959	0.404657	0.575309
C	-1.470887	-1.747041	0.570412
N	-0.473147	-2.635761	0.431540
N	2.518172	0.905473	0.438626
N	-2.045909	1.725952	0.437821
C	1.994170	-2.587736	-0.067870
C	2.887039	-1.532963	-0.062351
C	1.243641	3.018120	-0.066042
C	-0.116214	3.264119	-0.062647
C	-3.238758	-0.433607	-0.067080
C	-2.770037	-1.733433	-0.069562
B	-0.001331	-0.002672	1.672034
F	-0.738416	4.270169	-0.692149
F	2.177479	3.744553	-0.695294
F	4.068623	-1.494626	-0.693723
F	2.156870	-3.757680	-0.700804
F	-3.330512	-2.773495	-0.702033
F	-4.334604	0.012042	-0.696876
C	-0.002267	-0.003428	3.288315
N	-0.002900	-0.004593	4.452645
Br	0.002357	0.006589	-2.099551

28

I-CN-P-F...Br

C	2.838958	-1.621844	-0.136411
C	2.363727	-0.476301	0.581661
N	1.122717	-1.034010	1.168622
C	0.678144	-2.246867	0.458582
C	1.913242	-2.657999	-0.156864
P	-0.004480	0.002697	1.677356
C	-0.079167	-0.015591	3.465455
N	-0.550657	-2.688098	0.382130
C	-1.596838	-1.780526	0.514044
N	-1.404625	-0.449195	1.022050
C	-2.340436	0.520545	0.520388
C	-3.276599	-0.289452	-0.096248
C	-2.833822	-1.672764	-0.093789
N	-2.005562	1.864275	0.358314
C	-0.757796	2.227379	0.453920
N	0.309176	1.503346	1.168564
C	1.639499	1.764248	0.565331

C	1.362199	2.984944	-0.142228
C	0.010415	3.288147	-0.159477
N	2.515818	0.813161	0.293396
F	2.286003	3.646002	-0.852835
F	-0.542651	4.282338	-0.883102
F	-4.342830	0.125201	-0.804242
F	-3.463242	-2.635699	-0.793683
F	2.041915	-3.781856	-0.892492
F	3.965483	-1.619693	-0.861683
N	-0.161631	-0.041606	4.630009
Br	0.067082	0.026136	-2.031084

27

I-Cl-B-F...Br

N	-1.195607	0.690144	0.685557
N	0.000286	-1.380751	0.686439
N	1.195652	0.690433	0.687054
C	-1.138947	1.978632	0.195725
C	-2.282400	-0.003502	0.194713
C	-1.144330	-1.978200	0.201159
C	1.143806	-1.974561	0.193874
C	2.283926	-0.001925	0.198187
C	1.139629	1.979338	0.199283
N	0.000155	2.675477	0.055199
N	-2.316421	-1.338703	0.054814
N	2.317016	-1.336723	0.053603
C	-2.428789	2.200808	-0.425752
C	-3.119091	1.003667	-0.427469
C	-0.691311	-3.206548	-0.419824
C	0.690677	-3.203969	-0.425512
C	3.120787	1.004294	-0.423090
C	2.429015	2.200675	-0.423814
Cl	-0.000040	-0.001244	3.190157
B	-0.000123	-0.000136	1.257177
F	1.481531	-4.096210	-1.038764
F	-1.483031	-4.099080	-1.031817
F	-4.287658	0.765226	-1.039951
F	-2.805274	3.331985	-1.039339
F	2.804166	3.330943	-1.039930
F	4.287249	0.765291	-1.039523
Br	-0.000061	-0.001641	-2.486729

27

I-Cl-P-F...Br

N	0.312748	1.504190	1.181903
N	-1.396463	-0.446477	1.006312
N	1.126598	-1.033196	1.181745
C	1.646103	1.765528	0.570518
C	-0.756414	2.227165	0.466587

C	-2.338717	0.520187	0.511583
C	-1.595719	-1.779753	0.509327
C	0.680970	-2.248367	0.476214
C	2.367001	-0.472724	0.579561
N	2.518803	0.814122	0.292558
N	-2.005046	1.867380	0.371585
N	-0.546729	-2.689889	0.396713
C	1.363146	2.981657	-0.139097
C	0.010309	3.284882	-0.151290
C	-3.274618	-0.288019	-0.102889
C	-2.830250	-1.673603	-0.099324
C	1.913366	-2.659002	-0.144640
C	2.835278	-1.618749	-0.139824
P	-0.008061	0.001217	1.688511
F	-4.349876	0.123139	-0.803227
F	-3.467693	-2.639784	-0.790989
F	2.032435	-3.778814	-0.889438
F	3.954408	-1.617534	-0.877697
F	2.283381	3.640863	-0.857439
F	-0.546221	4.267857	-0.889025
Cl	-0.111311	-0.026045	3.763363
Br	0.073783	0.035018	-2.041531

57

II-CN-B-CN

B	0.000652	2.000920	-0.000346
N	-1.378511	1.370247	0.000374
N	0.688873	1.366282	1.192464
N	0.687968	1.365879	-1.193680
C	-1.991002	0.927236	-1.150681
C	-1.991321	0.929667	1.152386
C	-0.002272	0.928874	2.300107
C	1.991490	0.921906	1.147584
C	1.990357	0.921128	-1.148647
C	-0.003488	0.926765	-2.300952
N	-1.340068	0.784071	-2.318353
N	-1.339134	0.787132	2.319509
N	2.675078	0.776164	-0.000862
C	-3.269952	0.377473	-0.716096
C	-3.270070	0.377832	0.717547
C	1.013445	0.379429	3.191994
C	2.254437	0.374170	2.473848
C	2.252923	0.372834	-2.474754
C	1.012171	0.378340	-3.193028
C	-4.344804	-0.165850	-1.443020
C	-4.345630	-0.164525	1.443756
C	0.923028	-0.154227	4.490242
C	3.420648	-0.168596	3.043692

C	3.419823	-0.168885	-3.042907
C	0.922732	-0.154884	-4.491709
C	-5.446736	-0.689419	-0.714670
C	-5.446505	-0.690369	0.714837
C	2.104448	-0.678193	5.081657
C	3.341043	-0.685857	4.364763
C	3.341031	-0.686480	-4.364180
C	2.105007	-0.677910	-5.081716
C	0.003697	3.588994	-0.000211
N	0.005563	4.752153	0.000127
C	4.656427	-0.183788	2.328925
N	5.671466	-0.195091	1.758941
C	4.511198	-1.219961	4.986448
N	5.467529	-1.656767	5.486221
C	2.057647	-1.201012	6.410171
N	2.012336	-1.625256	7.493231
C	-0.310401	-0.152240	5.209132
N	-1.303753	-0.148876	5.816248
C	4.655230	-0.183504	-2.327189
N	5.672770	-0.195191	-1.761927
C	4.512015	-1.219122	-4.984771
N	5.470864	-1.650781	-5.484095
C	2.058560	-1.200496	-6.410375
N	2.011852	-1.624773	-7.493397
C	-0.310269	-0.152634	-5.211674
N	-1.306028	-0.148603	-5.814535
C	-4.344580	-0.174238	-2.870819
N	-4.361897	-0.179989	-4.034710
C	-6.569226	-1.224014	-1.418467
N	-7.479459	-1.661545	-1.997212
C	-6.569655	-1.224055	1.417684
N	-7.482551	-1.656314	1.996138
C	-4.345404	-0.173650	2.871506
N	-4.361562	-0.180185	4.035441

57

II-CN-P-CN

N	0.002877	1.442632	1.518847
N	-1.349915	-0.791879	1.717956
N	1.251815	-0.725293	1.484347
C	1.194496	2.022323	0.997546
C	-1.205221	2.052488	1.027605
C	-2.389617	0.018410	1.019054
C	-1.173833	-2.065230	0.936809
C	1.179598	-2.068198	0.959534
C	2.363123	0.022037	1.003437
N	2.355004	1.354725	0.875240
N	-2.310060	1.289433	0.780021
N	-0.031199	-2.620056	0.675398

C	0.723810	3.243577	0.406483
C	-0.733140	3.234792	0.402517
C	-3.230033	-1.016788	0.408880
C	-2.499099	-2.244981	0.341246
C	2.464052	-2.245717	0.378140
C	3.209822	-0.996823	0.440604
C	1.445982	4.270252	-0.245694
C	-1.444240	4.266136	-0.274516
C	-4.513554	-0.901994	-0.141547
C	-3.039967	-3.365370	-0.310544
C	3.028888	-3.367648	-0.290464
C	4.500683	-0.888159	-0.120826
C	0.728351	5.295601	-0.902684
C	-0.712208	5.286257	-0.912729
C	-5.081022	-2.046160	-0.788316
C	-4.350777	-3.257694	-0.876509
C	4.316593	-3.245230	-0.853139
C	5.061073	-2.017348	-0.762762
C	0.087066	0.007705	3.984095
N	0.244327	0.077784	5.140934
C	-2.318775	-4.592719	-0.397204
N	-1.755777	-5.610173	-0.460642
C	-4.933186	-4.388438	-1.526540
N	-5.405644	-5.310723	-2.057652
C	-6.394722	-1.962309	-1.340643
N	-7.468909	-1.883794	-1.783033
C	-5.256501	0.310630	-0.029813
N	-5.885576	1.283755	0.083760
C	2.313452	-4.599274	-0.362788
N	1.736885	-5.609978	-0.410941
C	4.909642	-4.364888	-1.515008
N	5.399230	-5.272286	-2.055604
C	6.373523	-1.947116	-1.317709
N	7.445236	-1.890306	-1.770269
C	5.242553	0.326651	-0.010775
N	5.864459	1.304486	0.100986
C	2.873576	4.278698	-0.240131
N	4.037494	4.307008	-0.245115
C	1.427994	6.347232	-1.566142
N	1.998892	7.204563	-2.109771
C	-1.406700	6.337516	-1.586502
N	-1.969112	7.193823	-2.139378
C	-2.870551	4.271279	-0.281387
N	-4.034994	4.281231	-0.268042
P	-0.016209	-0.027550	2.232469

45

II-CN-B-F

B	0.000274	1.821610	-0.000255
---	----------	----------	-----------

N	-1.378010	1.198724	0.000380
N	0.689357	1.198138	1.192797
N	0.688911	1.197795	-1.193763
C	-1.993183	0.762158	-1.153544
C	-1.993669	0.764433	1.155149
C	-0.002483	0.765155	2.303777
C	1.996577	0.762167	1.149018
C	1.995926	0.761232	-1.149667
C	-0.003116	0.763175	-2.304413
N	-1.342417	0.623573	-2.324524
N	-1.341981	0.626299	2.325674
N	2.684146	0.622018	-0.000505
C	-3.274252	0.222922	-0.720674
C	-3.274327	0.222963	0.722067
C	1.012915	0.225580	3.197316
C	2.262114	0.223363	2.475317
C	2.261265	0.221530	-2.475827
C	1.012394	0.224630	-3.198144
C	-4.346896	-0.331299	-1.421243
C	-4.347932	-0.329688	1.422121
C	0.943228	-0.324830	4.478020
C	3.404344	-0.331713	3.055130
C	3.404248	-0.332553	-3.054298
C	0.943371	-0.324753	-4.479643
C	-5.428858	-0.856734	-0.705440
C	-5.428250	-0.858828	0.705974
C	2.103146	-0.853386	5.056840
C	3.324816	-0.856581	4.350142
C	3.325114	-0.857849	-4.349640
C	2.103966	-0.852594	-5.057164
F	-4.369327	-0.356896	-2.767093
F	-4.370717	-0.355598	2.767968
F	-0.209937	-0.346370	5.172509
F	4.580587	-0.362061	2.400744
F	4.580428	-0.361393	-2.400044
F	-0.209441	-0.345660	-5.174433
F	-6.489131	-1.368653	-1.358803
F	-6.488554	-1.371023	1.358898
F	2.067540	-1.363041	6.302543
F	4.419849	-1.371099	4.941175
F	4.420462	-1.370690	-4.941312
F	2.069286	-1.361124	-6.303494
C	0.000045	3.418769	0.000015
N	-0.001087	4.582116	0.000629

45

II-CN-P-F

N	-1.441920	1.349576	0.001661
N	0.724933	1.326008	1.248422

N	0.778809	1.525556	-1.339413
C	-2.067992	0.901060	-1.210928
C	-2.025546	0.837115	1.196662
C	-0.020659	0.833727	2.357435
C	2.085003	0.866781	1.186190
C	2.067777	0.795318	-1.167147
C	-0.026542	0.831315	-2.382396
N	-1.302831	0.612535	-2.310728
N	-1.359135	0.708191	2.358949
N	2.642817	0.563778	-0.027618
C	-3.264258	0.292628	-0.732642
C	-3.261456	0.282674	0.729231
C	1.001337	0.290229	3.203944
C	2.266913	0.275575	2.471633
C	2.258419	0.204143	-2.495718
C	1.017912	0.233304	-3.219937
C	-4.299459	-0.374132	-1.414730
C	-4.295626	-0.363573	1.432770
C	0.906770	-0.321960	4.467229
C	3.370473	-0.386390	3.042091
C	3.371061	-0.419478	-3.050123
C	0.931842	-0.352152	-4.477909
C	-5.308634	-0.997427	-0.693053
C	-5.311959	-0.994441	0.729984
C	2.021256	-0.944136	5.012449
C	3.248520	-0.977892	4.293384
C	3.279381	-0.994293	-4.333051
C	2.071084	-0.958015	-5.041411
F	-4.324544	-0.401894	-2.765497
F	-4.304669	-0.374483	2.781014
F	-0.254303	-0.302489	5.152775
F	4.550165	-0.442334	2.384984
F	4.542377	-0.485039	-2.386723
F	-0.220952	-0.350303	-5.176056
F	-6.315980	-1.621634	-1.333815
F	-6.324082	-1.609762	1.377517
F	1.965700	-1.521721	6.231492
F	4.303630	-1.597519	4.857728
F	4.359119	-1.578155	-4.888031
F	2.002801	-1.504375	-6.270790
C	0.006546	3.825894	0.036175
N	-0.071074	4.987408	0.186434
P	0.018802	2.077801	-0.014148

58

II-CN-B-CN...Br

B	-0.000358	-0.000021	2.368066
---	-----------	-----------	----------

N	0.682420	1.215345	1.753879
N	-1.393101	-0.016692	1.751399
N	0.711220	-1.198885	1.754139
C	1.963554	1.163038	1.250550
C	-0.029183	2.280318	1.245807
C	-1.990053	1.119059	1.250731
C	-1.962972	-1.166229	1.250635
C	0.025077	-2.280567	1.246207
C	1.990652	-1.116086	1.250550
N	2.664617	0.031660	1.108403
N	-1.360370	2.291418	1.106612
N	-1.305510	-2.323361	1.106877
C	2.192950	2.444283	0.602963
C	0.946456	3.142766	0.599463
C	-3.216010	0.676280	0.606645
C	-3.199212	-0.752427	0.606621
C	1.021003	-3.119622	0.599871
C	2.250413	-2.391482	0.602763
C	3.325953	2.973174	-0.036338
C	0.810212	4.384085	-0.042791
C	-4.239999	1.392433	-0.034759
C	-4.206667	-1.492018	-0.034407
C	0.914412	-4.364100	-0.041974
C	3.395416	-2.893044	-0.037215
C	3.199530	4.233557	-0.681180
C	1.953938	4.931019	-0.685676
C	-5.269275	0.651940	-0.677343
C	-5.252810	-0.775550	-0.677029
C	2.070515	-4.883346	-0.685680
C	3.298901	-4.156121	-0.682028
C	-0.003851	0.000205	3.967950
N	-0.007587	0.000462	5.131467
C	-4.211765	-2.919621	-0.026567
N	-4.271557	-4.082062	-0.013478
C	-6.313782	-1.489281	-1.314717
N	-7.182849	-2.071252	-1.826117
C	-6.346207	1.340857	-1.315565
N	-7.228265	1.902594	-1.827343
C	-4.277601	2.819566	-0.027505
N	-4.363701	3.980364	-0.015367
C	-0.301462	-5.112232	-0.038384
N	-1.261136	-5.770914	-0.033915
C	2.011785	-6.158990	-1.326376
N	1.964927	-7.202812	-1.839957
C	4.448356	-4.717550	-1.318034
N	5.387931	-5.179059	-1.827374
C	4.635220	-2.185181	-0.023209
N	5.672424	-1.657151	-0.004815
C	4.582209	2.295061	-0.021362

N	5.631530	1.791461	-0.002167
C	4.335613	4.822333	-1.316372
N	5.264450	5.305913	-1.824955
C	1.865076	6.204946	-1.326265
N	1.793858	7.247400	-1.839727
C	-0.423628	5.102251	-0.040281
N	-1.399414	5.736857	-0.036276
Br	0.002132	-0.000687	-1.370432

58

II-CN-P-CN...Br

N	0.004154	1.482472	1.792141
N	-1.343841	-0.789287	1.914748
N	1.283048	-0.743059	1.760252
C	1.187498	2.007265	1.188457
C	-1.205321	2.040869	1.213132
C	-2.388849	0.014180	1.228870
C	-1.170950	-2.068133	1.169697
C	1.173485	-2.066002	1.175495
C	2.350591	0.019047	1.204421
N	2.350722	1.352365	1.101898
N	-2.306097	1.286006	0.984359
N	-0.030412	-2.635428	0.924521
C	0.718754	3.202163	0.541010
C	-0.734959	3.195157	0.542235
C	-3.198674	-1.007168	0.579887
C	-2.470655	-2.241255	0.533351
C	2.426819	-2.233863	0.538157
C	3.168385	-0.982197	0.576625
C	1.438959	4.196731	-0.148870
C	-1.445659	4.195905	-0.171472
C	-4.446451	-0.878196	-0.048749
C	-2.981497	-3.348349	-0.163321
C	2.961064	-3.344862	-0.168055
C	4.421074	-0.858899	-0.054840
C	0.721514	5.185554	-0.868987
C	-0.715089	5.176385	-0.875566
C	-4.970756	-2.002680	-0.761983
C	-4.246936	-3.218821	-0.820300
C	4.206739	-3.204333	-0.815860
C	4.944346	-1.972238	-0.758753
C	0.060110	0.003791	4.188038
N	0.148627	0.033588	5.352895
C	-2.285026	-4.592197	-0.197835
N	-1.768315	-5.635961	-0.206089
C	-4.793624	-4.331775	-1.528165
N	-5.242348	-5.240279	-2.102467
C	-6.241052	-1.901217	-1.406457
N	-7.280688	-1.814553	-1.924338

C	-5.205638	0.325406	0.049000
N	-5.874713	1.273495	0.149521
C	2.278468	-4.597345	-0.176177
N	1.760422	-5.640219	-0.155832
C	4.767794	-4.314393	-1.520401
N	5.234088	-5.215934	-2.090763
C	6.218087	-1.885767	-1.393429
N	7.260146	-1.822657	-1.910982
C	5.180808	0.346516	0.046303
N	5.844941	1.296340	0.157441
C	2.865887	4.236611	-0.109767
N	4.026055	4.325196	-0.068759
C	1.420456	6.207406	-1.576967
N	1.988127	7.045867	-2.153710
C	-1.412557	6.196676	-1.594013
N	-1.977246	7.029612	-2.179812
C	-2.870895	4.239593	-0.136921
N	-4.031287	4.319164	-0.075354
P	-0.015130	-0.019441	2.421951
Br	0.096588	0.090950	-1.282121

46

II-CN-B-F...Br

B	-0.001045	0.000908	2.147271
N	-1.388685	-0.015845	1.544875
N	0.706789	-1.192958	1.544956
N	0.678384	1.210358	1.543107
C	-1.995838	1.125202	1.069785
C	-1.969365	-1.171287	1.071301
C	0.021984	-2.288416	1.067315
C	1.997307	-1.117531	1.070509
C	1.970505	1.165440	1.069258
C	-0.031846	2.289295	1.065462
N	-1.368035	2.304507	0.939766
N	-1.313701	-2.335589	0.942677
N	2.678733	0.032077	0.944167
C	-3.242179	0.681350	0.469086
C	-3.226128	-0.756694	0.470361
C	1.029776	-3.145396	0.465624
C	2.267032	-2.412126	0.467824
C	2.209570	2.465984	0.466097
C	0.955180	3.169673	0.463773
C	-4.271351	1.370836	-0.172072
C	-4.241161	-1.469126	-0.168417
C	0.950650	-4.382415	-0.173805
C	3.392282	-2.933071	-0.170658
C	3.322110	3.014419	-0.171778
C	0.846112	4.404546	-0.175295
C	-5.293081	0.644096	-0.788237

C	-5.278358	-0.765476	-0.785887
C	2.091471	-4.902302	-0.790551
C	3.304641	-4.183873	-0.787069
C	3.204172	4.262731	-0.788222
C	1.974066	4.951867	-0.791738
F	-4.309021	2.720482	-0.207117
F	-4.250828	-2.819384	-0.199762
F	-0.197828	-5.092374	-0.208949
F	4.565587	-2.264485	-0.199803
F	4.511672	2.375088	-0.200354
F	-0.319232	5.086626	-0.209801
F	-6.322826	1.287144	-1.389703
F	-6.295274	-1.431344	-1.384414
F	2.050842	-6.116324	-1.391046
F	4.391181	-4.729879	-1.384763
F	4.277065	4.834888	-1.386002
F	1.904310	6.164681	-1.391848
C	-0.000632	0.002280	3.759664
N	-0.000416	0.003258	4.923745
Br	0.003250	-0.007046	-1.616866

46

II-CN-P-F...Br

N	-0.002372	1.541088	-1.711955
N	1.271851	-0.738733	-1.595723
N	-1.271009	-0.735866	-1.588141
C	-1.208246	2.040041	-1.021824
C	1.213044	2.050295	-1.037027
C	2.391218	0.017460	-1.082254
C	1.148010	-2.042695	-1.032969
C	-1.155173	-2.045591	-1.045061
C	-2.390620	0.014601	-1.083414
N	-2.287569	1.352982	-0.816332
N	2.280856	1.347719	-0.810111
N	0.000734	-2.730038	-0.951294
C	-0.716964	3.272319	-0.404267
C	0.720371	3.273864	-0.408879
C	3.164556	-0.987671	-0.435568
C	2.436770	-2.251671	-0.439448
C	-2.438707	-2.254146	-0.450702
C	-3.166783	-0.987307	-0.442706
C	-1.410256	4.272264	0.266955
C	1.411430	4.273395	0.266842
C	4.359234	-0.900627	0.300834
C	2.942631	-3.361796	0.255933
C	-2.944016	-3.363996	0.249113
C	-4.360046	-0.899458	0.299349
C	-0.700410	5.285975	0.932979
C	0.699614	5.285566	0.932137

C	4.833545	-2.012938	0.981668
C	4.135145	-3.248629	0.955390
C	-4.132028	-3.248366	0.952304
C	-4.832146	-2.010946	0.979246
F	-2.762595	4.288755	0.306885
F	2.764074	4.294107	0.303734
F	5.053799	0.262427	0.356239
F	2.278749	-4.540648	0.252718
F	-2.279637	-4.542642	0.244960
F	-5.052098	0.264752	0.357681
F	-1.367816	6.277615	1.572795
F	1.366780	6.276331	1.572945
F	5.993459	-1.944354	1.680534
F	4.662246	-4.313002	1.615864
F	-4.657728	-4.309924	1.618095
F	-5.988964	-1.944035	1.683817
C	-0.005311	-0.011381	-4.021571
N	-0.002234	-0.113607	-5.192245
P	0.000376	0.019715	-2.266239
Br	0.000775	-0.072865	1.512553

58

II-CN-B-CN...I

B	0.002301	0.000067	2.317838
N	0.681826	1.214458	1.704452
N	-1.387948	-0.016709	1.701558
N	0.710560	-1.198112	1.705137
C	1.966281	1.165592	1.209511
C	-0.032072	2.278503	1.193579
C	-1.999217	1.121619	1.224704
C	-1.971693	-1.169166	1.224160
C	0.022112	-2.279345	1.195162
C	1.993382	-1.118862	1.209936
N	2.664782	0.031516	1.061046
N	-1.365977	2.291495	1.065689
N	-1.311023	-2.324007	1.066560
C	2.198700	2.454072	0.576295
C	0.948400	3.148553	0.562323
C	-3.240917	0.676573	0.612142
C	-3.223675	-0.753731	0.611506
C	1.023007	-3.126052	0.564215
C	2.256192	-2.401646	0.577147
C	3.341640	2.997943	-0.031165
C	0.820991	4.400460	-0.061912
C	-4.279163	1.391877	-0.007675
C	-4.244920	-1.492813	-0.008875
C	0.925191	-4.380492	-0.060248
C	3.411498	-2.917942	-0.031158
C	3.217995	4.258944	-0.677084

C	1.970692	4.952419	-0.692259
C	-5.306445	0.651454	-0.653998
C	-5.289580	-0.776316	-0.654325
C	2.087420	-4.904759	-0.691405
C	3.317814	-4.181644	-0.676641
C	0.002134	0.000759	3.914755
N	0.006508	0.001475	5.078024
C	-4.264113	-2.919841	0.025703
N	-4.339357	-4.080603	0.073280
C	-6.344213	-1.489957	-1.303293
N	-7.202522	-2.071808	-1.832853
C	-6.377080	1.340713	-1.303068
N	-7.247939	1.903307	-1.832923
C	-4.332134	2.818025	0.028780
N	-4.434781	3.976628	0.078341
C	-0.286548	-5.134800	-0.050398
N	-1.241736	-5.800226	-0.036819
C	2.033629	-6.182754	-1.328921
N	1.992489	-7.226238	-1.843837
C	4.471828	-4.746205	-1.302280
N	5.413572	-5.206240	-1.809196
C	4.659330	-2.226978	0.025291
N	5.702918	-1.715398	0.092466
C	4.606007	2.337927	0.026985
N	5.662066	1.852709	0.095354
C	4.358206	4.850793	-1.302603
N	5.288555	5.333246	-1.809810
C	1.886961	6.229233	-1.328912
N	1.821442	7.271906	-1.842854
C	-0.408243	5.126019	-0.052163
N	-1.378571	5.769112	-0.038476
I	0.012306	-0.000741	-1.641088

46

II-CN-B-F...I

B	-0.000545	0.000898	2.137254
N	-1.386054	-0.015736	1.532298
N	0.705923	-1.191206	1.532320
N	0.677712	1.208640	1.530786
C	-1.997318	1.126182	1.065005
C	-1.971060	-1.172144	1.066805
C	0.021402	-2.289202	1.059693
C	1.998351	-1.118162	1.062894
C	1.971572	1.165990	1.061662
C	-0.032201	2.290384	1.058609
N	-1.369060	2.305804	0.935598
N	-1.314987	-2.336668	0.938244
N	2.679602	0.032008	0.936488
C	-3.246716	0.681433	0.471542

C	-3.230727	-0.756709	0.472955
C	1.031060	-3.148682	0.464668
C	2.268455	-2.415623	0.466736
C	2.211025	2.469395	0.465037
C	0.956614	3.173120	0.463349
C	-4.274413	1.370937	-0.171180
C	-4.243927	-1.469322	-0.167732
C	0.951727	-4.385927	-0.173490
C	3.393404	-2.936178	-0.171619
C	3.323229	3.017366	-0.172939
C	0.847146	4.407852	-0.175085
C	-5.293323	0.644019	-0.791567
C	-5.278385	-0.765632	-0.789479
C	2.091762	-4.904491	-0.792774
C	3.304900	-4.185929	-0.789921
C	3.204443	4.264682	-0.791087
C	1.974338	4.953891	-0.794023
F	-4.309026	2.720271	-0.206499
F	-4.250106	-2.819200	-0.199639
F	-0.197612	-5.093934	-0.207088
F	4.564855	-2.265122	-0.200997
F	4.510914	2.375384	-0.202259
F	-0.319183	5.087608	-0.208627
F	-6.319739	1.286891	-1.397701
F	-6.291656	-1.431412	-1.393076
F	2.050062	-6.116810	-1.395517
F	4.390226	-4.730178	-1.390298
F	4.276136	4.835125	-1.391518
F	1.903543	6.165017	-1.396291
C	-0.000780	0.002178	3.746400
N	-0.001270	0.003274	4.910197
I	0.004384	-0.006395	-1.856773

62

II-CN-B-CN...BF₄

B	0.000974	-0.000001	2.287305
N	0.674923	1.204811	1.662126
N	-1.384892	-0.016727	1.675434
N	0.703329	-1.188884	1.663129
C	1.970835	1.166558	1.202412
C	-0.032567	2.290205	1.199042
C	-2.000712	1.124647	1.215133
C	-1.973650	-1.172412	1.215376
C	0.021725	-2.290892	1.200241
C	1.998042	-1.120174	1.203616
N	2.673349	0.031334	1.069788
N	-1.367986	2.299109	1.072310
N	-1.313112	-2.331588	1.073217
C	2.210382	2.475593	0.612114

C	0.960972	3.175064	0.606341
C	-3.256511	0.676905	0.630016
C	-3.239689	-0.754374	0.629997
C	1.036085	-3.152139	0.607972
C	2.268507	-2.423314	0.613717
C	3.346612	3.013116	-0.012844
C	0.832464	4.419479	-0.030981
C	-4.286876	1.390103	-0.003380
C	-4.253343	-1.491016	-0.003755
C	0.937003	-4.399129	-0.029730
C	3.416860	-2.933169	-0.012263
C	3.224854	4.274309	-0.654580
C	1.978476	4.970169	-0.664987
C	-5.315390	0.651345	-0.647087
C	-5.298747	-0.776113	-0.647233
C	2.095581	-4.922142	-0.664377
C	3.325009	-4.196786	-0.654202
C	0.012519	0.000852	3.884775
N	0.020506	0.001442	5.048024
C	-4.262994	-2.919388	0.007142
N	-4.332313	-4.081235	0.025539
C	-6.348362	-1.489385	-1.304829
N	-7.203807	-2.068288	-1.842041
C	-6.380752	1.340681	-1.304849
N	-7.248414	1.900941	-1.842151
C	-4.330062	2.817892	0.008722
N	-4.426921	3.977713	0.028233
C	-0.279566	-5.147696	-0.038682
N	-1.235996	-5.811067	-0.047487
C	2.036898	-6.191294	-1.319138
N	1.994465	-7.225542	-1.851970
C	4.472988	-4.751867	-1.299532
N	5.407031	-5.204740	-1.826648
C	4.659619	-2.228921	0.011849
N	5.700042	-1.707962	0.042745
C	4.606403	2.339866	0.012565
N	5.659945	1.845899	0.044180
C	4.359404	4.857202	-1.299088
N	5.282205	5.333070	-1.825636
C	1.890107	6.238129	-1.318604
N	1.823694	7.271758	-1.850188
C	-0.401259	5.139445	-0.039814
N	-1.372421	5.781149	-0.048524
B	-0.011483	-0.001451	-1.891977
F	-0.021375	-0.002695	-3.284507
F	0.643381	1.170283	-1.382721
F	-1.348064	-0.022821	-1.367651
F	0.681041	-1.150574	-1.380965

II-CN-B-F...BF₄

B	0.000063	0.000980	2.111691
N	-1.381391	-0.015435	1.504764
N	0.703171	-1.186550	1.500619
N	0.675214	1.204315	1.499858
C	-2.002169	1.129039	1.056707
C	-1.975489	-1.174286	1.057390
C	0.021923	-2.296278	1.052352
C	2.002919	-1.121230	1.051204
C	1.976126	1.169433	1.050306
C	-0.031851	2.297433	1.051160
N	-1.370270	2.308578	0.925726
N	-1.315981	-2.338781	0.927002
N	2.681647	0.032188	0.922034
C	-3.264826	0.682442	0.491435
C	-3.248507	-0.757150	0.492217
C	1.039738	-3.166579	0.485660
C	2.278103	-2.431956	0.485088
C	2.220438	2.486252	0.483820
C	0.964926	3.191234	0.484210
C	-4.288376	1.369996	-0.158871
C	-4.257171	-1.467957	-0.156423
C	0.959775	-4.399874	-0.159203
C	3.398967	-2.950522	-0.161126
C	3.328448	3.031841	-0.162389
C	0.854868	4.421916	-0.160980
C	-5.302148	0.643823	-0.788630
C	-5.286892	-0.765156	-0.787025
C	2.096601	-4.915664	-0.786782
C	3.309064	-4.197142	-0.785613
C	3.208390	4.276049	-0.786713
C	1.979013	4.965242	-0.787980
F	-4.318697	2.719465	-0.203728
F	-4.258010	-2.817879	-0.198698
F	-0.192024	-5.104050	-0.201644
F	4.567797	-2.274942	-0.202385
F	4.513488	2.385037	-0.204105
F	-0.314077	5.097244	-0.204220
F	-6.318845	1.287106	-1.409978
F	-6.290084	-1.431331	-1.406287
F	2.049737	-6.121024	-1.402488
F	4.389883	-4.733923	-1.400231
F	4.275856	4.838884	-1.401260
F	1.903224	6.169243	-1.403331
C	0.001229	0.001849	3.723541
N	-0.000858	0.002798	4.887641
B	-0.001028	0.000220	-2.075619
F	0.000466	-0.000109	-3.480866

F	-1.342199	-0.017115	-1.574845
F	0.684180	-1.152256	-1.573413
F	0.653906	1.170391	-1.574026

78

III-CN-B-CN

B	-0.995069	0.026964	-3.893199
N	0.496554	0.080687	-3.621330
N	-1.454781	-1.198045	-3.123358
N	-1.547248	1.183692	-3.081213
C	1.163478	1.235716	-3.243116
C	1.256895	-1.053697	-3.365300
C	-0.616301	-2.249386	-2.791137
C	-2.622491	-1.217577	-2.370113
C	-2.664718	1.076823	-2.268234
C	-0.807475	2.322368	-2.789065
N	0.530901	2.385052	-2.934019
N	0.712906	-2.235526	-3.016566
N	-3.272623	-0.097013	-2.000030
C	2.523264	0.811963	-2.993513
C	2.594445	-0.563647	-3.144339
C	-1.423636	-3.118992	-1.966614
C	-2.668717	-2.536018	-1.787157
C	-2.771170	2.362895	-1.617674
C	-1.682137	3.138634	-1.985626
C	-3.394095	-3.394908	-0.744427
C	-1.358694	-4.234846	-0.923381
C	3.990107	-0.974134	-2.666677
C	3.836874	1.201981	-2.311234
C	-3.386385	3.088020	-0.419363
C	-1.716989	4.374871	-1.081997
C	3.828093	0.538771	-0.899156
C	3.971722	-0.835206	-1.142121
C	-2.329486	3.030502	0.722951
C	-1.298467	3.886009	0.309283
C	-2.731897	-3.074193	0.595892
C	-1.416311	-3.544310	0.477321
C	-0.507201	-3.349423	1.510240
C	-3.228910	-2.501296	1.759988
C	4.114857	-1.771583	-0.125655
C	3.744209	1.019197	0.402578
C	-0.203473	4.185635	1.110522
C	-2.256309	2.372755	1.944876
C	-0.970957	-2.728843	2.723764
C	-2.325770	-2.337813	2.861941
C	-1.119766	2.626111	2.789823
C	-0.113780	3.539861	2.389035

C	3.857974	0.077916	1.486059
C	4.068205	-1.299423	1.227587
H	-4.480683	-3.456562	-0.768539
H	-0.650984	-5.053093	-1.046034
H	4.457090	-1.863781	-3.086893
H	4.197005	2.227396	-2.378717
H	-1.287755	5.310332	-1.437193
H	-4.424381	2.902858	-0.148550
O	-3.170747	4.477088	-0.856284
O	-2.753543	-4.698053	-1.002122
O	4.735346	0.256462	-2.995000
C	-1.400830	0.036219	-5.429377
N	-1.705360	0.038463	-6.552150
C	3.750523	0.548934	2.830455
N	3.620596	0.953849	3.914728
C	4.261553	-2.206679	2.312884
N	4.424693	-2.947800	3.194862
C	4.365539	-3.133231	-0.481596
N	4.596579	-4.199163	-0.886551
C	3.547067	2.409472	0.657490
N	3.360236	3.543079	0.847057
C	0.728743	5.171487	0.659777
N	1.399592	6.013130	0.220076
C	0.976372	3.837849	3.261379
N	1.871362	4.089621	3.961635
C	-1.018167	1.941544	4.039283
N	-0.947463	1.339952	5.033744
C	-3.284701	1.465374	2.337994
N	-4.123859	0.707479	2.611778
C	-4.622675	-2.192313	1.826212
N	-5.774285	-2.029539	1.788654
C	-2.797127	-1.805137	4.099511
N	-3.193931	-1.372886	5.104701
C	-0.041897	-2.499935	3.783569
N	0.751155	-2.288016	4.610203
C	0.857418	-3.733477	1.353316
N	1.973792	-4.005529	1.171342

77

III-Cl-B-CN

Cl	0.010000	-0.400491	5.314044
B	0.007719	-0.266101	3.440996
N	1.025843	-1.128690	2.756904
N	0.285352	1.112373	2.919489
N	-1.290481	-0.647076	2.794233
C	0.725574	-2.369593	2.218961
C	2.260362	-0.655980	2.343550
C	1.540789	1.523175	2.502198
C	-0.715165	1.992281	2.540833

C	-2.249347	0.282076	2.424098
C	-1.525893	-1.899028	2.250300
N	-0.541263	-2.795805	2.032405
N	2.555401	0.659908	2.286525
N	-1.996978	1.606577	2.367198
C	1.981246	-2.838922	1.679273
C	2.904512	-1.806660	1.752670
C	1.351602	2.899352	2.102836
C	-0.006564	3.180174	2.122288
C	-3.318995	-0.512919	1.864797
C	-2.881319	-1.824190	1.754612
C	-0.157017	4.536366	1.433489
C	2.009553	4.092091	1.408780
C	4.101418	-2.264035	0.920029
C	2.631627	-3.912886	0.807026
C	-4.635503	-0.450647	1.091198
C	-3.933718	-2.539933	0.907445
C	2.694731	-3.329626	-0.621357
C	3.624675	-2.281844	-0.548791
C	-4.267915	-0.623081	-0.397215
C	-3.820990	-1.947637	-0.515538
C	0.193114	4.308461	-0.054105
C	1.568033	4.029359	-0.068650
C	2.258181	3.809238	-1.253683
C	-0.549941	4.373741	-1.225960
C	3.971404	-1.534586	-1.667160
C	2.076310	-3.677123	-1.815497
C	-3.431680	-2.478587	-1.738746
C	-4.346524	0.224855	-1.494245
C	1.516460	3.852656	-2.482974
C	0.128439	4.130237	-2.468871
C	-3.938126	-0.288081	-2.771978
C	-3.484846	-1.623913	-2.892457
C	2.403201	-2.916525	-2.989741
C	3.339405	-1.857129	-2.915879
H	-1.020169	5.162076	1.658198
H	3.053788	4.325559	1.613898
H	5.089262	-1.852356	1.124315
H	2.324655	-4.952725	0.914345
H	-4.054271	-3.619066	0.996554
H	-5.373329	0.310060	1.343988
O	-5.135257	-1.812358	1.353705
O	1.105559	5.164275	1.862817
O	4.041203	-3.712161	1.188191
C	-0.605865	4.182330	-3.692930
N	-1.221996	4.222487	-4.680066
C	2.191427	3.627358	-3.721456
N	2.756571	3.437242	-4.721544
C	3.672956	-1.110412	-4.086971

N	3.954200	-0.488959	-5.030525
C	1.785574	-3.244658	-4.235110
N	1.267776	-3.524414	-5.239784
C	-3.087411	-2.134999	-4.165701
N	-2.752815	-2.565036	-5.194688
C	-4.004922	0.554140	-3.923536
N	-4.061681	1.255061	-4.851507
C	-3.033300	-3.848277	-1.828947
N	-2.739904	-4.974946	-1.840835
C	-4.862572	1.547828	-1.331721
N	-5.313630	2.602853	-1.134283
C	1.180977	-4.790414	-1.856445
N	0.481874	-5.721122	-1.832118
C	4.957719	-0.506486	-1.554328
N	5.778795	0.302430	-1.389565
C	3.670895	3.594438	-1.224600
N	4.823075	3.451502	-1.137423
C	-1.936886	4.715138	-1.175153
N	-3.056223	5.018045	-1.070348

78

III-CN-P-CN

P	-1.027494	0.023983	-3.967363
N	0.574076	0.090163	-3.784144
N	-1.522340	-1.267414	-3.135136
N	-1.692781	1.302426	-3.240185
C	1.198727	1.320161	-3.230532
C	1.307943	-1.109106	-3.336981
C	-0.614606	-2.327914	-2.763024
C	-2.729830	-1.246743	-2.321811
C	-2.769446	1.086765	-2.241608
C	-0.828153	2.446073	-2.857924
N	0.510618	2.390143	-2.875106
N	0.756080	-2.241888	-3.001572
N	-3.377150	-0.058357	-2.025600
C	2.499092	0.831374	-2.926859
C	2.618688	-0.544984	-3.133805
C	-1.402813	-3.113717	-1.958771
C	-2.721105	-2.505292	-1.761877
C	-2.810575	2.379265	-1.632202
C	-1.705962	3.159010	-2.008835
C	-3.403842	-3.383392	-0.720954
C	-1.349288	-4.200271	-0.906892
C	3.993225	-0.931647	-2.597463
C	3.764135	1.221803	-2.169160
C	-3.370082	3.070589	-0.394878
C	-1.709445	4.361503	-1.065872
C	3.723509	0.510164	-0.788581
C	3.922563	-0.846587	-1.073224

C	-2.290343	2.980978	0.713563
C	-1.261119	3.832699	0.294860
C	-2.733986	-3.048605	0.602956
C	-1.410948	-3.493979	0.471107
C	-0.479266	-3.219383	1.462945
C	-3.214022	-2.459934	1.767594
C	4.107241	-1.798628	-0.078697
C	3.633545	0.955248	0.521798
C	-0.157241	4.123296	1.083930
C	-2.194799	2.304402	1.922480
C	-0.927586	-2.586705	2.670498
C	-2.292327	-2.250845	2.841450
C	-1.046343	2.540592	2.747279
C	-0.051406	3.466136	2.351963
C	3.792650	-0.002865	1.579781
C	4.048628	-1.362344	1.284286
H	-4.489645	-3.476093	-0.731036
H	-0.636097	-5.017355	-1.013975
H	4.508238	-1.790186	-3.028385
H	4.095188	2.259973	-2.178903
H	-1.281994	5.305021	-1.405520
H	-4.402658	2.887113	-0.097940
O	-3.156638	4.478141	-0.797674
O	-2.747083	-4.684093	-0.988364
O	4.725744	0.331064	-2.848581
C	-1.461431	-0.046265	-5.698187
N	-1.745292	-0.112197	-6.828240
C	3.747164	0.439840	2.936615
N	3.728650	0.824833	4.035192
C	4.338889	-2.279223	2.340575
N	4.632911	-3.014878	3.193411
C	4.462444	-3.129776	-0.461735
N	4.807083	-4.162748	-0.873044
C	3.444170	2.341350	0.798327
N	3.318100	3.483776	0.981411
C	0.743542	5.139284	0.635260
N	1.364955	6.019754	0.194509
C	1.017140	3.790826	3.241223
N	1.861183	4.097668	3.982006
C	-0.929607	1.854777	3.994226
N	-0.856972	1.289324	5.009493
C	-3.242021	1.427225	2.331821
N	-4.133427	0.741215	2.629808
C	-4.616436	-2.198758	1.867061
N	-5.775231	-2.085160	1.864830
C	-2.760672	-1.762041	4.098660
N	-3.164317	-1.414004	5.133436
C	0.015698	-2.330890	3.710858
N	0.810582	-2.140598	4.540105

C	0.887007	-3.588062	1.283521
N	1.988979	-3.914589	1.105512

69

IV-CN-B-CN-O

B	-0.023736	-0.020224	3.403966
N	-1.365536	-0.325809	2.755983
N	0.929392	-1.027743	2.777333
N	0.388429	1.313168	2.795478
C	-2.201047	0.662740	2.262284
C	-1.682549	-1.571673	2.238586
C	0.502362	-2.237093	2.251704
C	2.180883	-0.674765	2.299579
C	1.664770	1.550065	2.310729
C	-0.529207	2.218840	2.286459
N	-1.830890	1.943758	2.104479
N	-0.788124	-2.557776	2.065037
N	2.593367	0.594206	2.147912
C	-3.284878	-0.052188	1.627842
C	-2.972514	-1.394945	1.611861
C	1.676825	-2.808069	1.632904
C	2.687097	-1.870328	1.666214
C	1.590988	2.854166	1.693112
C	0.271684	3.254367	1.674889
O	3.867324	-1.997292	0.974986
O	1.742105	-3.970758	0.902777
O	-3.675788	-2.331771	0.893630
O	-4.333037	0.494759	0.928810
O	2.589789	3.494835	1.000917
O	-0.184564	4.333234	0.955900
C	-4.976848	-0.410183	0.095768
C	-4.656776	-1.783926	0.077658
C	2.121022	4.468706	0.129514
C	0.770096	4.873710	0.104838
C	3.892234	-3.087766	0.116676
C	2.857975	-4.046423	0.079590
C	2.923052	-5.129589	-0.812633
C	5.001452	-3.202056	-0.737886
C	-5.332872	-2.661128	-0.786907
C	-5.974977	0.101015	-0.750345
C	0.336939	5.852439	-0.805118
C	3.053844	5.041584	-0.750556
C	4.049277	-5.264053	-1.677680
C	5.085851	-4.303174	-1.639649
C	2.630754	6.047826	-1.668053
C	1.275847	6.451003	-1.695900
C	-6.677379	-0.780517	-1.623958
C	-6.357824	-2.157543	-1.641441
C	-0.045353	-0.039252	4.993566

N	-0.064176	-0.056766	6.156415
C	-7.693011	-0.262045	-2.484453
N	-8.516470	0.170582	-3.184522
C	-7.051830	-3.050400	-2.514138
N	-7.612857	-3.785624	-3.221410
C	-4.973151	-4.043132	-0.797363
N	-4.665114	-5.165498	-0.797110
C	-6.263593	1.499230	-0.717628
N	-6.484503	2.641463	-0.682306
C	-1.042741	6.220437	-0.826994
N	-2.171477	6.504256	-0.836620
C	0.835818	7.447368	-2.619829
N	0.467476	8.257102	-3.370901
C	3.578274	6.629490	-2.564691
N	4.357591	7.093118	-3.294656
C	4.410220	4.596403	-0.711136
N	5.510721	4.219531	-0.671480
C	6.023581	-2.206092	-0.682580
N	6.844399	-1.383449	-0.619044
C	6.213081	-4.418675	-2.509417
N	7.132929	-4.501700	-3.218178
C	4.117493	-6.367130	-2.582796
N	4.164924	-7.269134	-3.317127
C	1.849363	-6.070701	-0.845596
N	0.964200	-6.826023	-0.872863

69

IV-CN-B-CN-S

B	0.079864	0.411213	-4.070529
N	1.170417	-0.481367	-3.490708
N	-1.211634	-0.184549	-3.523000
N	0.232994	1.720849	-3.305581
C	2.312698	0.017910	-2.897530
C	0.944351	-1.785780	-3.101716
C	-1.325974	-1.506838	-3.143384
C	-2.210412	0.577731	-2.951353
C	-0.834831	2.394101	-2.746223
C	1.422158	2.118885	-2.728164
N	2.492293	1.316398	-2.607072
N	-0.277740	-2.337190	-3.024479
N	-2.071440	1.879098	-2.651891
C	3.011545	-1.132400	-2.343704
C	2.174147	-2.233235	-2.465698
C	-2.649854	-1.640821	-2.553513
C	-3.188295	-0.366848	-2.433076
C	-0.260834	3.497659	-1.992515
C	1.117397	3.329769	-1.980895
S	-4.639008	0.031914	-1.519890
S	-3.322648	-3.091319	-1.820553

S	2.435536	-3.795390	-1.699894
S	4.503790	-1.088570	-1.412813
S	-1.140797	4.652401	-0.997166
S	2.228938	4.234785	-0.959883
C	4.036426	-2.146790	-0.027940
C	3.172953	-3.256262	-0.143452
C	-0.174743	4.524808	0.520933
C	1.224766	4.352211	0.536101
C	-4.433313	-1.098911	-0.128172
C	-3.892323	-2.395245	-0.254617
C	-3.796981	-3.234917	0.883110
C	-4.872959	-0.640211	1.139068
C	2.873618	-4.036814	1.001885
C	4.612800	-1.830110	1.227769
C	1.913867	4.285809	1.772761
C	-0.886411	4.627248	1.742280
C	-4.261162	-2.789034	2.149957
C	-4.799982	-1.487417	2.278697
C	-0.196575	4.584595	2.984710
C	1.207958	4.413942	2.999606
C	4.343096	-2.631086	2.370694
C	3.468242	-3.736685	2.257879
C	0.122565	0.558197	-5.650060
N	0.159040	0.658835	-6.808025
C	4.936077	-2.303164	3.628317
N	5.416006	-2.027047	4.652179
C	3.166244	-4.537421	3.401470
N	2.913323	-5.188493	4.332811
C	1.971851	-5.142829	0.901724
N	1.236860	-6.041703	0.811841
C	5.486538	-0.704086	1.352568
N	6.204706	0.207213	1.451217
C	3.331764	4.099922	1.795003
N	4.487475	3.957428	1.801141
C	1.916287	4.356111	4.238635
N	2.502261	4.307331	5.243303
C	-0.921388	4.697784	4.210738
N	-1.512581	4.787692	5.209425
C	-2.308088	4.784178	1.737446
N	-3.464662	4.918456	1.740514
C	-5.406676	0.679371	1.284660
N	-5.847343	1.750504	1.404174
C	-5.257360	-1.019236	3.548558
N	-5.630873	-0.637041	4.582863
C	-4.169381	-3.648275	3.286767
N	-4.090707	-4.354159	4.208843
C	-3.245651	-4.549008	0.758835
N	-2.806027	-5.621712	0.648606

III-CN-B-F

B	0.008279	-0.282082	3.644295
N	1.034419	-1.151687	2.942702
N	0.290385	1.109734	3.110684
N	-1.301498	-0.662479	2.980197
C	0.723370	-2.371263	2.356075
C	2.253134	-0.669344	2.484650
C	1.536259	1.506480	2.643561
C	-0.706996	1.977704	2.686083
C	-2.239465	0.271951	2.560870
C	-1.523981	-1.899669	2.390200
N	-0.541736	-2.793819	2.160472
N	2.547692	0.644518	2.417784
N	-1.985803	1.594391	2.498388
C	1.949366	-2.817519	1.744344
C	2.875596	-1.787552	1.822878
C	1.347677	2.854546	2.170725
C	-0.010008	3.139741	2.196390
C	-3.279080	-0.498880	1.927112
C	-2.845380	-1.812508	1.822574
C	-0.190496	4.353048	1.283330
C	1.967429	3.899598	1.242892
C	3.947033	-2.120771	0.784310
C	2.475517	-3.758836	0.660517
C	-4.434233	-0.368996	0.934049
C	-3.743859	-2.456870	0.766392
C	2.323448	-2.985546	-0.672454
C	3.263763	-1.938619	-0.592707
C	-3.789312	-0.463085	-0.469908
C	-3.347500	-1.797255	-0.577405
C	0.081414	3.839792	-0.151985
C	1.460264	3.548805	-0.177137
C	2.054680	3.037766	-1.309112
C	-0.707270	3.622278	-1.259862
C	3.391809	-1.024252	-1.614455
C	1.506735	-3.120283	-1.772847
C	-2.693232	-2.236001	-1.706864
C	-3.579474	0.436173	-1.491433
C	1.261000	2.826396	-2.459621
C	-0.106993	3.116468	-2.435345
C	-2.926577	-0.005204	-2.664669
C	-2.487589	-1.328909	-2.771531
C	1.639720	-2.199819	-2.837621
C	2.573201	-1.161382	-2.758457
H	-1.039815	5.018231	1.431654
H	3.017274	4.166019	1.355245
H	4.956011	-1.729392	0.905168
H	2.189511	-4.809479	0.672682

H	-3.900244	-3.534480	0.775685
H	-5.198108	0.390935	1.091508
O	-4.991510	-1.726234	1.035178
O	1.085234	5.038026	1.540150
O	3.920422	-3.588431	0.874751
F	-2.035536	3.891070	-1.259372
F	-0.849198	2.923975	-3.543955
F	1.823046	2.358376	-3.591731
F	3.376828	2.744405	-1.355651
F	-3.990295	1.724994	-1.409364
F	-2.737096	0.845980	-3.692520
F	-1.878847	-1.740589	-3.901534
F	-2.254351	-3.512007	-1.832544
F	0.592340	-4.115514	-1.871405
F	0.875473	-2.327256	-3.940575
F	2.700303	-0.299158	-3.786757
F	4.286046	-0.007500	-1.559890
C	0.010176	-0.400221	5.237823
N	0.012944	-0.486663	6.398113

65

III-Cl-B-F

Cl	1.554706	-3.347426	-4.080168
B	1.026317	-2.203777	-2.673592
N	1.979291	-2.172067	-1.509028
N	-0.302976	-2.553334	-2.059081
N	0.882261	-0.760470	-3.076652
C	2.919677	-1.167086	-1.325415
C	1.775539	-2.893521	-0.339882
C	-0.429181	-3.258183	-0.869872
C	-1.485530	-1.906042	-2.391484
C	-0.340519	-0.175209	-3.373671
C	1.858381	0.197827	-2.838309
N	2.921276	-0.023531	-2.039247
N	0.611792	-3.508782	-0.051225
N	-1.521682	-0.771974	-3.118729
C	3.561230	-1.479707	-0.073164
C	2.867628	-2.522541	0.524257
C	-1.846217	-3.304286	-0.610335
C	-2.485554	-2.487876	-1.532464
C	-0.038872	1.208852	-3.637502
C	1.291225	1.435558	-3.313473
C	-3.869549	-2.211937	-0.944313
C	-2.852304	-3.505802	0.522647
C	3.267611	-2.487492	1.999928
C	4.369956	-0.831505	1.049982
C	-0.692598	2.589944	-3.677170
C	1.420538	2.952070	-3.163273
C	3.327480	-0.143245	1.963518

C	2.624035	-1.201085	2.573898
C	-0.718962	3.079348	-2.208365
C	0.632044	3.310641	-1.879942
C	-3.626911	-1.303443	0.285121
C	-2.974441	-2.129661	1.222425
C	-2.573000	-1.633845	2.442688
C	-3.885383	0.019242	0.567469
C	1.584722	-0.950814	3.442235
C	2.991447	1.167849	2.214801
C	0.992044	3.728403	-0.618057
C	-1.714880	3.264924	-1.275701
C	-2.848090	-0.282749	2.753753
C	-3.500607	0.535335	1.825632
C	-1.361546	3.710524	0.018222
C	-0.021286	3.941160	0.343730
C	1.939502	1.439883	3.118262
C	1.242225	0.391111	3.725966
H	-4.695350	-1.957754	-1.606904
H	-2.783281	-4.390392	1.153880
H	3.204787	-3.395920	2.596999
H	5.278500	-0.280546	0.812011
H	2.388270	3.428166	-3.313102
H	-1.586316	2.745063	-4.279664
O	0.443269	3.379391	-4.175016
O	-4.098689	-3.491477	-0.257154
O	4.655397	-2.023024	1.862169
F	-4.504340	0.836774	-0.319107
F	-3.773405	1.817328	2.140849
F	-2.492065	0.219936	3.953176
F	-1.932622	-2.403708	3.356461
F	-3.020576	3.040603	-1.562170
F	-2.317906	3.928300	0.943208
F	0.297892	4.382094	1.577066
F	2.284480	3.951512	-0.276230
F	3.642911	2.201890	1.629056
F	1.613135	2.715160	3.408505
F	0.247886	0.665527	4.594486
F	0.888003	-1.948967	4.038220

66

III-CN-P-F

O	-0.965609	0.276518	-3.843894
C	0.479401	0.186560	-3.572254
C	0.535612	-1.209170	-2.951356
C	-0.681787	-1.370482	-2.282474
C	-1.420784	-0.046151	-2.486365
C	1.525207	-2.058960	-2.348978
N	0.667520	-3.063558	-1.678493
C	-0.661826	-2.458066	-1.369756

C	-0.622819	1.020167	-1.685124
C	0.577517	1.185864	-2.404885
C	1.530240	2.097366	-2.008249
C	1.283444	2.883064	-0.861502
C	0.109372	2.698337	-0.123485
C	-0.856613	1.753678	-0.542562
P	1.324917	-4.131702	-0.652006
C	1.465896	-5.744901	-1.388450
N	1.587349	-6.799070	-1.873271
N	-1.342843	-2.724446	-0.266390
C	-0.902353	-3.506334	0.721982
N	0.445450	-4.152557	0.709908
C	1.125350	-3.936524	2.020839
C	0.003067	-3.682419	2.868837
C	-1.147065	-3.422486	2.115528
C	-2.114265	-2.718676	3.070904
C	-1.545727	-1.304726	3.269454
C	-0.345437	-1.494338	3.983932
C	-0.266417	-3.029239	4.224861
O	-1.703569	-3.327114	4.343701
C	-1.991745	-0.049860	2.922788
C	-1.217908	1.070391	3.294211
C	-0.001716	0.887490	3.961207
C	0.440382	-0.409975	4.311045
N	2.807287	-1.911446	-2.147281
C	3.429444	-2.499952	-1.046637
N	2.750615	-3.487469	-0.230264
C	3.254159	-3.514714	1.134301
C	4.426918	-2.809113	1.039720
C	4.506055	-2.154004	-0.270156
C	5.486137	-2.110183	1.880845
C	4.934960	-0.708449	2.166304
C	4.942066	-0.048743	0.919875
C	5.552196	-1.069104	-0.073327
O	6.473148	-1.781197	0.832421
C	4.417946	1.222697	0.806088
C	3.927403	1.868449	1.962127
C	3.956667	1.220505	3.204024
C	4.445364	-0.097406	3.300460
N	2.419060	-3.841817	2.198208
F	4.369316	1.872691	-0.385347
F	4.449528	-0.722407	4.503714
F	2.677761	2.281111	-2.705872
F	-1.992859	1.606877	0.185134
F	-3.167646	0.133705	2.274261
F	1.619219	-0.545183	4.970345
F	3.457021	3.130897	1.888557
F	3.536942	1.872051	4.306022
F	0.734324	1.965400	4.301713

F	-1.653813	2.316184	3.025993
F	-0.107931	3.447632	0.977420
F	2.166888	3.826694	-0.484664
H	5.948846	-2.651932	2.704757
H	6.075528	-0.672840	-0.942675
H	1.068539	0.395024	-4.464168
H	-2.506997	-0.024790	-2.407880
H	-3.185802	-2.816967	2.901497
H	0.286285	-3.368210	5.099892

79

III-CN-B-CN...Br

B	-1.015141	0.036681	-3.894862
N	0.467490	0.034200	-3.602721
N	-1.545463	-1.162931	-3.147028
N	-1.545343	1.222905	-3.126283
C	1.165198	1.172304	-3.240454
C	1.169024	-1.119228	-3.293737
C	-0.758332	-2.255932	-2.831919
C	-2.697173	-1.122435	-2.377054
C	-2.677722	1.163262	-2.332500
C	-0.762904	2.323777	-2.818868
N	0.574004	2.350322	-2.967453
N	0.575365	-2.292817	-3.011739
N	-3.329093	0.019399	-2.049833
C	2.502935	0.710815	-2.970775
C	2.511608	-0.671810	-3.029500
C	-1.614921	-3.111277	-2.055086
C	-2.797543	-2.437190	-1.797105
C	-2.764993	2.465280	-1.721102
C	-1.620213	3.177009	-2.041071
C	-3.499454	-3.236449	-0.704060
C	-1.594133	-4.288989	-1.095227
C	3.862720	-1.105466	-2.477841
C	3.835579	1.103822	-2.350819
C	-3.411399	3.230594	-0.573248
C	-1.602921	4.382827	-1.113634
C	3.826413	0.607329	-0.885973
C	3.859867	-0.791402	-0.972193
C	-2.457598	3.091643	0.635786
C	-1.318833	3.830853	0.292086
C	-2.665501	-3.044042	0.574050
C	-1.447635	-3.687616	0.320097
C	-0.447884	-3.749888	1.277556
C	-2.956236	-2.488969	1.811455
C	4.026986	-1.592362	0.148186
C	3.935650	1.259060	0.333949
C	-0.265299	4.012840	1.174136

C	-2.584334	2.500235	1.883677
C	-0.690276	-3.131870	2.548755
C	-1.938537	-2.526030	2.820705
C	-1.497666	2.636233	2.809394
C	-0.349636	3.383570	2.459101
C	4.057231	0.460050	1.520161
C	4.108522	-0.950725	1.428496
H	-4.583437	-3.185040	-0.606972
H	-0.996896	-5.170253	-1.326899
H	4.289038	-2.060476	-2.783547
H	4.245843	2.096861	-2.531998
H	-1.076596	5.288885	-1.412170
H	-4.478556	3.124221	-0.381253
O	-3.057804	4.609642	-0.972310
O	-3.040302	-4.597200	-1.057611
O	4.688670	0.039226	-2.927147
C	-1.376732	0.049604	-5.460800
N	-1.637990	0.058089	-6.594632
C	4.214235	1.098880	2.788666
N	4.370960	1.630114	3.812900
C	4.332013	-1.738095	2.599553
N	4.550019	-2.392080	3.538383
C	4.250478	-2.993350	-0.022521
N	4.499565	-4.107234	-0.251962
C	4.042998	2.682905	0.371071
N	4.187553	3.837454	0.332302
C	0.801659	4.891503	0.812956
N	1.596172	5.666730	0.462444
C	0.704687	3.570816	3.404964
N	1.564409	3.757975	4.167257
C	-1.604902	2.067264	4.115295
N	-1.711489	1.624615	5.186886
C	-3.811409	1.862802	2.239117
N	-4.857362	1.411456	2.479456
C	-4.279036	-2.013374	2.066603
N	-5.394582	-1.713325	2.211181
C	-2.218842	-2.015569	4.125323
N	-2.479107	-1.634303	5.194267
C	0.319321	-3.186047	3.557949
N	1.153433	-3.254106	4.367383
C	0.743707	-4.488965	1.009831
N	1.667191	-5.148199	0.749525
Br	-0.122885	0.006482	-0.068370

78

III-Cl-B-CN...Br

Cl	0.009992	-0.412811	5.445733
B	0.007489	-0.274344	3.538910
N	1.029674	-1.142233	2.880181

N	0.286286	1.107625	3.043522
N	-1.295589	-0.658743	2.917215
C	0.720943	-2.367145	2.314812
C	2.249042	-0.660090	2.439391
C	1.533929	1.505296	2.595648
C	-0.712938	1.972038	2.632827
C	-2.238299	0.273114	2.519021
C	-1.516294	-1.898629	2.344044
N	-0.540099	-2.801286	2.136748
N	2.552415	0.650185	2.391685
N	-1.994760	1.595500	2.469982
C	1.961351	-2.824763	1.742364
C	2.882669	-1.793299	1.815892
C	1.344483	2.864910	2.158255
C	-0.011928	3.144612	2.176693
C	-3.291956	-0.509829	1.925912
C	-2.853395	-1.818744	1.813987
C	-0.177429	4.442326	1.399821
C	1.990154	3.999676	1.376137
C	4.031126	-2.198355	0.904398
C	2.562651	-3.849009	0.790394
C	-4.548216	-0.419486	1.072350
C	-3.843780	-2.508352	0.886703
C	2.563176	-3.210538	-0.613334
C	3.491305	-2.161860	-0.539832
C	-4.102239	-0.566273	-0.395151
C	-3.653652	-1.889757	-0.514343
C	0.157058	4.130787	-0.073900
C	1.531815	3.852918	-0.088090
C	2.221747	3.639872	-1.272432
C	-0.582768	4.201895	-1.245266
C	3.840007	-1.417923	-1.657541
C	1.951736	-3.561045	-1.808093
C	-3.270547	-2.419988	-1.737773
C	-4.186426	0.278834	-1.491746
C	1.482670	3.689836	-2.501239
C	0.096292	3.966592	-2.487504
C	-3.782915	-0.233674	-2.769536
C	-3.330262	-1.567740	-2.890907
C	2.280879	-2.803186	-2.981392
C	3.212352	-1.742107	-2.906044
H	-1.040298	5.079984	1.589788
H	3.037434	4.246790	1.547337
H	5.026431	-1.788487	1.073443
H	2.263553	-4.894308	0.861553
H	-3.972283	-3.588989	0.940187
H	-5.297074	0.341096	1.291188
O	-5.077407	-1.787059	1.270400
O	1.091642	5.108395	1.767873

O	3.996316	-3.663816	1.106198
C	-0.621358	4.084959	-3.717276
N	-1.210830	4.213857	-4.713175
C	2.167760	3.531197	-3.744884
N	2.741804	3.431189	-4.752939
C	3.585817	-1.032993	-4.088836
N	3.919261	-0.466706	-5.050085
C	1.717514	-3.172562	-4.241297
N	1.276586	-3.504991	-5.266346
C	-2.997108	-2.095345	-4.176277
N	-2.751818	-2.544798	-5.222022
C	-3.907023	0.587639	-3.931943
N	-4.039833	1.256312	-4.875814
C	-2.924307	-3.802680	-1.840763
N	-2.700582	-4.944744	-1.875285
C	-4.754502	1.581438	-1.340964
N	-5.271515	2.609849	-1.166089
C	1.101860	-4.708428	-1.863231
N	0.460897	-5.680532	-1.861601
C	4.865916	-0.428115	-1.558618
N	5.739252	0.329160	-1.419503
C	3.641676	3.480529	-1.250011
N	4.801554	3.409744	-1.178349
C	-1.955485	4.596585	-1.201779
N	-3.054701	4.970075	-1.113785
Br	0.014837	0.005272	-0.314130

79

III-CN-P-CN...Br

P	-1.025712	0.022542	-3.971544
N	0.573487	0.091548	-3.774392
N	-1.525012	-1.272536	-3.147882
N	-1.703192	1.302635	-3.258162
C	1.191972	1.319813	-3.215527
C	1.308812	-1.104258	-3.327774
C	-0.612087	-2.323051	-2.760445
C	-2.733050	-1.252718	-2.336734
C	-2.774822	1.079324	-2.253965
C	-0.837147	2.443248	-2.864476
N	0.500090	2.389493	-2.865799
N	0.758254	-2.237686	-2.991911
N	-3.379182	-0.065183	-2.035236
C	2.491792	0.837472	-2.911850
C	2.617599	-0.538850	-3.123705
C	-1.400237	-3.109358	-1.958180
C	-2.721222	-2.507437	-1.769853
C	-2.817516	2.369096	-1.637427
C	-1.715663	3.150498	-2.012349
C	-3.394900	-3.369773	-0.711725

C	-1.335725	-4.175235	-0.888788
C	3.991294	-0.921627	-2.586686
C	3.751445	1.230042	-2.151174
C	-3.353174	3.038463	-0.378131
C	-1.699238	4.335385	-1.052112
C	3.706100	0.512222	-0.774769
C	3.913226	-0.843167	-1.063097
C	-2.255667	2.926535	0.710670
C	-1.231343	3.784756	0.293355
C	-2.724629	-3.007814	0.604925
C	-1.398278	-3.444645	0.476110
C	-0.471263	-3.172196	1.472091
C	-3.209750	-2.426974	1.770784
C	4.108177	-1.794963	-0.070431
C	3.622417	0.957011	0.535553
C	-0.129896	4.080098	1.083907
C	-2.162247	2.254748	1.921726
C	-0.924293	-2.543520	2.679910
C	-2.291806	-2.214503	2.847685
C	-1.016091	2.495517	2.748493
C	-0.021511	3.421842	2.352060
C	3.788767	-0.002386	1.592751
C	4.051242	-1.360111	1.293505
H	-4.479968	-3.466612	-0.718585
H	-0.614765	-4.986932	-0.981571
H	4.513436	-1.776187	-3.016792
H	4.078458	2.269569	-2.152157
H	-1.271329	5.281238	-1.382959
H	-4.379656	2.851413	-0.063279
O	-3.142075	4.453274	-0.757322
O	-2.730257	-4.671643	-0.954263
O	4.719579	0.345709	-2.830354
C	-1.445771	-0.052900	-5.705103
N	-1.731659	-0.125316	-6.834057
C	3.752031	0.438743	2.950477
N	3.737293	0.820942	4.050294
C	4.350532	-2.280024	2.345026
N	4.651060	-3.023270	3.188547
C	4.473651	-3.123279	-0.453414
N	4.826663	-4.154303	-0.862767
C	3.455249	2.347553	0.806573
N	3.354312	3.494525	0.975849
C	0.760024	5.111943	0.649305
N	1.373040	6.008574	0.230694
C	1.038629	3.764983	3.245595
N	1.876506	4.093579	3.984004
C	-0.915164	1.830964	4.008382
N	-0.859119	1.282214	5.033913
C	-3.226881	1.402544	2.338890

N	-4.139976	0.746034	2.638196
C	-4.615276	-2.182812	1.872880
N	-5.775032	-2.083992	1.875512
C	-2.773163	-1.748845	4.109227
N	-3.193773	-1.425451	5.145304
C	0.014345	-2.300231	3.727692
N	0.807917	-2.119359	4.560542
C	0.891380	-3.556201	1.298183
N	1.988265	-3.897010	1.115174
Br	-0.119993	0.083171	-0.213548

70

IV-CN-B-CN-O...Br

B	-0.024046	-0.020860	3.452183
N	-1.371119	-0.326227	2.816082
N	0.934702	-1.032533	2.842354
N	0.391654	1.321012	2.867123
C	-2.188184	0.664074	2.299611
C	-1.671092	-1.564161	2.273780
C	0.498092	-2.224725	2.289153
C	2.172948	-0.668600	2.342386
C	1.659421	1.540745	2.355354
C	-0.527257	2.208717	2.331598
N	-1.830335	1.947631	2.166435
N	-0.787764	-2.558627	2.120989
N	2.596786	0.595261	2.212923
C	-3.239696	-0.041869	1.613519
C	-2.928811	-1.379608	1.597794
C	1.651317	-2.772046	1.623238
C	2.658601	-1.838831	1.658343
C	1.578187	2.814435	1.688733
C	0.264305	3.214540	1.672519
O	3.813152	-1.937350	0.910685
O	1.690931	-3.905905	0.838937
O	-3.596953	-2.307984	0.826835
O	-4.252873	0.512980	0.860103
O	2.565710	3.416080	0.938206
O	-0.203587	4.255107	0.897596
C	-4.894723	-0.386284	0.038918
C	-4.573604	-1.766344	0.022118
C	2.099006	4.381793	0.075113
C	0.742455	4.789161	0.051876
C	3.836625	-3.019127	0.059961
C	2.797745	-3.982064	0.023635
C	2.885108	-5.086062	-0.842284
C	4.961583	-3.158585	-0.771682
C	-5.280305	-2.648042	-0.814734
C	-5.920566	0.112951	-0.782466
C	0.320845	5.796441	-0.833484

C	3.036037	4.985631	-0.780703
C	4.018588	-5.229735	-1.697844
C	5.052905	-4.269560	-1.662257
C	2.615603	6.003590	-1.688010
C	1.262817	6.406240	-1.715036
C	-6.635224	-0.772937	-1.643225
C	-6.317018	-2.148070	-1.658468
C	-0.051381	-0.046182	5.055751
N	-0.072864	-0.067324	6.219087
C	-7.675300	-0.263556	-2.479303
N	-8.522834	0.154277	-3.159674
C	-7.037663	-3.045277	-2.504562
N	-7.627777	-3.777507	-3.191162
C	-4.965480	-4.040286	-0.795663
N	-4.731286	-5.180342	-0.774892
C	-6.252360	1.500287	-0.727200
N	-6.546728	2.625411	-0.679506
C	-1.045104	6.211025	-0.827841
N	-2.152530	6.569467	-0.819642
C	0.833050	7.430374	-2.613012
N	0.482609	8.267066	-3.343059
C	3.568854	6.614450	-2.558536
N	4.349149	7.110143	-3.266499
C	4.405173	4.587347	-0.713238
N	5.527487	4.284411	-0.653081
C	6.014456	-2.197924	-0.691377
N	6.886902	-1.431375	-0.611688
C	6.195856	-4.409288	-2.507421
N	7.127194	-4.523283	-3.196952
C	4.107050	-6.354366	-2.573948
N	4.179019	-7.274938	-3.283291
C	1.845740	-6.064735	-0.843682
N	1.016230	-6.881379	-0.847388
Br	0.044847	0.039261	-0.338733

70

IV-CN-B-CN-S...Br

B	0.085981	0.434632	-4.276057
N	1.188038	-0.462416	-3.716046
N	-1.209459	-0.162655	-3.730537
N	0.246471	1.756997	-3.527896
C	2.314972	0.042039	-3.099961
C	0.950957	-1.753397	-3.290409
C	-1.304344	-1.473572	-3.311008
C	-2.185849	0.601898	-3.125995
C	-0.815972	2.404516	-2.929991
C	1.430025	2.127727	-2.922231
N	2.505685	1.337373	-2.824578
N	-0.263807	-2.309488	-3.214056

N	-2.054205	1.903876	-2.847114
C	2.988816	-1.088754	-2.487925
C	2.153752	-2.187369	-2.604304
C	-2.587150	-1.598970	-2.644008
C	-3.126358	-0.328593	-2.529279
C	-0.246724	3.457657	-2.109781
C	1.127641	3.287797	-2.103788
S	-4.452145	0.101173	-1.453078
S	-3.131822	-3.000430	-1.729236
S	2.321355	-3.672337	-1.673945
S	4.366040	-0.993402	-1.396221
S	-1.131911	4.442187	-0.949077
S	2.212295	4.023204	-0.927123
C	3.678190	-1.859403	0.025937
C	2.822431	-2.975493	-0.089637
C	-0.205539	4.033313	0.541561
C	1.194067	3.857817	0.550859
C	-4.028561	-0.919458	-0.030118
C	-3.469871	-2.210142	-0.145886
C	-3.228531	-2.979297	1.017407
C	-4.356819	-0.409076	1.249230
C	2.386505	-3.649770	1.076144
C	4.097126	-1.424099	1.305432
C	1.863459	3.616851	1.774157
C	-0.931349	3.967772	1.754299
C	-3.537689	-2.462882	2.305056
C	-4.107832	-1.174616	2.420961
C	-0.265165	3.712726	2.983781
C	1.137187	3.535497	2.993325
C	3.649931	-2.088920	2.479689
C	2.792730	-3.206818	2.364301
C	0.113535	0.577557	-5.868734
N	0.133708	0.677205	-7.027807
C	4.083617	-1.642565	3.765874
N	4.443434	-1.283188	4.813156
C	2.358203	-3.904778	3.533139
N	2.016021	-4.480247	4.485708
C	1.580384	-4.826178	0.963774
N	0.967400	-5.811116	0.861780
C	5.032432	-0.348820	1.426620
N	5.835835	0.488220	1.527378
C	3.289741	3.515160	1.801077
N	4.453780	3.485201	1.818577
C	1.824729	3.299749	4.223584
N	2.384729	3.117035	5.228014
C	-1.006599	3.662089	4.204161
N	-1.608965	3.634144	5.200264
C	-2.339754	4.217900	1.759792
N	-3.476461	4.470877	1.768451

C	-5.005635	0.860248	1.369350
N	-5.582017	1.868653	1.453082
C	-4.456591	-0.654642	3.705616
N	-4.753311	-0.239539	4.752207
C	-3.295326	-3.251364	3.471728
N	-3.106328	-3.896916	4.422078
C	-2.728534	-4.314339	0.899950
N	-2.370161	-5.417622	0.797157
Br	0.029904	0.099735	-0.382449

79

III-CN-B-CN...I

B	-0.995944	0.024907	-3.903299
N	0.494483	0.085261	-3.655999
N	-1.452055	-1.202723	-3.146066
N	-1.555070	1.182379	-3.106601
C	1.151656	1.237037	-3.259972
C	1.256062	-1.045344	-3.392374
C	-0.600104	-2.232043	-2.790732
C	-2.616697	-1.222654	-2.389315
C	-2.656621	1.062606	-2.279285
C	-0.812564	2.316231	-2.806141
N	0.521270	2.387988	-2.961341
N	0.723738	-2.226604	-3.037247
N	-3.275978	-0.108109	-2.026781
C	2.509913	0.820272	-3.015843
C	2.589635	-0.552806	-3.180545
C	-1.396084	-3.097732	-1.961037
C	-2.652367	-2.536014	-1.799240
C	-2.762165	2.339737	-1.620587
C	-1.682856	3.124021	-1.996222
C	-3.359930	-3.386227	-0.744069
C	-1.309861	-4.193320	-0.909039
C	3.963705	-0.963763	-2.666716
C	3.796168	1.208784	-2.297218
C	-3.362588	3.044019	-0.410184
C	-1.701037	4.339883	-1.075532
C	3.755732	0.535373	-0.895060
C	3.902527	-0.835643	-1.143526
C	-2.298740	2.981899	0.720682
C	-1.269823	3.835565	0.305921
C	-2.702544	-3.039336	0.591850
C	-1.383783	-3.494959	0.481306
C	-0.477442	-3.288052	1.511107
C	-3.202232	-2.459518	1.750454
C	4.033742	-1.774323	-0.129206
C	3.675940	1.013492	0.404352
C	-0.174975	4.128765	1.107628
C	-2.230312	2.328174	1.942200

C	-0.945996	-2.667954	2.718461
C	-2.301092	-2.281206	2.849755
C	-1.097633	2.578348	2.786810
C	-0.089250	3.486030	2.385701
C	3.779380	0.071304	1.482142
C	3.976424	-1.305490	1.222991
H	-4.445193	-3.475156	-0.766159
H	-0.584564	-4.998356	-1.020956
H	4.449165	-1.847393	-3.078723
H	4.155382	2.236327	-2.344342
H	-1.280297	5.282422	-1.422645
H	-4.397569	2.853794	-0.128637
O	-3.154586	4.445142	-0.829371
O	-2.699770	-4.687062	-0.982463
O	4.722858	0.270087	-2.962919
C	-1.420375	0.033886	-5.452839
N	-1.743452	0.046321	-6.570829
C	3.729847	0.543230	2.828293
N	3.705825	0.945541	3.920499
C	4.188131	-2.208419	2.309574
N	4.404197	-2.928021	3.198460
C	4.324444	-3.129225	-0.486422
N	4.616872	-4.181523	-0.890075
C	3.547227	2.411252	0.661654
N	3.473713	3.557168	0.852296
C	0.749962	5.125084	0.664927
N	1.404853	5.986255	0.235577
C	0.980733	3.811069	3.274778
N	1.831086	4.120966	4.006784
C	-1.013939	1.925580	4.054470
N	-0.969728	1.392285	5.088684
C	-3.287646	1.454199	2.337085
N	-4.186168	0.768065	2.611751
C	-4.602037	-2.174612	1.819775
N	-5.757924	-2.040405	1.785434
C	-2.786590	-1.766448	4.090416
N	-3.201014	-1.380991	5.107484
C	-0.034245	-2.471682	3.799930
N	0.721155	-2.331944	4.674948
C	0.879072	-3.706037	1.364067
N	1.969928	-4.076428	1.203045
I	0.054070	0.013125	0.058188

79

III-CN-P-CN...I

P	-1.027494	0.023983	-3.967363
N	0.574076	0.090163	-3.784144
N	-1.522340	-1.267414	-3.135136
N	-1.692781	1.302426	-3.240185

C	1.198727	1.320161	-3.230532
C	1.307943	-1.109106	-3.336981
C	-0.614606	-2.327914	-2.763024
C	-2.729830	-1.246743	-2.321811
C	-2.769446	1.086765	-2.241608
C	-0.828153	2.446073	-2.857924
N	0.510618	2.390143	-2.875106
N	0.756080	-2.241888	-3.001572
N	-3.377150	-0.058357	-2.025600
C	2.499092	0.831374	-2.926859
C	2.618688	-0.544984	-3.133805
C	-1.402813	-3.113717	-1.958771
C	-2.721105	-2.505292	-1.761877
C	-2.810575	2.379265	-1.632202
C	-1.705962	3.159010	-2.008835
C	-3.403842	-3.383392	-0.720954
C	-1.349288	-4.200271	-0.906892
C	3.993225	-0.931647	-2.597463
C	3.764135	1.221803	-2.169160
C	-3.370082	3.070589	-0.394878
C	-1.709445	4.361503	-1.065872
C	3.723509	0.510164	-0.788581
C	3.922563	-0.846587	-1.073224
C	-2.290343	2.980978	0.713563
C	-1.261119	3.832699	0.294860
C	-2.733986	-3.048605	0.602956
C	-1.410948	-3.493979	0.471107
C	-0.479266	-3.219383	1.462945
C	-3.214022	-2.459934	1.767594
C	4.107241	-1.798628	-0.078697
C	3.633545	0.955248	0.521798
C	-0.157241	4.123296	1.083930
C	-2.194799	2.304402	1.922480
C	-0.927586	-2.586705	2.670498
C	-2.292327	-2.250845	2.841450
C	-1.046343	2.540592	2.747279
C	-0.051406	3.466136	2.351963
C	3.792650	-0.002865	1.579781
C	4.048628	-1.362344	1.284286
H	-4.489645	-3.476093	-0.731036
H	-0.636097	-5.017355	-1.013975
H	4.508238	-1.790186	-3.028385
H	4.095188	2.259973	-2.178903
H	-1.281994	5.305021	-1.405520
H	-4.402658	2.887113	-0.097940
O	-3.156638	4.478141	-0.797674
O	-2.747083	-4.684093	-0.988364
O	4.725744	0.331064	-2.848581
C	-1.461431	-0.046265	-5.698187

N	-1.745292	-0.112197	-6.828240
C	3.747164	0.439840	2.936615
N	3.728650	0.824833	4.035192
C	4.338889	-2.279223	2.340575
N	4.632911	-3.014878	3.193411
C	4.462444	-3.129776	-0.461735
N	4.807083	-4.162748	-0.873044
C	3.444170	2.341350	0.798327
N	3.318100	3.483776	0.981411
C	0.743542	5.139284	0.635260
N	1.364955	6.019754	0.194509
C	1.017140	3.790826	3.241223
N	1.861183	4.097668	3.982006
C	-0.929607	1.854777	3.994226
N	-0.856972	1.289324	5.009493
C	-3.242021	1.427225	2.331821
N	-4.133427	0.741215	2.629808
C	-4.616436	-2.198758	1.867061
N	-5.775231	-2.085160	1.864830
C	-2.760672	-1.762041	4.098660
N	-3.164317	-1.414004	5.133436
C	0.015698	-2.330890	3.710858
N	0.810582	-2.140598	4.540105
C	0.887007	-3.588062	1.283521
N	1.988979	-3.914589	1.105512
I	0.001688	0.070786	-0.036644

83

III-CN-B-CN...BF4

B	-1.010885	0.045252	-3.926450
N	0.476763	0.100513	-3.657234
N	-1.471432	-1.179988	-3.168028
N	-1.568939	1.198866	-3.123729
C	1.131559	1.253962	-3.263152
C	1.238097	-1.034427	-3.408281
C	-0.628317	-2.228301	-2.846201
C	-2.634904	-1.202535	-2.408518
C	-2.678597	1.082211	-2.305429
C	-0.833659	2.341465	-2.835551
N	0.500539	2.410976	-2.988615
N	0.695817	-2.223511	-3.091768
N	-3.297286	-0.087374	-2.052448
C	2.481939	0.831181	-2.990937
C	2.569132	-0.541053	-3.167093
C	-1.425804	-3.097483	-2.021228
C	-2.672201	-2.520490	-1.827853
C	-2.784667	2.361623	-1.651702
C	-1.709740	3.151766	-2.031000
C	-3.355714	-3.351864	-0.740834
C	-1.314959	-4.173497	-0.953180

C	3.938649	-0.950996	-2.627841
C	3.733837	1.211441	-2.215763
C	-3.357391	3.036967	-0.414718
C	-1.723860	4.360534	-1.096540
C	3.645246	0.500824	-0.831686
C	3.846095	-0.858072	-1.105330
C	-2.257330	2.955212	0.681074
C	-1.258814	3.844279	0.267208
C	-2.656844	-2.987495	0.568589
C	-1.340000	-3.438884	0.420424
C	-0.403834	-3.215628	1.417871
C	-3.128239	-2.430072	1.747718
C	4.023578	-1.804579	-0.107323
C	3.485311	0.939869	0.473542
C	-0.172148	4.171294	1.065399
C	-2.135976	2.262764	1.875464
C	-0.833081	-2.574018	2.628651
C	-2.191528	-2.226211	2.812140
C	-0.989528	2.518550	2.698907
C	-0.038303	3.494346	2.320504
C	3.606854	-0.018369	1.536431
C	3.917907	-1.368418	1.253006
H	-4.442002	-3.432640	-0.729350
H	-0.597994	-4.985793	-1.068477
H	4.443553	-1.818532	-3.051081
H	4.086427	2.242331	-2.219980
H	-1.320415	5.311722	-1.441480
H	-4.382057	2.832292	-0.106123
O	-3.172486	4.446385	-0.815328
O	-2.709131	-4.660086	-0.974787
O	4.692338	0.297947	-2.872043
C	-1.410538	0.059501	-5.480218
N	-1.700924	0.071796	-6.607136
C	3.482615	0.423175	2.888488
N	3.400904	0.813946	3.981726
C	4.211384	-2.273545	2.318322
N	4.516383	-2.999156	3.175543
C	4.411762	-3.128912	-0.485047
N	4.788449	-4.149139	-0.899600
C	3.262835	2.322420	0.742572
N	3.111485	3.462185	0.917462
C	0.686032	5.235406	0.644068
N	1.269218	6.157516	0.238482
C	1.005552	3.860902	3.223314
N	1.819963	4.209603	3.978010
C	-0.849395	1.815385	3.933500
N	-0.769771	1.236307	4.939957
C	-3.165774	1.364241	2.281068
N	-4.052840	0.672989	2.577572

C	-4.535106	-2.202272	1.872673
N	-5.696984	-2.133603	1.888258
C	-2.647920	-1.749011	4.078368
N	-3.047920	-1.418320	5.119940
C	0.120449	-2.349429	3.667168
N	0.922934	-2.200020	4.496659
C	0.939995	-3.659628	1.246369
N	2.016206	-4.063627	1.071133
B	0.066362	0.032708	0.267685
F	-1.338895	-0.185605	0.154043
F	0.756058	-0.999017	-0.433267
F	0.392283	1.291209	-0.314985
F	0.445809	0.022323	1.630800

83

III-CN-P-CN...BF4

P	-1.044295	0.033727	-4.029526
N	0.556005	0.099531	-3.831069
N	-1.525828	-1.256371	-3.184068
N	-1.703739	1.305562	-3.282585
C	1.182806	1.329491	-3.283438
C	1.302506	-1.102762	-3.412626
C	-0.612405	-2.320208	-2.826438
C	-2.730638	-1.245379	-2.365958
C	-2.780220	1.088676	-2.282743
C	-0.839576	2.458367	-2.906000
N	0.495319	2.401616	-2.931019
N	0.752271	-2.243079	-3.099236
N	-3.371910	-0.056623	-2.047633
C	2.481384	0.841673	-2.980492
C	2.608612	-0.534444	-3.196224
C	-1.386951	-3.100512	-2.004185
C	-2.705494	-2.495657	-1.795806
C	-2.807683	2.371929	-1.654245
C	-1.708845	3.154947	-2.030106
C	-3.363342	-3.348500	-0.720664
C	-1.309185	-4.162044	-0.927709
C	3.967995	-0.922313	-2.618222
C	3.717109	1.225931	-2.176912
C	-3.347211	3.037163	-0.394313
C	-1.705541	4.347918	-1.070800
C	3.620157	0.498816	-0.807140
C	3.847060	-0.852577	-1.095930
C	-2.246662	2.935105	0.693940
C	-1.238150	3.813620	0.281936
C	-2.669609	-2.981422	0.583319
C	-1.348324	-3.424756	0.435765
C	-0.410527	-3.180287	1.428774
C	-3.137046	-2.408134	1.759241

C	4.036683	-1.803967	-0.102883
C	3.467998	0.927901	0.501546
C	-0.150368	4.134645	1.080908
C	-2.130037	2.243104	1.891183
C	-0.841347	-2.543983	2.639146
C	-2.202394	-2.198040	2.821328
C	-0.982274	2.490797	2.713870
C	-0.022427	3.459606	2.337421
C	3.612441	-0.034548	1.558160
C	3.930234	-1.379634	1.261449
H	-4.448973	-3.442706	-0.707401
H	-0.595228	-4.979920	-1.023795
H	4.500919	-1.774653	-3.038949
H	4.047225	2.264395	-2.161530
H	-1.288537	5.296128	-1.409027
H	-4.372409	2.841400	-0.080500
O	-3.150086	4.451748	-0.781890
O	-2.707140	-4.652917	-0.970178
O	4.704079	0.344400	-2.831439
C	-1.472326	-0.029427	-5.759911
N	-1.741865	-0.089165	-6.894146
C	3.514849	0.398397	2.915273
N	3.464365	0.777770	4.014500
C	4.241556	-2.289778	2.318453
N	4.561719	-3.017217	3.168584
C	4.448598	-3.118191	-0.487293
N	4.841735	-4.132225	-0.903473
C	3.249470	2.307610	0.782348
N	3.110137	3.446423	0.971292
C	0.705600	5.200274	0.660219
N	1.284774	6.123783	0.252240
C	1.010779	3.830383	3.251097
N	1.809888	4.183286	4.020141
C	-0.856293	1.805254	3.959905
N	-0.784625	1.253416	4.981964
C	-3.172651	1.366404	2.309053
N	-4.068686	0.696210	2.626544
C	-4.543601	-2.181016	1.884741
N	-5.705313	-2.109513	1.903111
C	-2.658523	-1.727754	4.090605
N	-3.051434	-1.404335	5.137253
C	0.105163	-2.334141	3.686823
N	0.895352	-2.204232	4.531325
C	0.936593	-3.609214	1.248625
N	2.014992	-4.000830	1.059907
B	0.075083	0.051464	0.255987
F	-1.325808	-0.196886	0.161885
F	0.777409	-0.925924	-0.507928
F	0.356570	1.342687	-0.274368

F	0.485342	-0.012827	1.609756
---	----------	-----------	----------

67

III-CN-B-F...Br

B	0.008217	-0.282345	3.648533
N	1.037220	-1.156083	2.967620
N	0.291356	1.112314	3.137997
N	-1.305879	-0.665642	3.006661
C	0.720052	-2.365252	2.368100
C	2.246150	-0.667925	2.496678
C	1.531974	1.499764	2.655549
C	-0.705333	1.969897	2.698092
C	-2.232418	0.270503	2.573251
C	-1.518850	-1.895428	2.402807
N	-0.542391	-2.796874	2.187741
N	2.548863	0.642993	2.445439
N	-1.986534	1.593303	2.526083
C	1.940977	-2.809666	1.749096
C	2.866648	-1.780766	1.827803
C	1.344861	2.843267	2.174641
C	-0.011578	3.128316	2.200369
C	-3.268349	-0.496028	1.932103
C	-2.835053	-1.808503	1.827694
C	-0.193334	4.337424	1.285918
C	1.964182	3.883688	1.245098
C	3.935633	-2.111410	0.789109
C	2.463942	-3.748822	0.665095
C	-4.419381	-0.364456	0.937962
C	-3.729035	-2.451980	0.770517
C	2.327572	-2.987407	-0.671066
C	3.266400	-1.942907	-0.591376
C	-3.791808	-0.465559	-0.468404
C	-3.350934	-1.797093	-0.575643
C	0.083311	3.842368	-0.149949
C	1.459360	3.551776	-0.175436
C	2.050892	3.039887	-1.305393
C	-0.703748	3.623108	-1.255374
C	3.391861	-1.029175	-1.610458
C	1.510843	-3.118940	-1.768563
C	-2.696015	-2.233533	-1.702444
C	-3.579654	0.431727	-1.487669
C	1.259645	2.832644	-2.452779
C	-0.104772	3.122102	-2.428122
C	-2.931188	-0.009452	-2.657992
C	-2.493666	-1.329849	-2.764657
C	1.645858	-2.202700	-2.830703
C	2.577394	-1.167383	-2.751675
H	-1.045249	5.000490	1.434220
H	3.015682	4.146821	1.356965

H	4.944081	-1.716835	0.910653
H	2.174164	-4.799181	0.677570
H	-3.882040	-3.530827	0.779801
H	-5.181356	0.398421	1.095451
O	-4.985008	-1.725005	1.048519
O	1.084267	5.030099	1.552617
O	3.915223	-3.585469	0.889242
F	-2.037858	3.885293	-1.249340
F	-0.850158	2.920681	-3.538036
F	1.820108	2.355433	-3.586729
F	3.375724	2.737956	-1.347505
F	-3.985061	1.726566	-1.399841
F	-2.732340	0.845813	-3.686110
F	-1.875582	-1.739350	-3.895282
F	-2.249037	-3.511866	-1.822770
F	0.587227	-4.112217	-1.861263
F	0.872988	-2.323237	-3.933400
F	2.697451	-0.297253	-3.779531
F	4.283559	-0.004649	-1.549423
C	0.010550	-0.402289	5.258111
N	0.012860	-0.488235	6.419326
Br	-0.000096	0.015957	-0.230295

66

III-Cl-B-F...Br

Cl	1.566305	-3.373785	-4.106844
B	1.024839	-2.202982	-2.672562
N	1.988913	-2.189862	-1.528118
N	-0.299267	-2.572649	-2.080599
N	0.889566	-0.775389	-3.101590
C	2.915055	-1.175859	-1.337883
C	1.774332	-2.897700	-0.355028
C	-0.422066	-3.261233	-0.883853
C	-1.475627	-1.912386	-2.401080
C	-0.334535	-0.188299	-3.380083
C	1.858036	0.183291	-2.845673
N	2.926239	-0.038765	-2.057762
N	0.617691	-3.523812	-0.070841
N	-1.515067	-0.786935	-3.137762
C	3.551721	-1.480212	-0.083670
C	2.859216	-2.522195	0.513297
C	-1.835887	-3.301466	-0.617465
C	-2.474699	-2.485590	-1.538264
C	-0.036951	1.196347	-3.635841
C	1.291712	1.422301	-3.311659
C	-3.854991	-2.205943	-0.949537
C	-2.837061	-3.499992	0.516929
C	3.255731	-2.485394	1.987268
C	4.357097	-0.828907	1.036757

C	-0.690699	2.574881	-3.670865
C	1.422592	2.935630	-3.156407
C	3.328504	-0.144908	1.962421
C	2.626733	-1.201382	2.571055
C	-0.715704	3.078129	-2.211190
C	0.632679	3.309413	-1.883169
C	-3.625659	-1.306382	0.283960
C	-2.974276	-2.131206	1.219328
C	-2.572989	-1.634837	2.436668
C	-3.881728	0.014110	0.566753
C	1.588658	-0.951206	3.436708
C	2.991663	1.163145	2.215715
C	0.989575	3.727414	-0.623141
C	-1.708941	3.261862	-1.279140
C	-2.849785	-0.288678	2.747850
C	-3.500038	0.527655	1.822069
C	-1.358110	3.711728	0.009211
C	-0.021625	3.943868	0.333784
C	1.945474	1.433086	3.119894
C	1.249804	0.386158	3.724219
H	-4.680029	-1.950678	-1.613987
H	-2.765018	-4.385365	1.148027
H	3.191668	-3.395158	2.583576
H	5.265007	-0.276892	0.795298
H	2.392671	3.408943	-3.305463
H	-1.585342	2.729547	-4.273436
O	0.448325	3.366340	-4.180289
O	-4.089603	-3.495598	-0.267179
O	4.653610	-2.028019	1.847327
F	-4.498535	0.833167	-0.326570
F	-3.763541	1.816211	2.135903
F	-2.485059	0.218973	3.946946
F	-1.926205	-2.407803	3.349388
F	-3.016536	3.026090	-1.567476
F	-2.316566	3.918613	0.940024
F	0.298732	4.377072	1.573890
F	2.287180	3.944555	-0.279899
F	3.642729	2.198935	1.622871
F	1.609813	2.711149	3.405314
F	0.244805	0.660865	4.586237
F	0.886824	-1.955788	4.025594
Br	-0.070920	0.152308	0.190949

67

III-CN-P-F...Br

O	-0.907120	0.232212	-3.928398
C	0.533369	0.186103	-3.592627
C	0.596057	-1.193983	-2.944545
C	-0.638329	-1.362708	-2.306467

C	-1.399642	-0.063706	-2.568857
C	1.576565	-2.044326	-2.331657
N	0.702487	-3.035747	-1.673211
C	-0.628376	-2.442286	-1.386957
C	-0.669653	1.052534	-1.785265
C	0.556491	1.220528	-2.454856
C	1.479732	2.143463	-2.024308
C	1.172766	2.941060	-0.904990
C	-0.038293	2.769448	-0.232585
C	-0.967855	1.805664	-0.673830
P	1.342264	-4.090374	-0.632935
C	1.401032	-5.725213	-1.371608
N	1.452872	-6.786525	-1.853621
N	-1.320929	-2.700786	-0.286572
C	-0.870443	-3.454199	0.718970
N	0.462782	-4.114451	0.719442
C	1.149883	-3.903565	2.023997
C	0.022807	-3.651178	2.869382
C	-1.120784	-3.374997	2.109503
C	-2.092187	-2.686355	3.064064
C	-1.518681	-1.287680	3.328590
C	-0.347138	-1.510510	4.075358
C	-0.269232	-3.048516	4.242902
O	-1.715937	-3.349601	4.327530
C	-1.916342	-0.020004	2.977888
C	-1.136001	1.073663	3.395200
C	0.033429	0.858291	4.125507
C	0.440702	-0.449415	4.459244
N	2.868661	-1.953199	-2.161210
C	3.477484	-2.541135	-1.052452
N	2.811401	-3.549412	-0.246571
C	3.283116	-3.545989	1.133782
C	4.459643	-2.847193	1.041280
C	4.549627	-2.199307	-0.271299
C	5.502018	-2.133406	1.889629
C	4.947746	-0.734072	2.165291
C	4.955963	-0.081678	0.917226
C	5.573912	-1.100307	-0.067296
O	6.504183	-1.801620	0.850219
C	4.404197	1.174633	0.791710
C	3.902049	1.819446	1.938064
C	3.943355	1.186369	3.182906
C	4.446310	-0.121283	3.290180
N	2.448210	-3.883234	2.195632
F	4.334997	1.811206	-0.407370
F	4.446793	-0.743160	4.502377
F	2.663403	2.326886	-2.671126
F	-2.133852	1.653563	0.006781
F	-3.054683	0.201243	2.265855

F	1.598494	-0.623670	5.151180
F	3.377127	3.062999	1.845339
F	3.505771	1.839368	4.284164
F	0.770817	1.921657	4.518129
F	-1.518322	2.336931	3.099451
F	-0.319299	3.542676	0.840896
F	2.041130	3.890963	-0.490147
H	5.961734	-2.668447	2.720466
H	6.101206	-0.699416	-0.932795
H	1.151322	0.387132	-4.467847
H	-2.488547	-0.072635	-2.529085
H	-3.162187	-2.764126	2.872539
H	0.264988	-3.428916	5.113326
Br	1.283117	-0.620828	0.892264

67

III-CN-B-F...I

O	-0.774559	0.173077	-3.908527
C	0.638181	0.250523	-3.483183
C	0.745802	-1.082533	-2.747522
C	-0.498482	-1.297921	-2.175552
C	-1.339515	-0.081236	-2.567674
C	1.698153	-1.931680	-2.084242
N	0.938539	-2.783037	-1.294260
C	-0.358853	-2.309503	-1.159229
C	-0.745447	1.130373	-1.812694
C	0.516618	1.338990	-2.398002
C	1.362689	2.314250	-1.926355
C	0.934086	3.130810	-0.861852
C	-0.318304	2.927450	-0.282383
C	-1.164518	1.904879	-0.756840
B	1.555965	-3.778170	-0.336484
C	1.600839	-5.290832	-0.893224
N	1.638872	-6.386433	-1.285306
N	-1.140059	-2.576929	-0.094969
C	-0.534201	-3.133962	0.970503
N	0.763501	-3.624719	0.943048
C	1.360181	-3.526003	2.190957
C	0.279317	-3.263280	3.104915
C	-0.872513	-3.043647	2.366300
C	-1.858361	-2.383542	3.327416
C	-1.314490	-0.970664	3.615054
C	-0.139234	-1.177063	4.360159
C	-0.020078	-2.712944	4.499065
O	-1.455301	-3.055864	4.580604
C	-1.717049	0.295040	3.261865
C	-0.948104	1.396597	3.686209
C	0.217483	1.193668	4.425112
C	0.635007	-0.111343	4.755315

N	3.027524	-1.773150	-1.944392
C	3.584639	-2.319425	-0.846975
N	2.920834	-3.208975	-0.015628
C	3.424947	-3.154381	1.275487
C	4.675319	-2.452968	1.162153
C	4.763390	-1.928252	-0.117342
C	5.707102	-1.695089	1.991995
C	5.183805	-0.252625	2.133411
C	5.270337	0.295016	0.840583
C	5.840194	-0.843862	-0.037229
O	6.735216	-1.478837	0.952153
C	4.847725	1.580564	0.596125
C	4.339997	2.347041	1.664571
C	4.246141	1.798682	2.943828
C	4.663936	0.473920	3.177692
N	2.690182	-3.416934	2.372184
F	4.899584	2.129849	-0.645853
F	4.543698	-0.051018	4.425934
F	2.599136	2.507769	-2.457663
F	-2.364093	1.703888	-0.150279
F	-2.836408	0.511015	2.520520
F	1.794046	-0.280772	5.444336
F	3.918868	3.613154	1.448382
F	3.735047	2.536995	3.954856
F	0.960492	2.257241	4.804618
F	-1.326636	2.653558	3.362499
F	-0.704880	3.696132	0.759769
F	1.747895	4.096611	-0.379455
H	6.130134	-2.167405	2.877700
H	6.380101	-0.558770	-0.939583
H	1.298779	0.451156	-4.325920
H	-2.424967	-0.168413	-2.603406
H	-2.927973	-2.483394	3.147209
H	0.531546	-3.097374	5.356565
I	1.468053	-0.029284	1.099604

71

III-CN-B-F...BF₄

O	-0.841461	0.116010	-4.040553
C	0.556440	0.243628	-3.577472
C	0.674563	-1.056011	-2.782856
C	-0.587367	-1.284456	-2.252616
C	-1.440081	-0.102171	-2.707440
C	1.622721	-1.851267	-2.046772
N	0.848606	-2.677093	-1.244208
C	-0.471787	-2.256645	-1.197548
C	-0.889546	1.144746	-1.974566
C	0.378019	1.368435	-2.541170
C	1.184399	2.389538	-2.096651

C	0.714025	3.228724	-1.069321
C	-0.541155	3.005952	-0.500515
C	-1.347707	1.940735	-0.950223
B	1.442873	-3.633865	-0.239298
C	1.541589	-5.159107	-0.750109
N	1.607503	-6.262275	-1.116434
N	-1.300010	-2.532024	-0.171395
C	-0.725493	-3.020951	0.944085
N	0.593441	-3.448243	0.994662
C	1.127366	-3.318856	2.267337
C	-0.005641	-3.063423	3.118163
C	-1.129721	-2.905761	2.320512
C	-2.180785	-2.250396	3.213844
C	-1.697871	-0.809914	3.463269
C	-0.543232	-0.945356	4.254949
C	-0.383707	-2.468710	4.472669
O	-1.808467	-2.859272	4.508220
C	-2.124122	0.424589	3.033476
C	-1.391606	1.565627	3.412604
C	-0.239832	1.433550	4.190531
C	0.196452	0.159905	4.607426
N	2.945317	-1.672933	-1.864608
C	3.459888	-2.153874	-0.716288
N	2.767481	-3.009357	0.127038
C	3.221265	-2.920318	1.435083
C	4.463154	-2.197910	1.347259
C	4.596001	-1.716965	0.052712
C	5.449530	-1.390395	2.189175
C	4.888670	0.041586	2.260969
C	4.998849	0.542867	0.951665
C	5.640513	-0.605491	0.137378
O	6.511150	-1.185182	1.181210
C	4.518009	1.793779	0.640015
C	3.940085	2.576336	1.659890
C	3.834326	2.076329	2.959194
C	4.308433	0.785810	3.260703
N	2.446587	-3.184850	2.504588
F	4.578954	2.291565	-0.622219
F	4.174577	0.303597	4.524534
F	2.419811	2.604461	-2.621366
F	-2.552338	1.728083	-0.360379
F	-3.226135	0.568564	2.250004
F	1.336248	0.057278	5.338235
F	3.475908	3.812979	1.382904
F	3.264574	2.831476	3.922712
F	0.461165	2.533532	4.535456
F	-1.793143	2.792174	3.015346
F	-0.976729	3.814556	0.487799
F	1.479074	4.248189	-0.623538

H	5.847968	-1.823717	3.105524
H	6.207616	-0.337726	-0.753475
H	1.236467	0.425222	-4.408542
H	-2.522142	-0.215050	-2.767458
H	-3.236437	-2.399462	2.991455
H	0.143908	-2.797775	5.367189
B	1.196602	0.407332	1.155292
F	1.996141	0.351680	-0.020989
F	1.095842	1.747524	1.605981
F	1.795075	-0.400846	2.162744
F	-0.098292	-0.106419	0.859059