Supporting Information

"DFT Investigation of Electronic Modulation and Site Specific CFC-11 Sensing on Difuran Functionalized Heptazine Based g-C_3N_4"

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A. Coordinates of the designed Hz and Hz-df structures with the (CFC-11)-(Hz-df) complexes, the H_20 adsorbed, H_20-CFC-11 co-adsorbed complexes at Sites A, B and C

Atomic Numbers
1: Hydrogen, 6: Carbon, 7: Nitrogen, 8: Oxygen, 9: Fluorine, 17: Chlorine

1. Hz optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.876436	6.026207	1.146774
2	6	0	-2.706775	7.498812	-0.128732
3	6	0	-1.757309	5.410805	0.692492
4	6	0	-0.552653	6.716113	-0.978395
5	6	0	0.211345	4.739464	-0.183002
6	7	0	-2.869531	5.187587	1.382774
7	7	0	-3.834411	7.214920	0.522921
8	7	0	-1.672510	6.538598	-0.140940
9	7	0	-0.729823	4.568725	0.744886
10	7	0	0.346677	5.730765	-1.057327
11	7	0	-2.552963	8.626890	-0.806536
12	6	0	-1.419749	8.741683	-1.529716
13	7	0	-0.434777	7.829229	-1.682729
14	6	0	2.527538	3.985064	-0.502892
15	6	0	4.240868	5.461799	-0.349115
16	6	0	4.539953	3.169134	-1.118324
17	6	0	6.470731	4.646115	-0.930489
18	6	0	6.657152	2.410546	-1.288541
19	7	0	3.222770	3.007682	-1.087365
20	7	0	2.959437	5.180302	-0.104683
21	7	0	5.083108	4.425351	-0.800213
22	7	0	5.355256	2.157374	-1.400092
23	7	0	7.264663	3.602244	-1.171730
24	7	0	4.744183	6.668808	-0.147283
25	7	0	6.951941	5.868078	-0.760414
26	6	0	-2.597282	-0.643454	0.239166

27	6	0	-0.953464	0.872257	-0.109857
28	6	0	-0.526163	-1.336422	0.827685
29	6	0	1.265806	0.291916	0.711237
30	6	0	1.644830	-1.916603	0.994138
31	7	0	-1.839300	-1.571714	0.819947
32	7	0	-2.221917	0.516592	-0.305319
33	7	0	-0.071601	-0.058169	0.461823
34	7	0	0.364678	-2.264434	1.145992
35	7	0	2.137653	-0.669468	0.993739
36	7	0	-0.480704	2.068578	-0.455746
37	6	0	0.746119	2.365585	-0.016549
38	7	0	1.617778	1.573001	0.603194
39	6	0	-5.707616	-4.036023	0.516551
40	6	0	-5.122512	-6.221647	-0.407015
41	6	0	-3.830669	-4.248869	-1.025674
42	6	0	-3.171810	-6.334759	-1.560601
43	7	0	-6.205561	-6.738584	0.152672
44	7	0	-6.765343	-4.575530	1.100033
45	7	0	-4.881115	-4.835351	-0.298759
46	7	0	-4.212825	-6.982435	-1.021807
47	7	0	-3.024023	-5.023228	-1.740852
48	7	0	-5.374768	-2.755238	0.702708
49	6	0	-4.371577	-2.292691	-0.035714
50	7	0	-3.644718	-2.933171	-0.951419
51	6	0	-7.468431	3.167690	0.713608
52	6	0	-7.022965	0.860204	0.033586
53	6	0	-5.289260	2.166156	1.142099
54	6	0	-4.934255	0.062123	0.404828
55	7	0	-8.283939	0.739476	-0.349561
56	7	0	-8.735003	3.018311	0.355526
57	7	0	-6.591820	2.065096	0.626537
58	7	0	-6.129963	-0.113635	-0.156070
59	7	0	-4.503514	1.096947	1.129488
60	7	0	-6.980104	4.344156	1.108258
61	6	0	-5.675697	4.367574	1.428684
62	7	0	-4.852131	3.335851	1.594809
63	6	0	3.986376	-2.573687	0.877618
64	6	0	5.630910	-1.375097	-0.076618
65	6	0	5.926263	-2.581619	2.025433
66	6	0	7.762341	-1.270291	1.096464
67	6	0	8.015174	-2.611452	2.913244
68	7	0	4.623859	-2.911672	1.983273
69	7	0	4.420179	-1.921454	-0.194598
70	7	0	6.433295	-1.739587	1.018101
71	7	0	6.723448	-3.011707	2.984063
72	7	0	8.566282	-1.750719	2.034326
73	7	0	6.063551	-0.455959	-0.930224
74	6	0	7.223062	0.120419	-0.615917
75	7	0	8.146681	-0.308116	0.258693

76	6	0	-0.782743	-6.878729	-1.686321
77	6	0	0.734622	-5.428745	-0.850764
78	6	0	1.324096	-7.708617	-1.453179
79	6	0	2.994101	-6.221413	-0.433853
80	6	0	3.489461	-8.326867	-1.132509
81	7	0	0.058249	-7.916340	-1.829501
82	7	0	-0.497046	-5.646820	-1.272017
83	7	0	1.684214	-6.457136	-0.904598
84	7	0	2.250918	-8.648042	-1.565246
85	7	0	3.904533	-7.172904	-0.563901
86	7	0	1.073909	-4.250617	-0.351978
87	6	0	2.282585	-4.152115	0.184597
88	7	0	3.273641	-5.050777	0.150340
89	7	0	2.586072	-2.938546	0.821309
90	7	0	1.171126	3.698982	-0.251304
91	7	0	-3.984330	-0.947569	0.189504
92	7	0	7.542731	1.338429	-1.208112
93	7	0	-2.115019	-7.160704	-1.944275
94	7	0	-5.159539	5.654724	1.533979
95	7	0	-1.255222	9.899629	-2.191955
96	7	0	6.550380	8.062717	-0.265276
97	1	0	5.933581	8.803774	0.024329
98	1	0	7.532029	8.227149	-0.415999
99	7	0	-10.375038	1.652586	-0.461288
100	1	0	-10.680141	0.778451	-0.856509
101	1	0	-11.008671	2.426868	-0.350313
102	7	0	-8.096276	-6.409019	1.393982
103	1	0	-8.287923	-7.390223	1.275872
104	1	0	-8.691688	-5.823399	1.956248
105	6	0	6.062106	6.818082	-0.402180
106	6	0	-9.080669	1.808565	-0.133547
107	6	0	-6.980930	-5.886400	0.856466
108	1	0	-1.975281	10.601572	-2.144701
109	1	0	-0.442280	10.021945	-2.773052
110	1	0	-5.850567	6.363596	1.313656
111	1	0	8.479209	1.649049	-0.971965
112	1	0	-2.332655	-8.149569	-1.973817
113	7	0	8.837526	-3.122054	3.843483
114	7	0	4.427291	-9.278473	-1.278057
115	1	0	9.802311	-2.834495	3.861640
116	1	0	8.465102	-3.747618	4.539189
117	1	0	5.366097	-9.097300	-0.963102
118	1	0	4.173687	-10.161900	-1.688787

2. Hz-df optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.980566	-6.058706	0.949053
2	6	0	-6.989584	-5.468948	0.068285
3	6	0	-5.299946	-3.840206	0.725649
4	6	0	-7.245489	-3.118604	-0.552551
5	6	0	-5.573999	-1.708641	0.042458
6	7	0	-4.558158	-4.825827	1.217221
7	7	0	-6.185453	-6.442474	0.497969
8	7	0	-6.509439	-4.141796	0.077865
9	7	0	-4.900925	-2.574965	0.798229
10	7	0	-6.698009	-1.904056	-0.643133
11	7	0	-8.197289	-5.718255	-0.415063
12	6	0	-8.864379	-4.665504	-0.933798
13	7	0	-8.434439	-3.391587	-1.064843
14	6	0	-5.831171	0.718247	-0.140976
15	6	0	-7.746000	1.746326	0.501477
16	6	0	-6.018410	2.865756	-0.803975
17	6	0	-7.994796	4.103641	-0.094438
18	6	0	-6.171767	5.104058	-1.008856
19	7	0	-5.367432	1.710874	-0.898932
20	7	0	-6.957656	0.670533	0.566106
21	7	0	-7.250377	2.904934	-0.129491
22	7	0	-5.508626	3.987467	-1.299272
23	7	0	-7.419840	5.225765	-0.529021
24	7	0	-8.954353	1.762990	1.040043
25	7	0	-9.216977	4.093781	0.416194
26	6	0	0.531331	-2.036641	-0.543473
27	6	0	-1.574663	-1.196973	-0.529153
28	6	0	0.369947	0.178579	-0.127959
29	6	0	-1.819521	1.067965	0.384447
30	6	0	0.044620	2.355943	0.374264
31	7	0	1.137405	-0.888864	-0.257088
32	7	0	-0.767543	-2.210156	-0.841192
33	7	0	-1.015418	0.015959	-0.087868
34	7	0	0.874327	1.398499	-0.028379
35	7	0	-1.245401	2.224289	0.716848
36	7	0	-2.902775	-1.272605	-0.619649
37	6	0	-3.590218	-0.272032	-0.063018
38	7	0	-3.129463	0.851598	0.494168
39	6	0	4.350624	-3.947980	1.168047
40	6	0	6.311279	-2.541843	1.534726
41	6	0	4.565465	-1.827811	-0.015289
42	6	0	6.294041	-0.491018	0.569830
43	7	0	6.837563	-3.490789	2.292758
44	7	0	4.890009	-4.889598	1.925348

45	7	0	5.069773	-2.766312	0.904158
46	7	0	6.906352	-1.357927	1.376408
47	7	0	5.222743	-0.690398	-0.205740
48	7	0	3.112438	-4.055959	0.681685
49	6	0	2.717716	-3.103468	-0.165247
50	7	0	3.426486	-2.092426	-0.653449
51	6	0	-1.044264	-8.070353	-0.345629
52	6	0	0.774448	-6.634165	-1.124536
53	6	0	-0.927517	-5.748969	0.380989
54	6	0	0.745378	-4.480309	-0.432346
55	7	0	1.318761	-7.669209	-1.740803
56	7	0	-0.465973	-9.104875	-0.937401
57	7	0	-0.400171	-6.813675	-0.367299
58	7	0	1.291185	-5.402978	-1.216737
59	7	0	-0.265473	-4.594255	0.418576
60	7	0	-2.244596	-8.164612	0.227619
61	6	0	-2.730005	-7.040363	0.778607
62	7	0	-2.088101	-5.895186	1.003919
63	6	0	-0.219942	4.794490	0.317521
64	6	0	-2.136384	5.665839	-0.486681
65	6	0	-0.617832	6.936056	0.935908
66	6	0	-2.719215	7.934026	0.178945
67	6	0	-1.153794	9.106490	1.337428
68	7	0	0.144172	5.842914	1.050640
69	7	0	-1.251942	4.672702	-0.509422
70	7	0	-1.825249	6.841555	0.214220
71	7	0	-0.286147	8.083646	1.503115
72	7	0	-2.356366	9.085069	0.725084
73	7	0	-3.314641	5.547091	-1.081931
74	6	0	-4.175645	6.541546	-0.874233
75	7	0	-3.925325	7.757939	-0.362544
76	6	0	6.083803	1.916565	0.226900
77	6	0	4.058252	2.902423	0.452818
78	6	0	5.861035	3.889978	-0.864780
79	6	0	3.637659	4.894353	-0.889748
80	6	0	5.416360	5.848215	-1.929776
81	7	0	6.640269	2.857918	-0.534190
82	7	0	4.882746	1.924878	0.814913
83	7	0	4.515211	3.887996	-0.442115
84	7	0	6.310792	4.891382	-1.604459
85	7	0	4.099857	5.887738	-1.631020
86	7	0	2.805896	2.964195	0.900394
87	6	0	2.007823	3.813234	0.259096
88	7	0	2.341152	4.783722	-0.588992
89	7	0	0.607371	3.644531	0.445141
90	7	0	-4.999743	-0.421833	-0.059975
91	7	0	1.344002	-3.182687	-0.523587
92	7	0	-5.517937	6.323911	-1.156953
93	7	0	6.877673	0.783471	0.487613

94	7	0	-4.082581	-7.113421	1.086860
95	7	0	-10.102537	-4.918215	-1.391428
96	7	0	-10.893388	2.909605	1.421293
97	1	0	-11.246676	2.069244	1.848481
98	1	0	-11.438568	3.755639	1.401016
99	7	0	1.289101	-9.915500	-2.156317
100	1	0	2.140614	-9.778749	-2.675864
101	1	0	0.850225	-10.819769	-2.099499
102	7	0	6.679633	-5.599953	3.157243
103	1	0	7.576404	-5.438260	3.585423
104	1	0	6.166963	-6.450481	3.322353
105	6	0	-9.640523	2.921829	0.934825
106	6	0	0.692024	-8.856610	-1.584178
107	6	0	6.115574	-4.623495	2.426444
108	1	0	-10.461437	-5.857857	-1.350489
109	1	0	-10.631048	-4.173971	-1.816042
110	1	0	-4.491003	-8.006481	0.833668
111	1	0	-6.102093	7.112910	-0.902862
112	7	0	-0.777947	10.285715	1.860721
113	7	0	5.890532	6.881426	-2.646028
114	1	0	-1.398973	11.075299	1.794581
115	1	0	0.097976	10.348468	2.353094
116	1	0	5.255915	7.600822	-2.951517
117	1	0	6.855707	6.879400	-2.932676
118	6	0	8.258917	0.920025	0.647335
119	6	0	9.020442	1.654610	1.506147
120	8	0	9.043938	0.209878	-0.214311
121	6	0	10.377028	1.385209	1.158903
122	1	0	8.649906	2.296333	2.290915
123	6	0	10.340177	0.491638	0.118118
124	1	0	11.269564	1.780421	1.619081
125	6	0	11.358382	-0.173425	-0.643107
126	6	0	11.317419	-1.071704	-1.677040
127	8	0	12.656963	0.106859	-0.313074
128	6	0	12.678500	-1.364018	-2.004495
129	1	0	10.423168	-1.464636	-2.136196
130	6	0	13.445137	-0.627253	-1.153032
131	1	0	13.036389	-2.033503	-2.773061
132	1	0	14.508932	-0.512653	-1.016963

3. Site-A complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.317059	5.968731	0.911202
2	6	0	7.360848	5.356694	0.131490
3	6	0	5.612480	3.748523	0.675526

4	6	0	7.611679	3.010419	-0.507065
5	6	0	5.888344	1.621826	-0.021318
6	7	0	4.861226	4.739844	1.140016
7	7	0	6.550423	6.338005	0.530739
8	7	0	6.859601	4.037668	0.097417
9	7	0	5.189594	2.489343	0.709011
10	7	0	7.050044	1.806386	-0.643562
11	7	0	8.596489	5.591767	-0.283329
12	6	0	9.273391	4.534667	-0.780025
13	7	0	8.830483	3.269887	-0.951356
14	6	0	6.109910	-0.809464	-0.207801
15	6	0	7.968732	-1.873065	0.533746
16	6	0	6.288832	-2.962218	-0.856835
17	6	0	8.202074	-4.236129	-0.045501
18	6	0	6.410199	-5.203667	-1.052601
19	7	0	5.666776	-1.794881	-0.987514
20	7	0	7.199255	-0.781964	0.556204
21	7	0	7.483617	-3.023448	-0.120105
22	7	0	5.782905	-4.075186	-1.375433
23	7	0	7.629545	-5.347730	-0.509158
24	7	0	9.147194	-1.911689	1.133658
25	7	0	9.396027	-4.248742	0.527974
26	6	0	-0.168454	2.054490	-0.988634
27	6	0	1.922329	1.186756	-0.846214
28	6	0	-0.057001	-0.176992	-0.629179
29	6	0	2.071543	-1.086698	0.067713
30	6	0	0.194409	-2.347817	-0.068988
31	7	0	-0.803721	0.898953	-0.809626
32	7	0	1.151138	2.218315	-1.186411
33	7	0	1.318902	-0.026291	-0.465951
34	7	0	-0.581604	-1.391241	-0.570619
35	7	0	1.454663	-2.229837	0.369883
36	7	0	3.254374	1.242804	-0.846079
37	6	0	3.888597	0.225449	-0.257240
38	7	0	3.373192	-0.890843	0.266788
39	6	0	-3.982823	4.076107	0.658107
40	6	0	-6.017061	2.760202	0.951151
41	6	0	-4.240881	1.956826	-0.514969
42	6	0	-6.021917	0.683143	0.046861
43	7	0	-6.533383	3.738690	1.677746
44	7	0	-4.507224	5.042102	1.394152
45	7	0	-4.742305	2.925960	0.371254
46	7	0	-6.649466	1.597372	0.787837
47	7	0	-4.922502	0.834088	-0.700023
48	7	0	-2.726701	4.132628	0.209982
49	6	0	-2.344997	3.164614	-0.625388
50	7	0	-3.073623	2.173191	-1.121966
51	6	0	1.497050	8.055396	-0.585701
52	6	0	-0.287400	6.654666	-1.495526

53	6	0	1.301007	5.728785	0.106792
54	6	0	-0.338185	4.496577	-0.820403
55	7	0	-0.775768	7.703160	-2.134928
56	7	0	0.972037	9.104548	-1.200942
57	7	0	0.837445	6.808809	-0.661551
58	7	0	-0.815844	5.432159	-1.632373
59	7	0	0.619085	4.584611	0.092193
60	7	0	2.660659	8.125275	0.061711
61	6	0	3.095641	6.987412	0.626526
62	7	0	2.424063	5.850017	0.799684
63	6	0	0.397477	-4.789618	-0.074110
64	6	0	2.340951	-5.697516	-0.766529
65	6	0	0.722877	-6.934791	0.573150
66	6	0	2.847279	-7.971035	-0.058340
67	6	0	1.198575	-9.111981	1.012698
68	7	0	-0.025401	-5.828207	0.641265
69	7	0	1.475838	-4.690766	-0.844120
70	7	0	1.970803	-6.864122	-0.079219
71	7	0	0.340232	-8.073973	1.124855
72	7	0	2.434466	-9.113367	0.470360
73	7	0	3.553138	-5.600913	-1.294014
74	6	0	4.384648	-6.607252	-1.031111
75	7	0	4.085483	-7.816817	-0.529445
76	6	0	-5.834168	-1.737953	-0.233130
77	6	0	-3.830609	-2.769908	-0.010801
78	6	0	-5.665827	-3.729480	-1.303454
79	6	0	-3.470109	-4.793573	-1.323497
80	6	0	-5.277720	-5.710652	-2.347453
81	7	0	-6.416299	-2.673179	-0.981694
82	7	0	-4.630034	-1.768427	0.346366
83	7	0	-4.318338	-3.756879	-0.887040
84	7	0	-6.145261	-4.727073	-2.028934
85	7	0	-3.961740	-5.781882	-2.052021
86	7	0	-2.577348	-2.855976	0.426967
87	6	0	-1.806419	-3.746033	-0.193532
88	7	0	-2.170260	-4.719325	-1.024172
89	7	0	-0.404591	-3.620605	0.005679
90	7	0	5.297749	0.346349	-0.170935
91	7	0	-0.961125	3.210316	-0.956546
92	7	0	5.744379	-6.412126	-1.235880
93	7	0	-6.609623	-0.586940	0.019717
94	7	0	4.429019	7.035790	1.013588
95	7	0	10.538200	4.772223	-1.167194
96	7	0	11.040899	-3.094977	1.617044
97	1	0	11.387849	-2.260630	2.060908
98	1	0	11.569608	-3.951595	1.626717
99	7	0	-0.689876	9.953353	-2.520481
100	1	0	-1.509022	9.834502	-3.093721
101	1	0	-0.244783	10.851153	-2.423464

102	7	0	-6.310839	5.838654	2.550531
103	1	0	-7.227247	5.716517	2.949217
104	1	0	-5.761202	6.659166	2.745816
105	6	0	9.815014	-3.084057	1.066204
106	6	0	-0.145014	8.880134	-1.923766
107	6	0	-5.764248	4.835050	1.843379
108	1	0	10.910046	5.704756	-1.092762
109	1	0	11.077142	4.024396	-1.571953
110	1	0	4.864282	7.925247	0.794659
111	1	0	6.299975	-7.210434	-0.948906
112	7	0	0.773342	-10.282410	1.517512
113	7	0	-5.781306	-6.737961	-3.051501
114	1	0	1.383648	-11.082577	1.489769
115	1	0	-0.130383	-10.328432	1.958842
116	1	0	-5.167669	-7.478683	-3.348875
117	1	0	-6.747871	-6.714996	-3.332604
118	6	0	-7.981289	-0.723376	0.252742
119	6	0	-8.687029	-1.377239	1.217540
120	8	0	-8.818489	-0.115787	-0.637160
121	6	0	-10.063540	-1.163938	0.911287
122	1	0	-8.266406	-1.927067	2.045855
123	6	0	-10.091658	-0.382367	-0.216476
124	1	0	-10.926280	-1.522418	1.451399
125	6	0	-11.157467	0.181392	-0.994531
126	6	0	-11.182592	0.962228	-2.120136
127	8	0	-12.433419	-0.082322	-0.574745
128	6	0	-12.563078	1.195014	-2.412249
129	1	0	-10.318451	1.317132	-2.660692
130	6	0	-13.274312	0.543016	-1.450612
131	1	0	-12.969696	1.771037	-3.230693
132	1	0	-14.328154	0.427111	-1.252348
133	6	0	-3.105510	0.019604	3.338784
134	9	0	-2.527412	0.716806	4.330879
135	17	0	-2.319220	0.455029	1.800880
136	17	0	-2.910603	-1.721084	3.695560
137	17	0	-4.847234	0.466798	3.299288

4. Site-B complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.263059	6.194599	-0.254083
2	6	0	-6.310492	5.818984	0.655415
3	6	0	-4.902328	4.034628	-0.223988
4	6	0	-6.894640	3.481669	1.067364
5	6	0	-5.469105	1.909287	0.272373
6	7	0	-4.037886	4.945330	-0.654821

7	7	0	-5.384377	6.702690	0.282286
8	7	0	-6.033449	4.443441	0.502434
9	7	0	-4.698834	2.737414	-0.431075
10	7	0	-6.531085	2.197570	1.021373
11	7	0	-7.452925	6.192444	1.212572
12	6	0	-8.252925	5.202411	1.661087
13	7	0	-8.013906	3.872732	1.654462
14	6	0	-6.077704	-0.460743	0.272924
15	6	0	-8.142235	-1.149725	-0.358613
16	6	0	-6.563520	-2.597815	0.804187
17	6	0	-8.722302	-3.480212	0.095573
18	6	0	-7.042142	-4.797780	0.870312
19	7	0	-5.744704	-1.560982	0.946183
20	7	0	-7.204400	-0.199381	-0.385313
21	7	0	-7.806691	-2.409236	0.177492
22	7	0	-6.212304	-3.813651	1.206581
23	7	0	-8.307814	-4.702190	0.433293
24	7	0	-9.354946	-0.951730	-0.849014
25	7	0	-9.944181	-3.255724	-0.363642
26	6	0	0.625692	1.321743	0.594026
27	6	0	-1.575777	0.782850	0.613955
28	6	0	0.138346	-0.789835	-0.042233
29	6	0	-2.176848	-1.344876	-0.452586
30	6	0	-0.512461	-2.873846	-0.623166
31	7	0	1.048436	0.157584	0.111467
32	7	0	-0.619068	1.634154	0.985388
33	7	0	-1.211889	-0.448606	0.040876
34	7	0	0.468130	-2.050080	-0.266372
35	7	0	-1.790177	-2.548383	-0.875817
36	7	0	-2.873858	1.036735	0.773396
37	6	0	-3.718585	0.194336	0.171708
38	7	0	-3.445850	-0.938925	-0.481416
39	6	0	4.798862	2.631357	-0.798882
40	6	0	6.528441	0.943331	-1.110889
41	6	0	4.582268	0.462974	0.287755
42	6	0	6.113195	-1.113324	-0.253406
43	7	0	7.248604	1.821275	-1.792145
44	7	0	5.526467	3.498336	-1.483381
45	7	0	5.297453	1.342048	-0.548217
46	7	0	6.915222	-0.325176	-0.970069
47	7	0	5.031711	-0.774405	0.457481
48	7	0	3.567812	2.929198	-0.379410
49	6	0	2.964847	2.029003	0.399193
50	7	0	3.461534	0.889641	0.868455
51	6	0	-0.026710	7.500825	1.024485
52	6	0	1.610301	5.766679	1.563494
53	6	0	-0.275148	5.259400	0.104364
54	6	0	1.227222	3.700055	0.724255
55	7	0	2.331042	6.660197	2.216417

56	7	0	0.713841	8.385594	1.672644
57	7	0	0.435657	6.172058	0.899224
58	7	0	1.942167	4.469420	1.537273
59	7	0	0.209887	4.030856	-0.061240
60	7	0	-1.224909	7.810641	0.527528
61	6	0	-1.887035	6.820735	-0.090527
62	7	0	-1.430213	5.618679	-0.436531
63	6	0	-1.157747	-5.243703	-0.672619
64	6	0	-3.153197	-5.890483	0.147157
65	6	0	-1.889483	-7.243434	-1.439664
66	6	0	-4.083657	-7.990798	-0.660161
67	6	0	-2.749291	-9.275387	-1.977945
68	7	0	-0.978826	-6.265177	-1.504097
69	7	0	-2.131006	-5.039631	0.205248
70	7	0	-3.042014	-7.037232	-0.655155
71	7	0	-1.749404	-8.375209	-2.108472
72	7	0	-3.911899	-9.133680	-1.307560
73	7	0	-4.280219	-5.653328	0.802144
74	6	0	-5.284827	-6.493351	0.557631
75	7	0	-5.231710	-7.688484	-0.052611
76	6	0	5.499775	-3.469358	-0.076335
77	6	0	3.366352	-4.091102	-0.507327
78	6	0	4.879321	-5.440613	0.853316
79	6	0	2.526598	-6.058347	0.661801
80	6	0	4.044032	-7.361412	1.736290
81	7	0	5.836971	-4.532474	0.652314
82	7	0	4.363609	-3.245787	-0.745576
83	7	0	3.587924	-5.188744	0.344919
84	7	0	5.103574	-6.547414	1.543466
85	7	0	2.764531	-7.160847	1.353374
86	7	0	2.157638	-3.914112	-1.036904
87	6	0	1.184752	-4.644062	-0.501285
88	7	0	1.292088	-5.709283	0.292680
89	7	0	-0.154703	-4.228736	-0.740165
90	7	0	-5.088726	0.548700	0.235986
91	7	0	1.608416	2.324207	0.698377
92	7	0	-6.570984	-6.107262	0.911337
93	7	0	6.480554	-2.467765	-0.200626
94	7	0	-3.223827	7.115735	-0.333314
95	7	0	-9.425282	5.586120	2.194946
96	7	0	-11.454712	-1.770879	-1.222140
97	1	0	-11.691423	-0.859708	-1.578904
98	1	0	-12.120157	-2.526197	-1.232563
99	7	0	2.646686	8.845503	2.800654
100	1	0	3.512942	8.554153	3.222758
101	1	0	2.346982	9.806120	2.828723
102	7	0	7.477412	3.955270	-2.581673
103	1	0	8.364315	3.669281	-2.962980
104	1	0	7.114178	4.881154	-2.739256

105	6	0	-10.203421	-2.001180	-0.789233
106	6	0	1.868662	7.930404	2.199979
107	6	0	6.725095	3.057826	-1.924455
108	1	0	-9.640405	6.567464	2.259001
109	1	0	-10.044256	4.888699	2.574362
110	1	0	-3.487756	8.030659	0.015525
111	1	0	-7.271893	-6.782825	0.627155
112	7	0	-2.567959	-10.449165	-2.606136
113	7	0	4.290130	-8.504185	2.398623
114	1	0	-3.294584	-11.145110	-2.571042
115	1	0	-1.730358	-10.593937	-3.145709
116	1	0	3.526626	-9.126450	2.607099
117	1	0	5.218768	-8.681956	2.744747
118	6	0	7.831826	-2.816951	-0.268669
119	6	0	8.537016	-3.616900	-1.117005
120	8	0	8.644662	-2.289495	0.692605
121	6	0	9.885846	-3.588532	-0.655315
122	1	0	8.136321	-4.147747	-1.967067
123	6	0	9.903796	-2.758282	0.437175
124	1	0	10.740362	-4.097285	-1.074291
125	6	0	10.947748	-2.310152	1.313563
126	6	0	10.963380	-1.478658	2.402569
127	8	0	12.209103	-2.776619	1.058156
128	6	0	12.322032	-1.429538	2.846280
129	1	0	10.107009	-0.974037	2.823183
130	6	0	13.030954	-2.229599	2.001897
131	1	0	12.716179	-0.872458	3.683713
132	1	0	14.071267	-2.506224	1.934450
133	6	0	2.463615	7.390466	-1.904718
134	9	0	2.375810	8.118105	-0.772118
135	17	0	0.805152	7.210018	-2.562153
136	17	0	3.170507	5.811563	-1.509649
137	17	0	3.500350	8.304361	-3.054318

5. Site-C complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.310224	6.450434	-0.913406
2	6	0	-7.377886	6.031336	-0.071215
3	6	0	-5.839995	4.266917	-0.751359
4	6	0	-7.864059	3.701028	0.483298
5	6	0	-6.324408	2.154459	-0.128192
6	7	0	-5.001739	5.190022	-1.208055
7	7	0	-6.479956	6.934803	-0.466570
8	7	0	-7.024911	4.665317	-0.110210
9	7	0	-5.561550	2.971515	-0.852935

10	7	0	-7.435257	2.438081	0.547855
11	7	0	-8.563130	6.381890	0.404842
12	6	0	-9.334221	5.384522	0.887261
13	7	0	-9.029100	4.072412	0.988331
14	6	0	-6.812208	-0.239944	0.007372
15	6	0	-8.807021	-1.076296	-0.668846
16	6	0	-7.211136	-2.365205	0.647610
17	6	0	-9.285855	-3.404176	-0.098156
18	6	0	-7.578112	-4.580197	0.829382
19	7	0	-6.454683	-1.278514	0.761148
20	7	0	-7.919312	-0.079670	-0.713594
21	7	0	-8.432023	-2.281770	-0.042441
22	7	0	-6.816360	-3.534023	1.138810
23	7	0	-8.825251	-4.579467	0.332576
24	7	0	-10.004258	-0.973869	-1.222434
25	7	0	-10.494679	-3.274385	-0.623717
26	6	0	-0.233351	1.918537	0.531195
27	6	0	-2.403008	1.264619	0.480160
28	6	0	-0.579964	-0.254744	0.022464
29	6	0	-2.838598	-0.954306	-0.474999
30	6	0	-1.092962	-2.399875	-0.466701
31	7	0	0.272763	0.746514	0.161241
32	7	0	-1.511781	2.189519	0.837291
33	7	0	-1.947881	0.020033	0.009724
34	7	0	-0.177145	-1.507746	-0.102066
35	7	0	-2.369396	-2.157439	-0.804744
36	7	0	-3.719048	1.457531	0.559143
37	6	0	-4.487018	0.534335	-0.026396
38	7	0	-4.123318	-0.619769	-0.592413
39	6	0	3.899211	3.390110	-0.816007
40	6	0	5.717545	1.776284	-0.983688
41	6	0	3.770218	1.276192	0.396893
42	6	0	5.400021	-0.244537	-0.002661
43	7	0	6.412540	2.646638	-1.697588
44	7	0	4.606474	4.253992	-1.526778
45	7	0	4.456595	2.141585	-0.476634
46	7	0	6.169787	0.541897	-0.756949
47	7	0	4.284096	0.079057	0.658074
48	7	0	2.641030	3.639799	-0.447996
49	6	0	2.069388	2.750953	0.364553
50	7	0	2.612936	1.672833	0.921171
51	6	0	-1.215502	8.072954	0.454476
52	6	0	0.459289	6.465957	1.224529
53	6	0	-1.309366	5.759272	-0.298126
54	6	0	0.230081	4.329384	0.513871
55	7	0	1.093936	7.439924	1.854017
56	7	0	-0.548079	9.042739	1.061738
57	7	0	-0.690168	6.762210	0.464455
58	7	0	0.857182	5.191185	1.307947

59	7	0	-0.758533	4.548372	-0.343803
60	7	0	-2.397827	8.284577	-0.125209
61	6	0	-2.980444	7.217116	-0.694835
62	7	0	-2.446200	6.019249	-0.927545
63	6	0	-1.608135	-4.800344	-0.408365
64	6	0	-3.607219	-5.503917	0.354588
65	6	0	-2.199115	-6.877545	-1.086153
66	6	0	-4.390599	-7.692910	-0.368952
67	6	0	-2.930619	-8.978106	-1.545456
68	7	0	-1.335552	-5.858585	-1.165186
69	7	0	-2.633840	-4.597642	0.408360
70	7	0	-3.398939	-6.687391	-0.371309
71	7	0	-1.970291	-8.036417	-1.679837
72	7	0	-4.130803	-8.859658	-0.939810
73	7	0	-4.775586	-5.289744	0.941774
74	6	0	-5.723440	-6.194312	0.701632
75	7	0	-5.580926	-7.417415	0.165801
76	6	0	4.915956	-2.613503	0.312943
77	6	0	2.837133	-3.382029	-0.148985
78	6	0	4.370060	-4.554902	1.346414
79	6	0	2.065573	-5.321085	1.110936
80	6	0	3.611106	-6.463847	2.319472
81	7	0	5.282768	-3.607218	1.120692
82	7	0	3.794425	-2.497110	-0.406595
83	7	0	3.087243	-4.411167	0.777692
84	7	0	4.629199	-5.601593	2.113790
85	7	0	2.338536	-6.363656	1.878262
86	7	0	1.640885	-3.307565	-0.728907
87	6	0	0.691311	-4.060351	-0.182686
88	7	0	0.828093	-5.068264	0.678120
89	7	0	-0.659065	-3.737096	-0.492729
90	7	0	-5.875480	0.816993	-0.049955
91	7	0	0.687187	2.980174	0.603319
92	7	0	-7.043258	-5.857445	0.972755
93	7	0	5.844571	-1.567355	0.154157
94	7	0	-4.316499	7.419739	-1.015732
95	7	0	-10.548912	5.742108	1.337710
96	7	0	-12.038248	-1.927961	-1.637596
97	1	0	-12.305045	-1.053861	-2.059862
98	1	0	-12.661983	-2.718123	-1.631242
99	7	0	1.268318	9.674378	2.296597
100	1	0	2.101522	9.454058	2.817091
101	1	0	0.914994	10.615854	2.248335
102	7	0	6.571648	4.742386	-2.591349
103	1	0	7.485603	4.477493	-2.921132
104	1	0	6.179577	5.644920	-2.804192
105	6	0	-10.798661	-2.063158	-1.136293
106	6	0	0.579365	8.681489	1.709529
107	6	0	5.836672	3.849537	-1.909106

108	1	0	-10.816015	6.712535	1.318859
109	1	0	-11.151254	5.041006	1.736669
110	1	0	-4.644483	8.342086	-0.750873
111	1	0	-7.694342	-6.585226	0.699142
112	7	0	-2.661517	-10.173693	-2.096210
113	7	0	3.895530	-7.547043	3.061612
114	1	0	-3.354354	-10.902981	-2.055355
115	1	0	-1.791696	-10.305088	-2.585937
116	1	0	3.161450	-8.200115	3.281279
117	1	0	4.818657	-7.648069	3.450757
118	6	0	7.214689	-1.841086	0.145769
119	6	0	7.981739	-2.697056	-0.587208
120	8	0	7.976246	-1.156069	1.047610
121	6	0	9.315962	-2.535190	-0.112719
122	1	0	7.630120	-3.350207	-1.371143
123	6	0	9.265975	-1.576054	0.866921
124	1	0	10.208172	-3.027910	-0.465700
125	6	0	10.267503	-0.931935	1.666061
126	6	0	10.209987	0.035046	2.635405
127	8	0	11.565216	-1.317066	1.461871
128	6	0	11.558113	0.260413	3.053875
129	1	0	9.312718	0.517151	2.992103
130	6	0	12.335096	-0.580511	2.315106
131	1	0	11.901554	0.956509	3.805154
132	1	0	13.396007	-0.768458	2.269287
133	6	0	10.967070	0.669194	-1.675387
134	17	0	11.582517	1.158599	-3.300159
135	17	0	11.789822	1.618903	-0.392223
136	17	0	9.205371	0.858725	-1.580664
137	9	0	11.285973	-0.621974	-1.497443

6. H_20 adsorbed Site-A complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.048755	-5.978402	0.883895
2	6	0	-6.954885	-5.405414	-0.212403
3	6	0	-5.309714	-3.769657	0.521342
4	6	0	-7.113766	-3.080307	-0.958541
5	6	0	-5.491182	-1.652785	-0.262699
6	7	0	-4.631334	-4.736985	1.127088
7	7	0	-6.211291	-6.366594	0.338374
8	7	0	-6.457554	-4.083959	-0.216524
9	7	0	-4.894168	-2.508661	0.577057
10	7	0	-6.546393	-1.875308	-1.040796
11	7	0	-8.112108	-5.662807	-0.800644
12	6	0	-8.707959	-4.627976	-1.431726

13	7	0	-8.248125	-3.365614	-1.575190
14	6	0	-5.702670	0.768431	-0.565075
15	6	0	-7.687091	1.827830	-0.291422
16	6	0	-5.729053	2.917301	-1.249892
17	6	0	-7.787925	4.183429	-0.935423
18	6	0	-5.808193	5.157151	-1.473519
19	7	0	-5.090255	1.752799	-1.223154
20	7	0	-6.939460	0.743365	-0.074343
21	7	0	-7.066520	2.975676	-0.823603
22	7	0	-5.116159	4.031787	-1.631937
23	7	0	-7.124953	5.296428	-1.251449
24	7	0	-8.975446	1.862878	0.008143
25	7	0	-9.085674	4.190796	-0.670178
26	6	0	0.576225	-2.089705	-0.018523
27	6	0	-1.462934	-1.171133	-0.322985
28	6	0	0.375662	0.042813	0.673181
29	6	0	-1.819998	1.025584	0.692252
30	6	0	0.051434	2.235707	1.090823
31	7	0	1.106997	-1.063434	0.632208
32	7	0	-0.618426	-2.163936	-0.613630
33	7	0	-0.970902	-0.028521	0.319935
34	7	0	0.893955	1.211612	1.006610
35	7	0	-1.289965	2.163947	1.134390
36	7	0	-2.750516	-1.190209	-0.673334
37	6	0	-3.504641	-0.231618	-0.135884
38	7	0	-3.135033	0.840498	0.560693
39	6	0	4.608578	-3.853155	1.293160
40	6	0	6.563455	-2.395269	1.349532
41	6	0	4.594952	-1.750508	0.056357
42	6	0	6.361261	-0.369321	0.355925
43	7	0	7.214421	-3.310504	2.049818
44	7	0	5.268941	-4.757056	1.998346
45	7	0	5.251045	-2.660931	0.906936
46	7	0	7.104252	-1.205239	1.079158
47	7	0	5.192338	-0.602624	-0.246499
48	7	0	3.323320	-4.015695	0.969933
49	6	0	2.794553	-3.103510	0.158448
50	7	0	3.388076	-2.057728	-0.413284
51	6	0	-1.028030	-8.097288	0.107848
52	6	0	0.891760	-6.719387	-0.537622
53	6	0	-0.961002	-5.741014	0.699848
54	6	0	0.814701	-4.519550	0.009968
55	7	0	1.484757	-7.793336	-1.029351
56	7	0	-0.402985	-9.166558	-0.358300
57	7	0	-0.366716	-6.849278	0.086948
58	7	0	1.431939	-5.501125	-0.639502
59	7	0	-0.303105	-4.587052	0.738264
60	7	0	-2.285891	-8.148382	0.551081
61	6	0	-2.811147	-6.992942	0.986514

62	7	0	-2.181813	-5.839665	1.207314
63	6	0	-0.238908	4.667624	0.945094
64	6	0	-1.949144	5.614313	-0.169237
65	6	0	-0.797646	6.736055	1.665286
66	6	0	-2.670930	7.829746	0.540303
67	6	0	-1.415033	8.872883	2.121800
68	7	0	-0.064795	5.628762	1.842206
69	7	0	-1.068949	4.618393	-0.087241
70	7	0	-1.806673	6.721897	0.682752
71	7	0	-0.609705	7.821723	2.394637
72	7	0	-2.441584	8.926007	1.247991
73	7	0	-2.972540	5.560494	-1.010458
74	6	0	-3.862266	6.546091	-0.907605
75	7	0	-3.727278	7.717462	-0.265406
76	6	0	6.075828	2.042690	0.117592
77	6	0	4.073538	2.928018	0.691203
78	6	0	5.668329	4.104233	-0.733402
79	6	0	3.439305	5.030942	-0.361959
80	6	0	5.050181	6.151308	-1.504988
81	7	0	6.503581	3.069728	-0.617793
82	7	0	4.964178	1.958920	0.857788
83	7	0	4.388849	4.013101	-0.146443
84	7	0	5.997319	5.193783	-1.409463
85	7	0	3.784351	6.116639	-1.036626
86	7	0	2.879885	2.883691	1.279513
87	6	0	1.984599	3.755876	0.834039
88	7	0	2.196846	4.841841	0.083052
89	7	0	0.615987	3.522109	1.119958
90	7	0	-4.910453	-0.376631	-0.336151
91	7	0	1.402044	-3.240529	-0.081653
92	7	0	-5.119394	6.366989	-1.473387
93	7	0	6.909300	0.916687	0.163659
94	7	0	-4.188191	-7.035251	1.162436
95	7	0	-9.896291	-4.888916	-2.000828
96	7	0	-10.938118	3.032399	0.000345
97	1	0	-11.376378	2.199793	0.358324
98	1	0	-11.459115	3.884126	-0.128316
99	7	0	1.464885	-10.057799	-1.327218
100	1	0	2.374406	-9.958845	-1.747760
101	1	0	1.010547	-10.954297	-1.267554
102	7	0	7.225091	-5.389709	2.997214
103	1	0	8.167149	-5.195625	3.294770
104	1	0	6.759096	-6.242796	3.259080
105	6	0	-9.614793	3.027793	-0.235179
106	6	0	0.825167	-8.963979	-0.882622
107	6	0	6.544214	-4.450377	2.319225
108	1	0	-10.273793	-5.820927	-1.951077
109	1	0	-10.370409	-4.158451	-2.506208
110	1	0	-4.585943	-7.936308	0.920688

111	1	0	-5.732505	7.157852	-1.307808
112	7	0	-1.170503	9.995626	2.817797
113	7	0	5.409067	7.272004	-2.154547
114	1	0	-1.759878	10.800093	2.679880
115	1	0	-0.433089	9.998437	3.503344
116	1	0	4.727376	7.999369	-2.294854
117	1	0	6.327450	7.330563	-2.562942
118	6	0	8.294722	1.049788	0.039270
119	6	0	9.224185	1.771365	0.726272
120	8	0	8.879161	0.333299	-0.965172
121	6	0	10.477918	1.488111	0.108855
122	1	0	9.029026	2.416850	1.568807
123	6	0	10.219620	0.599237	-0.904093
124	1	0	11.449896	1.872652	0.377182
125	6	0	11.052431	-0.072364	-1.860013
126	6	0	10.789247	-0.960335	-2.869962
127	8	0	12.394713	0.189500	-1.800222
128	6	0	12.050793	-1.265227	-3.470668
129	1	0	9.814803	-1.337877	-3.139864
130	6	0	12.984881	-0.545551	-2.788747
131	1	0	12.235193	-1.931405	-4.300852
132	1	0	14.055499	-0.444765	-2.871965
133	8	0	-2.095255	-2.331084	2.038505
134	1	0	-1.619924	-3.136186	1.777746
135	1	0	-3.002709	-2.507256	1.742433

7. H_20 adsorbed Site-B complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.852081	6.006260	1.056322
2	6	0	6.922864	5.457556	0.299085
3	6	0	5.217006	3.796115	0.814812
4	6	0	7.250199	3.122819	-0.349063
5	6	0	5.567790	1.679698	0.119104
6	7	0	4.429948	4.761868	1.271327
7	7	0	6.080818	6.412018	0.695738
8	7	0	6.461587	4.124190	0.252193
9	7	0	4.834203	2.523241	0.842576
10	7	0	6.727421	1.902199	-0.494441
11	7	0	8.155778	5.731025	-0.101866
12	6	0	8.867657	4.697761	-0.598355
13	7	0	8.464549	3.421035	-0.780876
14	6	0	5.868115	-0.745073	-0.070393
15	6	0	7.761937	-1.752016	0.661383
16	6	0	6.107333	-2.893044	-0.717712
17	6	0	8.063189	-4.107591	0.082674

18	6	0	6.295510	-5.129980	-0.913067
19	7	0	5.450040	-1.745219	-0.846021
20	7	0	6.960373	-0.684486	0.687392
21	7	0	7.308034	-2.917357	0.011476
22	7	0	5.631860	-4.021571	-1.232138
23	7	0	7.521970	-5.236477	-0.376885
24	7	0	8.944586	-1.754582	1.254420
25	7	0	9.260413	-4.083598	0.648990
26	6	0	-0.499086	1.892976	-0.872693
27	6	0	1.618732	1.102505	-0.714902
28	6	0	-0.316433	-0.326173	-0.493342
29	6	0	1.843524	-1.149597	0.228518
30	6	0	0.011373	-2.475570	0.111254
31	7	0	-1.097090	0.716535	-0.713118
32	7	0	0.814325	2.106418	-1.059588
33	7	0	1.054052	-0.123840	-0.318556
34	7	0	-0.796747	-1.559654	-0.414995
35	7	0	1.265838	-2.308677	0.547659
36	7	0	2.948292	1.203163	-0.718266
37	6	0	3.616404	0.216527	-0.116254
38	7	0	3.137742	-0.908437	0.424371
39	6	0	-4.285334	3.893543	0.903245
40	6	0	-6.228662	2.517248	1.420789
41	6	0	-4.522275	1.705358	-0.128329
42	6	0	-6.232151	0.408341	0.586957
43	7	0	-6.730660	3.514642	2.133189
44	7	0	-4.801086	4.887448	1.608220
45	7	0	-5.004791	2.700604	0.741858
46	7	0	-6.824030	1.326520	1.354283
47	7	0	-5.183781	0.563294	-0.232255
48	7	0	-3.062066	3.975888	0.375197
49	6	0	-2.673584	2.965675	-0.420342
50	7	0	-3.398085	1.926564	-0.808741
51	6	0	1.004176	7.942948	-0.523089
52	6	0	-0.703717	6.473203	-1.446811
53	6	0	0.862606	5.635821	0.210669
54	6	0	-0.712992	4.337467	-0.726579
55	7	0	-1.227645	7.494004	-2.100253
56	7	0	0.448350	8.968701	-1.151914
57	7	0	0.413419	6.669226	-0.620929
58	7	0	-1.187271	5.228283	-1.583315
59	7	0	0.203562	4.475672	0.217723
60	7	0	2.148600	8.065989	0.151943
61	6	0	2.604819	6.953617	0.745503
62	7	0	1.959513	5.803793	0.933931
63	6	0	0.281190	-4.910825	0.121074
64	6	0	2.246325	-5.754278	-0.593360
65	6	0	0.676984	-7.050562	0.748251
66	6	0	2.829028	-8.015273	0.095796

67	6	0	1.224286	-9.214579	1.169800
68	7	0	-0.104509	-5.968558	0.830270
69	7	0	1.350264	-4.774423	-0.657216
70	7	0	1.917847	-6.936600	0.088285
71	7	0	0.334067	-8.205301	1.294150
72	7	0	2.456021	-9.173483	0.619724
73	7	0	3.450866	-5.616444	-1.129301
74	6	0	4.315552	-6.597716	-0.879268
75	7	0	4.058313	-7.819212	-0.382854
76	6	0	-6.020794	-2.005302	0.298834
77	6	0	-3.985221	-2.989464	0.396486
78	6	0	-5.870599	-3.982712	-0.796331
79	6	0	-3.657095	-4.997187	-0.948431
80	6	0	-5.498941	-5.946917	-1.877397
81	7	0	-6.625617	-2.945468	-0.423538
82	7	0	-4.786617	-2.010186	0.808605
83	7	0	-4.501504	-3.982177	-0.457109
84	7	0	-6.368695	-4.985061	-1.501555
85	7	0	-4.167670	-5.990960	-1.656595
86	7	0	-2.707134	-3.046566	0.759356
87	6	0	-1.954650	-3.921053	0.092669
88	7	0	-2.344674	-4.897693	-0.721026
89	7	0	-0.548384	-3.765871	0.219773
90	7	0	5.020992	0.384566	-0.032454
91	7	0	-1.320990	3.031940	-0.821482
92	7	0	5.666673	-6.358738	-1.093136
93	7	0	-6.801992	-0.867977	0.605825
94	7	0	3.932823	7.044644	1.151719
95	7	0	10.128588	4.974596	-0.972857
96	7	0	10.876076	-2.879549	1.727380
97	1	0	11.200816	-2.034222	2.167244
98	1	0	11.431051	-3.719403	1.733383
99	7	0	-1.229125	9.745348	-2.495748
100	1	0	-2.021350	9.587592	-3.096387
101	1	0	-0.813539	10.658009	-2.407494
102	7	0	-6.543727	5.673337	2.862287
103	1	0	-7.413188	5.531619	3.350321
104	1	0	-6.011048	6.519325	2.983753
105	6	0	9.647146	-2.906179	1.183800
106	6	0	-0.647142	8.696811	-1.887195
107	6	0	-6.007513	4.652986	2.173179
108	1	0	10.471801	5.917362	-0.890581
109	1	0	10.692438	4.245398	-1.377557
110	1	0	4.342766	7.945966	0.932459
111	1	0	6.249572	-7.139636	-0.812558
112	7	0	0.839751	-10.401263	1.669646
113	7	0	-6.019212	-6.979323	-2.561280
114	1	0	1.475097	-11.181305	1.632892
115	1	0	-0.059088	-10.478795	2.116450

116	1	0	-5.407582	-7.704451	-2.898662
117	1	0	-7.000373	-6.975667	-2.787362
118	6	0	-8.162222	-1.019912	0.890309
119	6	0	-8.827727	-1.712845	1.856473
120	8	0	-9.035971	-0.390332	0.051988
121	6	0	-10.215903	-1.501356	1.607288
122	1	0	-8.374403	-2.289825	2.648154
123	6	0	-10.291129	-0.681673	0.509205
124	1	0	-11.055508	-1.886180	2.165405
125	6	0	-11.388626	-0.099328	-0.208606
126	6	0	-11.460782	0.720418	-1.304153
127	8	0	-12.646269	-0.387672	0.248427
128	6	0	-12.852645	0.952336	-1.536683
129	1	0	-10.619918	1.100814	-1.863761
130	6	0	-13.523238	0.261232	-0.573143
131	1	0	-13.293299	1.553369	-2.318691
132	1	0	-14.568197	0.129854	-0.340504
133	8	0	-1.978488	6.690165	1.066652
134	1	0	-2.719864	7.093534	0.598102
135	1	0	-2.245704	5.755246	1.096573

8. H_20 adsorbed Site-C complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.816467	6.227422	0.924757
2	6	0	6.863593	5.718699	0.081933
3	6	0	5.235696	4.023240	0.726364
4	6	0	7.231547	3.376825	-0.514092
5	6	0	5.613655	1.900215	0.066830
6	7	0	4.443458	4.979483	1.196603
7	7	0	6.011015	6.659645	0.490304
8	7	0	6.441400	4.371981	0.095472
9	7	0	4.891339	2.742288	0.804264
10	7	0	6.738709	2.138918	-0.602980
11	7	0	8.067043	6.016500	-0.384184
12	6	0	8.787795	4.989648	-0.882564
13	7	0	8.415784	3.697149	-1.009381
14	6	0	5.978825	-0.514637	-0.095361
15	6	0	7.928074	-1.454706	0.577488
16	6	0	6.267929	-2.655729	-0.742700
17	6	0	8.287253	-3.801919	-0.001499
18	6	0	6.521646	-4.886156	-0.932862
19	7	0	5.568585	-1.530896	-0.852950
20	7	0	7.092676	-0.414097	0.625928
21	7	0	7.491702	-2.637225	-0.052810

22	7	0	5.813634	-3.801341	-1.237362
23	7	0	7.767634	-4.950436	-0.436952
24	7	0	9.128974	-1.415493	1.131184
25	7	0	9.501108	-3.735906	0.524492
26	6	0	-0.490419	1.955470	-0.614759
27	6	0	1.649618	1.208811	-0.560352
28	6	0	-0.239290	-0.246353	-0.173053
29	6	0	1.979337	-1.035276	0.377293
30	6	0	0.173553	-2.403587	0.351718
31	7	0	-1.050249	0.785833	-0.322670
32	7	0	0.803735	2.182474	-0.895312
33	7	0	1.137066	-0.023334	-0.115604
34	7	0	-0.691611	-1.486156	-0.069387
35	7	0	1.451477	-2.213189	0.710941
36	7	0	2.974162	1.342156	-0.631450
37	6	0	3.696398	0.377373	-0.055804
38	7	0	3.276657	-0.760941	0.504093
39	6	0	-4.426244	3.724073	0.993675
40	6	0	-6.318329	2.226646	1.345580
41	6	0	-4.516539	1.572948	-0.157909
42	6	0	-6.194515	0.165903	0.413778
43	7	0	-6.901360	3.162691	2.077135
44	7	0	-5.024327	4.652768	1.719111
45	7	0	-5.081267	2.501319	0.736833
46	7	0	-6.860823	1.017955	1.196584
47	7	0	-5.118809	0.403399	-0.342754
48	7	0	-3.184229	3.878703	0.529481
49	6	0	-2.727675	2.931349	-0.290954
50	7	0	-3.379614	1.880031	-0.777059
51	6	0	0.820729	8.053179	-0.456654
52	6	0	-0.918830	6.531688	-1.253465
53	6	0	0.790608	5.736779	0.293710
54	6	0	-0.811052	4.389115	-0.535314
55	7	0	-1.495495	7.535563	-1.891111
56	7	0	0.209412	9.055643	-1.069912
57	7	0	0.232022	6.769647	-0.476099
58	7	0	-1.379862	5.278096	-1.341648
59	7	0	0.177231	4.555274	0.333092
60	7	0	2.005198	8.205061	0.136824
61	6	0	2.528759	7.108539	0.708184
62	7	0	1.932532	5.938980	0.934944
63	6	0	0.546935	-4.828653	0.316228
64	6	0	2.509219	-5.621081	-0.458167
65	6	0	1.031521	-6.944935	0.958807
66	6	0	3.183291	-7.855777	0.234215
67	6	0	1.658208	-9.085797	1.386844
68	7	0	0.220492	-5.885619	1.054530
69	7	0	1.582338	-4.667762	-0.499440
70	7	0	2.241739	-6.803454	0.249611

71	7	0	0.744357	-8.100810	1.533178
72	7	0	2.865232	-9.016827	0.786999
73	7	0	3.687767	-5.455769	-1.041332
74	6	0	4.589417	-6.409292	-0.814394
75	7	0	4.386731	-7.631221	-0.295076
76	6	0	-5.874055	-2.233578	0.103054
77	6	0	-3.812141	-3.127794	0.371550
78	6	0	-5.547811	-4.203637	-0.967513
79	6	0	-3.282938	-5.110524	-0.945567
80	6	0	-5.000787	-6.150520	-2.005112
81	7	0	-6.376524	-3.202659	-0.659986
82	7	0	-4.685243	-2.184659	0.712001
83	7	0	-4.210994	-4.139497	-0.521947
84	7	0	-5.941165	-5.229724	-1.704853
85	7	0	-3.689236	-6.130001	-1.684194
86	7	0	-2.566181	-3.129933	0.839060
87	6	0	-1.720623	-3.948063	0.217997
88	7	0	-1.997703	-4.940066	-0.625444
89	7	0	-0.332737	-3.715425	0.423544
90	7	0	5.097633	0.588707	-0.033151
91	7	0	-1.352406	3.065646	-0.621581
92	7	0	5.924132	-6.134476	-1.082398
93	7	0	-6.720713	-1.132179	0.340508
94	7	0	3.871329	7.243024	1.038429
95	7	0	10.021223	5.292291	-1.322165
96	7	0	11.111265	-2.474153	1.543529
97	1	0	11.422090	-1.616823	1.970030
98	1	0	11.693165	-3.295581	1.535066
99	7	0	-1.556167	9.777026	-2.329018
100	1	0	-2.393251	9.598895	-2.859341
101	1	0	-1.160611	10.700940	-2.270013
102	7	0	-6.880562	5.294070	2.906923
103	1	0	-7.784933	5.067758	3.330098
104	1	0	-6.403754	6.166025	3.070838
105	6	0	9.866517	-2.543765	1.041498
106	6	0	-0.924398	8.750960	-1.735040
107	6	0	-6.246440	4.347676	2.210176
108	1	0	10.338504	6.246875	-1.283048
109	1	0	10.588785	4.568263	-1.731045
110	1	0	4.244814	8.150874	0.783840
111	1	0	6.539192	-6.895390	-0.815787
112	7	0	1.329067	-10.275523	1.917626
113	7	0	-5.418097	-7.209825	-2.718240
114	1	0	1.985823	-11.036881	1.867323
115	1	0	0.452133	-10.371999	2.402719
116	1	0	-4.748645	-7.905206	-3.004494
117	1	0	-6.377915	-7.252969	-3.019333
118	6	0	-8.094966	-1.327828	0.498164
119	6	0	-8.826326	-2.087625	1.361374

120	8	0	-8.908043	-0.652764	-0.365718
121	6	0	-10.192894	-1.872563	1.014876
122	1	0	-8.430422	-2.710493	2.148941
123	6	0	-10.192214	-0.982751	-0.029740
124	1	0	-11.068639	-2.300302	1.478252
125	6	0	-11.236024	-0.358102	-0.790614
126	6	0	-11.230344	0.532033	-1.832521
127	8	0	-12.522865	-0.676139	-0.449288
128	6	0	-12.602200	0.778113	-2.153333
129	1	0	-10.352035	0.947444	-2.302628
130	6	0	-13.339483	0.024903	-1.290374
131	1	0	-12.986189	1.428325	-2.925840
132	1	0	-14.398166	-0.122741	-1.146508
133	8	0	-9.164798	3.789624	3.655076
134	1	0	-8.551467	3.196934	3.172618
135	1	0	-9.906541	3.898453	3.046135

9. H_20-CFC-11 co-adsorbed Site-A complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.446137	-5.879791	0.960621
2	6	0	-7.496173	-5.227119	0.231364
3	6	0	-5.693194	-3.656761	0.700658
4	6	0	-7.707870	-2.883899	-0.432910
5	6	0	-5.936435	-1.534215	-0.018701
6	7	0	-4.953476	-4.659619	1.157877
7	7	0	-6.698797	-6.222919	0.621186
8	7	0	-6.963634	-3.921577	0.163606
9	7	0	-5.237720	-2.408357	0.702346
10	7	0	-7.120594	-1.695883	-0.602856
11	7	0	-8.748903	-5.436529	-0.143858
12	6	0	-9.413975	-4.369587	-0.635480
13	7	0	-8.945244	-3.118504	-0.837273
14	6	0	-6.096267	0.903289	-0.164751
15	6	0	-7.877253	1.990830	0.722515
16	6	0	-6.249625	3.082894	-0.726380
17	6	0	-8.067003	4.381174	0.251558
18	6	0	-6.314549	5.333962	-0.835980
19	7	0	-5.673022	1.903997	-0.936789
20	7	0	-7.142379	0.877969	0.658338
21	7	0	-7.394245	3.151584	0.085885
22	7	0	-5.743030	4.200783	-1.235883
23	7	0	-7.489380	5.492920	-0.206248
24	7	0	-9.017071	2.039922	1.392381
25	7	0	-9.222517	4.407063	0.898016

26	6	0	0.069675	-2.126698	-1.231044
27	6	0	-1.998457	-1.220116	-1.018622
28	6	0	0.008002	0.120749	-0.997835
29	6	0	-2.051710	1.075382	-0.159140
30	6	0	-0.168603	2.297231	-0.441402
31	7	0	0.726791	-0.968870	-1.204172
32	7	0	-1.262958	-2.281827	-1.340732
33	7	0	-1.352702	-0.006265	-0.719174
34	7	0	0.549685	1.330793	-1.006498
35	7	0	-1.394630	2.209200	0.086839
36	7	0	-3.331122	-1.244368	-0.952081
37	6	0	-3.911325	-0.198392	-0.357434
38	7	0	-3.341034	0.911192	0.122761
39	6	0	3.753299	-4.235920	0.636464
40	6	0	5.805232	-2.977429	1.045101
41	6	0	4.136004	-2.123401	-0.515060
42	6	0	5.933876	-0.909649	0.125733
43	7	0	6.249831	-3.968421	1.801796
44	7	0	4.208223	-5.215833	1.400161
45	7	0	4.559099	-3.106225	0.396510
46	7	0	6.482972	-1.836706	0.912476
47	7	0	4.869222	-1.030882	-0.676530
48	7	0	2.525398	-4.260794	0.115048
49	6	0	2.208937	-3.272317	-0.726057
50	7	0	2.987015	-2.295654	-1.171484
51	6	0	-1.729184	-8.070127	-0.630956
52	6	0	0.053087	-6.719130	-1.614801
53	6	0	-1.451143	-5.745269	0.039854
54	6	0	0.183964	-4.561496	-0.952326
55	7	0	0.492156	-7.782207	-2.265023
56	7	0	-1.251719	-9.135715	-1.256612
57	7	0	-1.042610	-6.840540	-0.738340
58	7	0	0.606739	-5.510240	-1.777648
59	7	0	-0.741050	-4.618623	-0.005611
60	7	0	-2.871345	-8.106953	0.056028
61	6	0	-3.259257	-6.954717	0.625775
62	7	0	-2.553173	-5.834205	0.770553
63	6	0	-0.256129	4.742810	-0.409462
64	6	0	-2.224811	5.727721	-0.904460
65	6	0	-0.444989	6.904021	0.272247
66	6	0	-2.592949	8.003382	-0.118978
67	6	0	-0.808520	9.086061	0.784597
68	7	0	0.273820	5.774972	0.256766
69	7	0	-1.405265	4.694673	-1.070868
70	7	0	-1.753260	6.874405	-0.245350
71	7	0	0.028097	8.022387	0.792193
72	7	0	-2.094734	9.125994	0.378002
73	7	0	-3.481875	5.674200	-1.314310
74	6	0	-4.257482	6.695215	-0.952045

75	7	0	-3.876817	7.886577	-0.460380
76	6	0	5.859099	1.510205	-0.209743
77	6	0	3.872286	2.589407	-0.174000
78	6	0	5.822064	3.481153	-1.327654
79	6	0	3.653006	4.558601	-1.589527
80	6	0	5.558641	5.439512	-2.447302
81	7	0	6.521300	2.414542	-0.926652
82	7	0	4.618414	1.586521	0.280288
83	7	0	4.444419	3.535201	-1.038263
84	7	0	6.381329	4.457390	-2.023509
85	7	0	4.217596	5.515932	-2.300733
86	7	0	2.589549	2.707830	0.155531
87	6	0	1.894491	3.590109	-0.557382
88	7	0	2.325644	4.492677	-1.424169
89	7	0	0.481258	3.545143	-0.383345
90	7	0	-5.317000	-0.274815	-0.205014
91	7	0	0.840957	-3.290086	-1.120011
92	7	0	-5.632271	6.533439	-1.028265
93	7	0	6.572849	0.334893	0.112955
94	7	0	-4.581500	-6.966582	1.052850
95	7	0	-10.694981	-4.580514	-0.982295
96	7	0	-10.838661	3.259783	2.035905
97	1	0	-11.188272	2.418069	2.463518
98	1	0	-11.338245	4.130682	2.109549
99	7	0	0.340530	-10.032456	-2.629544
100	1	0	1.141384	-9.936743	-3.232262
101	1	0	-0.120513	-10.919292	-2.508838
102	7	0	5.916956	-6.058266	2.663089
103	1	0	6.812521	-5.961620	3.112864
104	1	0	5.335189	-6.863779	2.824698
105	6	0	-9.648304	3.233993	1.412842
106	6	0	-0.157174	-8.943014	-2.021559
107	6	0	5.441524	-5.042077	1.923159
108	1	0	-11.087021	-5.502616	-0.884811
109	1	0	-11.226831	-3.825182	-1.382535
110	1	0	-5.043930	-7.847588	0.856394
111	1	0	-6.144622	7.335421	-0.678295
112	7	0	-0.298213	10.235449	1.254550
113	7	0	6.138427	6.451394	-3.113179
114	1	0	-0.881298	11.055371	1.292955
115	1	0	0.652142	10.253002	1.587205
116	1	0	5.567207	7.204480	-3.459545
117	1	0	7.133767	6.436392	-3.263653
118	6	0	7.930223	0.424405	0.436259
119	6	0	8.596335	1.095380	1.417312
120	8	0	8.798744	-0.254241	-0.367726
121	6	0	9.980229	0.816349	1.214783
122	1	0	8.145053	1.702245	2.187571
123	6	0	10.051279	-0.017300	0.127032

124	1	0	10.819059	1.167360	1.795908
125	6	0	11.142365	-0.657753	-0.549989
126	6	0	11.210207	-1.494902	-1.632552
127	8	0	12.397671	-0.419182	-0.058881
128	6	0	12.596685	-1.791270	-1.820247
129	1	0	10.369902	-1.845654	-2.211991
130	6	0	13.268776	-1.117501	-0.845604
131	1	0	13.032932	-2.421995	-2.581091
132	1	0	14.311212	-1.029322	-0.583162
133	6	0	2.769534	-0.056565	3.145690
134	9	0	2.093158	-0.717333	4.098828
135	17	0	2.077654	-0.476638	1.560110
136	17	0	2.618332	1.696705	3.480112
137	17	0	4.488277	-0.570585	3.233902
138	8	0	3.166855	5.527296	1.293032
139	1	0	2.914461	4.818889	1.898291
140	1	0	2.307618	5.862449	0.982499

10. H_20-CFC-11 co-adsorbed Site-B complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.212143	6.160794	0.254168
2	6	0	6.214945	5.825521	-0.765697
3	6	0	4.835584	4.002979	0.068828
4	6	0	6.767514	3.508148	-1.325332
5	6	0	5.379071	1.891508	-0.542536
6	7	0	3.993899	4.889218	0.587027
7	7	0	5.312128	6.691086	-0.301491
8	7	0	5.937566	4.443950	-0.674182
9	7	0	4.627439	2.698660	0.216989
10	7	0	6.405617	2.223591	-1.319775
11	7	0	7.330541	6.223439	-1.356255
12	6	0	8.101550	5.255687	-1.897271
13	7	0	7.856380	3.927816	-1.947026
14	6	0	5.988935	-0.478802	-0.641358
15	6	0	8.109053	-1.173062	-0.243383
16	6	0	6.384453	-2.642410	-1.141328
17	6	0	8.609658	-3.524821	-0.681895
18	6	0	6.831203	-4.849780	-1.170458
19	7	0	5.565404	-1.599920	-1.225415
20	7	0	7.189326	-0.211879	-0.132472
21	7	0	7.699468	-2.446266	-0.687244
22	7	0	5.972066	-3.869604	-1.437659
23	7	0	8.145379	-4.753350	-0.913132
24	7	0	9.376011	-0.972201	0.081139
25	7	0	9.882399	-3.298112	-0.393418

26	6	0	-0.683136	1.347911	-0.455705
27	6	0	1.486455	0.755461	-0.642463
28	6	0	-0.164463	-0.665988	0.405609
29	6	0	2.159068	-1.269669	0.554071
30	6	0	0.495659	-2.735374	1.014412
31	7	0	-1.063261	0.298558	0.260521
32	7	0	0.502675	1.571966	-1.029616
33	7	0	1.164052	-0.400982	0.078721
34	7	0	-0.498199	-1.875204	0.819958
35	7	0	1.805067	-2.440842	1.079818
36	7	0	2.764772	0.958662	-0.965568
37	6	0	3.645705	0.178841	-0.338734
38	7	0	3.430447	-0.883064	0.434411
39	6	0	-4.949777	2.528472	0.731154
40	6	0	-6.649467	0.792135	0.904711
41	6	0	-4.599566	0.379005	-0.361265
42	6	0	-6.128189	-1.238686	0.045492
43	7	0	-7.433360	1.637787	1.555347
44	7	0	-5.738094	3.361614	1.390040
45	7	0	-5.394650	1.229963	0.431193
46	7	0	-6.996485	-0.482245	0.715449
47	7	0	-5.007503	-0.865801	-0.579555
48	7	0	-3.708904	2.873074	0.381574
49	6	0	-3.033210	2.003164	-0.368407
50	7	0	-3.454036	0.840340	-0.859431
51	6	0	-0.069072	7.531788	-0.764451
52	6	0	-1.722058	5.816932	-1.333368
53	6	0	0.224850	5.246762	0.009014
54	6	0	-1.306896	3.705455	-0.619066
55	7	0	-2.467875	6.740604	-1.910013
56	7	0	-0.839126	8.445421	-1.330366
57	7	0	-0.521371	6.194905	-0.697483
58	7	0	-2.051405	4.519718	-1.357129
59	7	0	-0.241969	4.007621	0.127256
60	7	0	1.148946	7.819016	-0.300389
61	6	0	1.838855	6.800607	0.232928
62	7	0	1.398506	5.578033	0.526955
63	6	0	1.174620	-5.092353	1.083873
64	6	0	3.053127	-5.829955	0.088557
65	6	0	2.033637	-6.980462	1.982483
66	6	0	4.098341	-7.835021	0.993744
67	6	0	2.972458	-8.945022	2.626693
68	7	0	1.125712	-5.998037	2.051737
69	7	0	2.021210	-4.988309	0.069199
70	7	0	3.061737	-6.876407	1.025363
71	7	0	1.998066	-8.022759	2.793886
72	7	0	4.024612	-8.896024	1.783701
73	7	0	4.083386	-5.674013	-0.731103
74	6	0	5.116779	-6.489442	-0.528255

75	7	0	5.150357	-7.613623	0.205183
76	6	0	-5.460384	-3.583743	-0.007461
77	6	0	-3.354245	-4.090294	0.648881
78	6	0	-4.715785	-5.614996	-0.684818
79	6	0	-2.375722	-6.142627	-0.224872
80	6	0	-3.767225	-7.592868	-1.281819
81	7	0	-5.706331	-4.720462	-0.659542
82	7	0	-4.389938	-3.264511	0.729142
83	7	0	-3.478305	-5.275143	-0.098954
84	7	0	-4.855469	-6.793326	-1.271304
85	7	0	-2.531947	-7.319789	-0.810364
86	7	0	-2.195093	-3.811111	1.240645
87	6	0	-1.164014	-4.561619	0.872410
88	7	0	-1.187232	-5.722762	0.209855
89	7	0	0.143915	-4.089635	1.148039
90	7	0	5.014983	0.534991	-0.523074
91	7	0	-1.680303	2.342288	-0.619800
92	7	0	6.347124	-6.151983	-1.079742
93	7	0	-6.463582	-2.604911	-0.054276
94	7	0	3.184965	7.080520	0.435974
95	7	0	9.245798	5.663819	-2.470267
96	7	0	11.501142	-1.801489	0.208645
97	1	0	11.787683	-0.882225	0.502439
98	1	0	12.156505	-2.564254	0.162689
99	7	0	-2.814884	8.952474	-2.359140
100	1	0	-3.697763	8.679769	-2.758979
101	1	0	-2.523898	9.916100	-2.339648
102	7	0	-7.759986	3.743584	2.384221
103	1	0	-8.658262	3.425438	2.709345
104	1	0	-7.428071	4.671767	2.589758
105	6	0	10.202584	-2.032584	-0.050195
106	6	0	-2.011211	8.011393	-1.839713
107	6	0	-6.948579	2.881762	1.749984
108	1	0	9.465658	6.646122	-2.489285
109	1	0	9.844305	4.984782	-2.911222
110	1	0	3.438928	8.014085	0.131775
111	1	0	7.073984	-6.816077	-0.836012
112	7	0	2.888085	-10.035427	3.406860
113	7	0	-3.932411	-8.804593	-1.839314
114	1	0	3.604531	-10.740388	3.349377
115	1	0	2.136860	-10.105912	4.073526
116	1	0	-3.141731	-9.422967	-1.916444
117	1	0	-4.821889	-9.040345	-2.247884
118	6	0	-7.808955	-2.965425	-0.164190
119	6	0	-8.612548	-3.792392	0.561927
120	8	0	-8.497343	-2.402959	-1.200118
121	6	0	-9.893322	-3.745049	-0.062978
122	1	0	-8.319115	-4.356552	1.433778
123	6	0	-9.778230	-2.877029	-1.119465

124	1	0	-10.791636	-4.267145	0.228654
125	6	0	-10.705415	-2.394952	-2.102328
126	6	0	-10.587000	-1.522212	-3.152170
127	8	0	-11.987264	-2.869126	-2.025607
128	6	0	-11.879286	-1.454208	-3.760924
129	1	0	-9.686368	-1.003106	-3.442569
130	6	0	-12.685921	-2.285132	-3.043731
131	1	0	-12.166888	-0.864985	-4.619463
132	1	0	-13.725437	-2.562880	-3.118320
133	6	0	-2.520840	7.162506	2.218186
134	9	0	-2.446710	7.976865	1.143703
135	17	0	-0.848759	6.910060	2.817630
136	17	0	-3.255607	5.628709	1.712063
137	17	0	-3.516405	7.994453	3.459525
138	8	0	1.823926	2.182295	1.631472
139	1	0	1.229457	2.872128	1.294671
140	1	0	2.699478	2.490751	1.348436

11. H_20-CFC-11 co-adsorbed Site-C complex optimized coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.943836	6.428957	1.130825
2	6	0	7.151314	6.090032	0.717579
3	6	0	5.559614	4.266062	0.999976
4	6	0	7.805440	3.796688	0.179372
5	6	0	6.222156	2.191775	0.411945
6	7	0	4.617291	5.151277	1.304786
7	7	0	6.165769	6.956826	0.955908
8	7	0	6.837732	4.716755	0.630615
9	7	0	5.305642	2.962861	0.997121
10	7	0	7.434971	2.529694	-0.020491
11	7	0	8.397804	6.484913	0.507351
12	6	0	9.278411	5.525491	0.150964
13	7	0	9.036974	4.214213	-0.065175
14	6	0	6.793093	-0.188203	0.280026
15	6	0	8.670035	-1.006924	1.249716
16	6	0	7.334147	-2.290250	-0.335372
17	6	0	9.293212	-3.305445	0.700149
18	6	0	7.780918	-4.492020	-0.510960
19	7	0	6.583560	-1.213320	-0.545353
20	7	0	7.762937	-0.029445	1.176640
21	7	0	8.428958	-2.200989	0.540976
22	7	0	7.047839	-3.453999	-0.907524
23	7	0	8.937606	-4.476488	0.171245
24	7	0	9.761347	-0.896079	1.989274
25	7	0	10.401784	-3.164760	1.411806

26	6	0	0.335237	1.732200	-1.365443
27	6	0	2.489840	1.189275	-0.917788
28	6	0	0.719502	-0.454625	-0.958568
29	6	0	2.835649	-1.018836	0.083905
30	6	0	1.193947	-2.542186	-0.243892
31	7	0	-0.130724	0.487501	-1.326381
32	7	0	1.629618	2.100702	-1.363231
33	7	0	2.017468	-0.093380	-0.584656
34	7	0	0.374267	-1.736233	-0.912455
35	7	0	2.352420	-2.232438	0.349222
36	7	0	3.791094	1.436763	-0.753892
37	6	0	4.477683	0.533162	-0.053299
38	7	0	4.058020	-0.633543	0.444999
39	6	0	-3.745891	3.464208	0.041840
40	6	0	-5.533848	1.923608	0.627871
41	6	0	-3.699439	1.177349	-0.778431
42	6	0	-5.292846	-0.236834	-0.019885
43	7	0	-6.168065	2.907934	1.248829
44	7	0	-4.398590	4.448201	0.646456
45	7	0	-4.341710	2.195284	-0.061343
46	7	0	-5.993244	0.673270	0.663471
47	7	0	-4.234331	-0.035820	-0.809353
48	7	0	-2.515723	3.632046	-0.438058
49	6	0	-1.974475	2.590559	-1.083988
50	7	0	-2.550247	1.439881	-1.397927
51	6	0	1.238225	7.893277	-1.117516
52	6	0	-0.176845	6.212320	-2.183574
53	6	0	1.158833	5.626954	-0.227321
54	6	0	-0.141426	4.135078	-1.295637
55	7	0	-0.640133	7.133421	-3.009145
56	7	0	0.730349	8.815360	-1.922233
57	7	0	0.742833	6.572167	-1.180122
58	7	0	-0.543256	4.926541	-2.279465
59	7	0	0.609750	4.412886	-0.239559
60	7	0	2.245226	8.158780	-0.285648
61	6	0	2.688218	7.131898	0.457475
62	7	0	2.114554	5.942768	0.635952
63	6	0	1.699848	-4.935211	-0.168664
64	6	0	3.812573	-5.552202	-0.663208
65	6	0	2.252245	-7.032845	0.483303
66	6	0	4.556165	-7.750031	0.074847
67	6	0	2.979576	-9.133941	0.949589
68	7	0	1.355053	-6.042239	0.485271
69	7	0	2.829318	-4.673885	-0.823090
70	7	0	3.540108	-6.775647	-0.031104
71	7	0	1.977313	-8.228269	0.978661
72	7	0	4.254458	-8.950968	0.545475
73	7	0	5.049033	-5.275465	-1.055750
74	6	0	5.980213	-6.162972	-0.714223

75	7	0	5.803359	-7.414042	-0.257855
76	6	0	-4.852038	-2.628068	-0.196663
77	6	0	-2.735461	-3.413604	-0.065666
78	6	0	-4.505055	-4.599170	-1.258137
79	6	0	-2.202522	-5.399026	-1.379294
80	6	0	-3.936365	-6.529201	-2.314392
81	7	0	-5.358739	-3.632917	-0.907668
82	7	0	-3.629879	-2.511075	0.326200
83	7	0	-3.145341	-4.463849	-0.908004
84	7	0	-4.898433	-5.653521	-1.954342
85	7	0	-2.608892	-6.442560	-2.083437
86	7	0	-1.461248	-3.343342	0.308996
87	6	0	-0.623336	-4.162375	-0.325353
88	7	0	-0.907958	-5.177953	-1.134049
89	7	0	0.758214	-3.883208	-0.153106
90	7	0	5.836553	0.850460	0.205274
91	7	0	-0.605856	2.771670	-1.397516
92	7	0	7.313783	-5.776943	-0.769156
93	7	0	-5.737748	-1.558189	0.073930
94	7	0	3.921340	7.371338	1.052702
95	7	0	10.548605	5.926879	-0.027275
96	7	0	11.729987	-1.816993	2.693364
97	1	0	11.902984	-0.951009	3.176695
98	1	0	12.367868	-2.592557	2.764136
99	7	0	-0.725221	9.337349	-3.605462
100	1	0	-1.396105	9.068452	-4.306497
101	1	0	-0.403946	10.288236	-3.526439
102	7	0	-6.258891	5.124234	1.795401
103	1	0	-7.184330	4.944991	2.150231
104	1	0	-5.905614	6.064197	1.722078
105	6	0	10.588341	-1.964358	1.999390
106	6	0	-0.193435	8.394418	-2.810250
107	6	0	-5.586222	4.123781	1.195115
108	1	0	10.779499	6.899899	0.088184
109	1	0	11.239291	5.256279	-0.321859
110	1	0	4.273858	8.300603	0.850110
111	1	0	7.940336	-6.495706	-0.423984
112	7	0	2.671691	-10.364818	1.392877
113	7	0	-4.348413	-7.613462	-2.992335
114	1	0	3.387668	-11.071850	1.422672
115	1	0	1.741458	-10.546890	1.732033
116	1	0	-3.666574	-8.279220	-3.317121
117	1	0	-5.323458	-7.707177	-3.225194
118	6	0	-7.074741	-1.833065	0.375765
119	6	0	-7.660158	-2.522293	1.395359
120	8	0	-8.013632	-1.370860	-0.501121
121	6	0	-9.062657	-2.486982	1.141916
122	1	0	-7.145395	-2.981923	2.225433
123	6	0	-9.228409	-1.765185	-0.013034

124	1	0	-9.855459	-2.906781	1.740913
125	6	0	-10.384652	-1.341179	-0.748451
126	6	0	-10.545830	-0.628494	-1.907565
127	8	0	-11.605546	-1.692977	-0.238324
128	6	0	-11.955649	-0.534303	-2.124651
129	1	0	-9.750012	-0.227382	-2.516283
130	6	0	-12.548224	-1.192866	-1.089335
131	1	0	-12.459459	-0.041286	-2.943224
132	1	0	-13.573937	-1.385117	-0.817388
133	6	0	-10.623586	0.994782	2.200347
134	17	0	-11.015799	1.855183	3.739432
135	17	0	-11.669500	1.599978	0.872533
136	17	0	-8.905174	1.171975	1.795614
137	9	0	-10.904967	-0.303591	2.384442
138	8	0	-3.412354	2.271245	2.725800
139	1	0	-3.038286	3.155300	2.832242
140	1	0	-4.230261	2.292636	3.238840

B. Coordinates of the designed single unit Heptazine, Hz and the Hz-df structures. Also the coordinates of the designed single unit Heptazine-SO_2 complex at four distances : 3, 3.5, 4 and 4.5 angstroms are:

1. (Heptazine-df)-SO_2 complex (Functional – B3LYP)

C	3.1151	3.0663	-0.26599
C	1.54652	1.42653	-0.26593
C	3.94673	0.95343	-0.26602
C	2.33789	-0.88447	-0.26596
C	4.58705	-1.22717	-0.26606
N	4.18479	2.27395	-0.26603
N	1.82344	2.73693	-0.26594
N	2.61109	0.50373	-0.26596
N	4.9372	0.07744	-0.26607
N	3.34619	-1.74806	-0.266
N	0.29409	0.98839	-0.26587
C	0.11831	-0.34586	-0.26581
N	1.07366	-1.29456	-0.2659
N	5.60298	-2.1077	-0.26612
H	5.40091	-3.09378	-0.26606
H	6.54985	-1.76602	-0.26611
H	3.32481	4.13496	-0.26602
C	-1.2358	-0.8421	-0.26591
C	-1.7369	-2.12672	-0.26604
O	-2.27168	0.05618	-0.26598
C	-3.14491	-2.01625	-0.26604
H	-1.13606	-3.02336	-0.26606
C	-3.42161	-0.66223	-0.26605
H	-3.87497	-2.81119	-0.26606

C	-4.6477	0.08018	-0.26606
C	-4.9307	1.42284	-0.26619
O	-5.80975	-0.64537	-0.2659
C	-6.35379	1.5291	-0.26611
H	-4.20427	2.22157	-0.26632
C	-6.83383	0.25277	-0.26594
H	-6.9414	2.43537	-0.26618
H	-7.82641	-0.16922	-0.26583
S	3.52389	1.44569	-3.49806
O	3.86776	2.86836	-3.48978
O	2.12722	1.05167	-3.68878

2. Heptazine-SO_2 complex (Functional – B3LYPD3)

C	1.80023	2.25679	0.48115
C	1.90217	-0.00875	0.48122
C	-0.21687	1.21169	0.48108
C	-0.21687	-1.2292	0.48122
C	-2.1349	-0.00876	0.48111
N	0.47389	2.36139	0.48109
N	2.55557	1.1558	0.4812
N	0.49434	-0.00876	0.48116
N	-1.53888	1.20247	0.48107
N	-1.53889	-1.21998	0.48119
N	2.55557	-1.17331	0.4813
C	1.80023	-2.2743	0.4812
N	0.47389	-2.3789	0.48127
N	-3.47668	-0.00875	0.48116
H	-3.97032	-0.88655	0.48106
H	-3.97031	0.86905	0.48097
H	2.34558	3.19919	0.48112
H	2.34559	-3.2167	0.48159
S	-0.5436	0.05206	-2.86084
O	0.15132	1.33304	-2.99679
O	0.23883	-1.18486	-2.84867

3. (Heptazine-df)-SO_2 complex (Functional – B3LYPD3)

C	-3.14433	3.02456	0.21439
C	-1.57394	1.38629	0.21442
C	-3.97493	0.91104	0.21439
C	-2.36417	-0.92681	0.21441
C	-4.61325	-1.2703	0.21439
N	-4.214	2.23146	0.21438
N	-1.85182	2.69647	0.21441
N	-2.63835	0.46207	0.21441
N	-4.96474	0.03453	0.21438
N	-3.37176	-1.79099	0.2144
N	-0.3213	0.94906	0.21444

C	-0.14543	-0.38563	0.21446
N	-1.09988	-1.33601	0.21443
N	-5.62862	-2.15143	0.21438
H	-5.42651	-3.13756	0.21433
H	-6.57597	-1.8109	0.21431
H	-3.35481	4.09292	0.21438
C	1.20784	-0.88055	0.21444
C	1.70732	-2.16597	0.21444
O	2.2445	0.01741	0.21444
C	3.1159	-2.05692	0.21441
H	1.10242	-3.05978	0.21444
C	3.393	-0.70318	0.21442
H	3.84799	-2.84984	0.21439
C	4.61881	0.0362	0.21441
C	4.89859	1.37911	0.21445
O	5.78093	-0.68883	0.21432
C	6.3219	1.48757	0.2144
H	4.16775	2.1737	0.2145
C	6.80403	0.21151	0.21434
H	6.9086	2.39441	0.21442
H	7.79789	-0.20785	0.21428
S	-3.85122	1.00332	3.71143
O	-4.05879	2.45074	3.77621
O	-2.48465	0.47912	3.71099

4. Hz-SO_2 complex (Functional – B3LYPD3)

C	-3.55108	-0.70833	0.72745
C	-2.05375	0.9956	0.56521
C	-1.37834	-1.36501	0.56583
C	0.3017	0.39919	0.37718
C	0.8486	-1.83498	0.39971
N	-2.65235	-1.71221	0.67814
N	-3.31947	0.61891	0.67813
N	-1.04125	0.00956	0.5024
N	-0.41607	-2.27825	0.51356
N	1.24099	-0.54002	0.31806
N	-1.71626	2.2795	0.51186
C	-0.40554	2.55703	0.39423
N	0.62121	1.6823	0.31523
N	-0.07347	3.85953	0.34029
H	-0.79556	4.55377	0.43974
H	0.89853	4.11942	0.31066
N	-4.84012	-1.07771	0.83999
H	-5.55318	-0.36919	0.88975
H	-5.0694	-2.05643	0.89024
N	1.81847	-2.75675	0.35556
H	2.79036	-2.47173	0.30617
H	1.55785	-3.72531	0.44336

S	-0.97519	0.21778	3.75018
O	-1.9317	1.22828	3.25144
O	0.43781	0.42767	3.42228

5. (Hz-df)-SO_2 complex (Functional – B3LYPD3)

C	0.41856	-1.38753	-0.83041
C	2.68919	-1.22242	-0.83088
C	1.21792	0.73374	-0.83013
C	3.64735	1.03046	-0.83057
C	2.1989	2.78454	-0.82982
N	0.16181	-0.07567	-0.83007
N	1.61798	-2.00595	-0.83078
N	2.51761	0.18129	-0.83057
N	1.06686	2.05066	-0.82977
N	3.47188	2.34711	-0.83018
N	3.91518	-1.7312	-0.83124
C	4.9315	-0.84702	-0.83132
N	4.86331	0.49886	-0.83094
N	6.17149	-1.37371	-0.83207
H	6.28184	-2.37386	-0.83068
H	6.96747	-0.75814	-0.83046
N	-0.6279	-2.26765	-0.83038
H	-0.33091	-3.23381	-0.83053
N	2.03219	4.12107	-0.82945
H	2.84202	4.71837	-0.8294
H	1.10033	4.50073	-0.82909
C	-1.99582	-2.06106	-0.83011
C	-3.01753	-2.97655	-0.82937
O	-2.47398	-0.79911	-0.83087
C	-4.22275	-2.20902	-0.82959
H	-2.91857	-4.05198	-0.8287
C	-3.84836	-0.89209	-0.83046
H	-5.23725	-2.5774	-0.82914
C	-4.54489	0.35991	-0.831
C	-4.10599	1.65863	-0.83182
O	-5.9128	0.31932	-0.83065
C	-5.28281	2.47187	-0.83199
H	-3.07155	1.96911	-0.83222
C	-6.34368	1.61732	-0.83126
H	-5.3312	3.55119	-0.83257
H	-7.41334	1.75535	-0.83108
S	2.66625	0.05635	2.16314
O	2.49803	1.50461	2.03452
O	1.4822	-0.80357	2.13359

6. Heptazine-SO_2 at 3.0 angstrom:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.608234	-2.703201	-0.456525
2	6	0	0.896496	-0.579365	-1.190295
3	6	0	-1.092429	-1.282158	0.034594
4	6	0	-0.899969	1.018508	-0.752452
5	6	0	-2.700331	0.277259	0.417288
6	7	0	-0.575945	-2.517597	0.115388
7	7	0	1.374893	-1.819618	-1.104047
8	7	0	-0.364089	-0.283339	-0.644762
9	7	0	-2.265912	-0.990719	0.568950
10	7	0	-2.078670	1.289374	-0.226540
11	7	0	1.605196	0.400469	-1.763539
12	6	0	1.005439	1.595213	-1.842103
13	7	0	-0.191121	1.958167	-1.401120
14	7	0	-3.890559	0.567699	0.963907
15	1	0	-4.251486	1.504950	0.890007
16	1	0	-4.391781	-0.148077	1.464490
17	1	0	1.012069	-3.711444	-0.388460
18	1	0	1.584533	2.375647	-2.332534
19	16	0	2.358258	0.725920	1.483730
20	8	0	1.987223	-0.682185	1.653413
21	8	0	1.276943	1.704137	1.322351

7. Heptazine-SO_2 at 3.5 angstrom:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.606131	2.703575	0.457467
2	6	0	0.896055	0.579445	1.189734
3	6	0	-1.093583	1.281578	-0.034194
4	6	0	-0.900074	-1.019118	0.752402
5	6	0	-2.700577	-0.278541	-0.417648
6	7	0	-0.578300	2.517698	-0.113711
7	7	0	1.373931	1.819858	1.103592
8	7	0	-0.364491	0.282958	0.644479
9	7	0	-2.266552	0.989571	-0.569316
10	7	0	-2.078981	-1.290144	0.227108
11	7	0	1.605288	-0.400271	1.762642
12	6	0	1.005979	-1.595229	1.841277
13	7	0	-0.190658	-1.958559	1.400717
14	7	0	-3.890122	-0.569717	-0.965241
15	1	0	-4.250875	-1.507001	-0.890884

16	1	0	-4.391858	0.145945	-1.465472
17	1	0	1.009211	3.712170	0.390169
18	1	0	1.585548	-2.375553	2.331322
19	16	0	2.360313	-0.722860	-1.482066
20	8	0	1.983138	0.683305	-1.654401
21	8	0	1.282935	-1.705782	-1.322874

8. Heptazine-SO_2 at 4.0 angstrom:

Center Numb	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.608482	-2.703166	0.457326
2	6	0	-0.897013	-0.579253	1.190739
3	6	0	1.091832	-1.281883	-0.034266
4	6	0	0.899442	1.018713	0.753138
5	6	0	2.699754	0.277544	-0.416800
6	7	0	0.575405	-2.517317	-0.115088
7	7	0	-1.375211	-1.819604	1.104795
8	7	0	0.363669	-0.283216	0.645541
9	7	0	2.265209	-0.990341	-0.568826
10	7	0	2.078111	1.289604	0.227174
11	7	0	-1.606046	0.400681	1.763476
12	6	0	-1.006347	1.595426	1.842155
13	7	0	0.190464	1.958330	1.401710
14	7	0	3.890063	0.567973	-0.963243
15	1	0	4.250854	1.505303	-0.889684
16	1	0	4.390931	-0.147633	-1.464433
17	1	0	-1.012028	-3.711552	0.389674
18	1	0	-1.585636	2.375940	2.332229
19	16	0	-2.357092	0.723385	-1.485392
20	8	0	-1.978532	-0.682762	-1.654907
21	8	0	-1.281144	1.707352	-1.323099

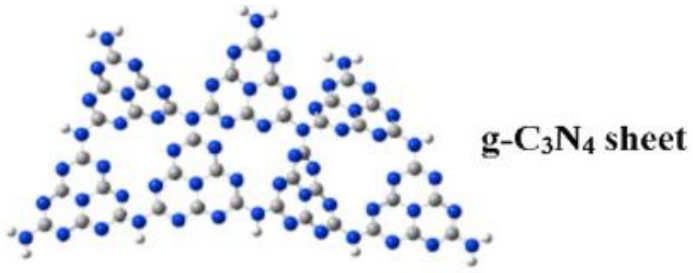
9. Heptazine-SO_2 at 4.5 angstrom:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.606908	-2.703767	0.455571
2	6	0	-0.895920	-0.580208	1.189838
3	6	0	1.093333	-1.282021	-0.035058
4	6	0	0.899985	1.018421	0.752602
5	6	0	2.700500	0.278220	-0.417579
6	7	0	0.577356	-2.517650	-0.116051

7	7	0	-1.373973	-1.820591	1.103131
8	7	0	0.364517	-0.283603	0.644442
9	7	0	2.266684	-0.989968	-0.569350
10	7	0	2.078513	1.289895	0.226606
11	7	0	-1.604919	0.399161	1.763560
12	6	0	-1.005530	1.594023	1.842672
13	7	0	0.190909	1.957541	1.401758
14	7	0	3.890459	0.569332	-0.964433
15	1	0	4.250939	1.506752	-0.890486
16	1	0	4.391877	-0.146103	-1.465309
17	1	0	-1.010383	-3.712132	0.387167
18	1	0	-1.584795	2.374071	2.333515
19	16	0	-2.359604	0.726145	-1.482698
20	8	0	-1.988234	-0.681762	-1.653300
21	8	0	-1.278461	1.704545	-1.321405

C. The reference structures and computational details of the works:

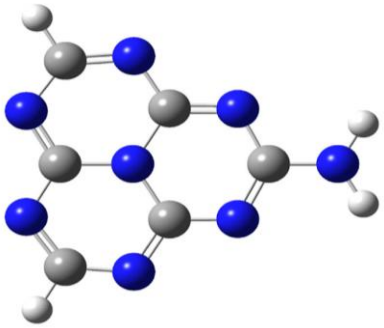
1. s-heptazine based g-C_3N_4 sheet. [9] R. Dutta, B. Dey and D. J. Kalita, Chemical Physics Letters, 2018, 707, 101-107.



For ground state optimization:
BASIS SET - 6-311G(d), FUNCTIONAL- B3LYP
HOMO-LUMO energy gap (Δ_{H-L}) obtained = 3.65 eV

For excited state calculations:
BASIS SET - 6-311G(d)
FUNCTIONAL - CAM-B3LYP
λ_{max} = 360 nm

2. Single heptazine unit. [16] M. Ashiq, R. A. Shehzad, J. Iqbal and K. Ayub, Physica B: Condensed Matter, 2024, 676, 415661.



For ground state optimization:
BASIS SET - 6-31G(d,p), FUNCTIONAL - B3LYP
HOMO-LUMO energy gap (Δ_{H-L}) obtained = 4.20 eV

For excited state calculations:
BASIS SET - 6-31G(d,p)
FUNCTIONAL - B3LYP
λ_{max} = 255 nm

D. BCP data of QTAIM plots:

Site-A

---------- **CP 217, Type (3,-1)** ----------
Position (Bohr): 6.25727347652398 -2.39661676686270 1.04402650112166
Density of all electrons: 0.6280661683E-02
Density of Alpha electrons: 0.3140330841E-02
Density of Beta electrons: 0.3140330841E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.4550544470E-02
G(r) in X,Y,Z: 0.1311891184E-02 0.1033090190E-02 0.2205563096E-02
Hamiltonian kinetic energy K(r): -0.1397620178E-02
Potential energy density V(r): -0.3152924292E-02
Energy density E(r) or H(r): 0.1397620178E-02
Laplacian of electron density: 0.2379265859E-01
---------- **CP 221, Type (3,-1)** ----------
Position (Bohr): 10.80456697419681 -1.98506580606838 3.65259141282210
Density of all electrons: 0.7866368988E-02
Density of Alpha electrons: 0.3933184494E-02
Density of Beta electrons: 0.3933184494E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.5569675983E-02
G(r) in X,Y,Z: 0.1822869542E-02 0.9365300880E-03 0.2810276353E-02
Hamiltonian kinetic energy K(r): -0.1082225405E-02
Potential energy density V(r): -0.4487450577E-02
Energy density E(r) or H(r): 0.1082225405E-02
Laplacian of electron density: 0.2660760555E-01
---------- **CP 228, Type (3,-1)** ----------
Position (Bohr): 2.92661265270508 -1.29144918944122 0.89180003936812
Density of all electrons: 0.1064873490E-01

Density of Alpha electrons: 0.5324367452E-02
Density of Beta electrons: 0.5324367452E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.8154083206E-02
G(r) in X,Y,Z: 0.2103300829E-02 0.7744490252E-03 0.5276333352E-02
Hamiltonian kinetic energy K(r): -0.1399032715E-02
Potential energy density V(r): -0.6755050491E-02
Energy density E(r) or H(r): 0.1399032715E-02
Laplacian of electron density: 0.3821246368E-01

---------- **CP 250, Type (3,-1)** ----------

Position (Bohr): 8.90545399367368 1.26501683496189 3.32262287342263
Density of all electrons: 0.3786752381E-02
Density of Alpha electrons: 0.1893376191E-02
Density of Beta electrons: 0.1893376191E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.2612296672E-02
G(r) in X,Y,Z: 0.1743987194E-03 0.9307977359E-03 0.1507100217E-02
Hamiltonian kinetic energy K(r): -0.6630696236E-03
Potential energy density V(r): -0.1949227048E-02
Energy density E(r) or H(r): 0.6630696236E-03
Laplacian of electron density: 0.1310146518E-01

---------- **CP 252, Type (3,-1)** ----------

Position (Bohr): 6.69204334962054 1.28257708675240 1.98424155022089
Density of all electrons: 0.5273903595E-02
Density of Alpha electrons: 0.2636951797E-02
Density of Beta electrons: 0.2636951797E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.3617407836E-02
G(r) in X,Y,Z: 0.1583089023E-02 0.1386324339E-02 0.6479944734E-03
Hamiltonian kinetic energy K(r): -0.8123092023E-03
Potential energy density V(r): -0.2805098633E-02
Energy density E(r) or H(r): 0.8123092023E-03
Laplacian of electron density: 0.1771886815E-01

---------- **CP 265, Type (3,-1)** ----------

Position (Bohr): 4.59613009445444 2.40527873640644 2.08311635463793
Density of all electrons: 0.4532331719E-02
Density of Alpha electrons: 0.2266165859E-02
Density of Beta electrons: 0.2266165859E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.3131005435E-02
G(r) in X,Y,Z: 0.1971091285E-03 0.2424911362E-02 0.5089849443E-03
Hamiltonian kinetic energy K(r): -0.7470942381E-03
Potential energy density V(r): -0.2383911197E-02
Energy density E(r) or H(r): 0.7470942381E-03
Laplacian of electron density: 0.1551239869E-01

---------- **CP 277, Type (3,-1)** ----------

Position (Bohr): 7.09926962654259 3.29584797027481 3.64478114888441
Density of all electrons: 0.3240860750E-02
Density of Alpha electrons: 0.1620430375E-02

Density of Beta electrons: 0.1620430375E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.2340869079E-02
G(r) in X,Y,Z: 0.5881711428E-03 0.2094477352E-03 0.1543250201E-02
Hamiltonian kinetic energy K(r): -0.6023373108E-03
Potential energy density V(r): -0.1738531768E-02
Energy density E(r) or H(r): 0.6023373108E-03
Laplacian of electron density: 0.1177282556E-01

---------- **CP 287, Type (3,-1)** ----------

Position (Bohr): 5.12003510874732 4.35105010329584 3.75907651326349
Density of all electrons: 0.5767161526E-02
Density of Alpha electrons: 0.2883580763E-02
Density of Beta electrons: 0.2883580763E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.3855515972E-02
G(r) in X,Y,Z: 0.2218618498E-03 0.4974130935E-03 0.3136241028E-02
Hamiltonian kinetic energy K(r): -0.8142986356E-03
Potential energy density V(r): -0.3041217336E-02
Energy density E(r) or H(r): 0.8142986356E-03
Laplacian of electron density: 0.1867925843E-01

Site-B

---------- **CP 293, Type (3,-1)** ----------

Position (Bohr): -6.21868583346694 8.22607601432939 1.71454733266637
Density of all electrons: 0.9685653773E-02
Density of Alpha electrons: 0.4842826886E-02
Density of Beta electrons: 0.4842826886E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.7222256183E-02
G(r) in X,Y,Z: 0.5744550588E-03 0.5429513769E-02 0.1218287355E-02
Hamiltonian kinetic energy K(r): -0.1306157598E-02
Potential energy density V(r): -0.5916098585E-02
Energy density E(r) or H(r): 0.1306157598E-02
Laplacian of electron density: 0.3411365512E-01

---------- **CP 294, Type (3,-1)** ----------

Position (Bohr): -8.36293007504986 8.87972922547885 2.91778676789631
Density of all electrons: 0.6879978261E-02
Density of Alpha electrons: 0.3439989130E-02
Density of Beta electrons: 0.3439989130E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.4968890460E-02
G(r) in X,Y,Z: 0.2272520990E-02 0.2365855782E-02 0.3305136882E-03
Hamiltonian kinetic energy K(r): -0.1038236564E-02
Potential energy density V(r): -0.3930653897E-02
Energy density E(r) or H(r): 0.1038236564E-02
Laplacian of electron density: 0.2402850810E-01

---------- **CP 307, Type (3,-1)** ----------

Position (Bohr): -4.44986012712975 10.62638722164961 -0.23967476784660
Density of all electrons: 0.5638377456E-02

Density of Alpha electrons: 0.2819188728E-02
Density of Beta electrons: 0.2819188728E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.3920428872E-02
G(r) in X,Y,Z: 0.8410643215E-03 0.4791311591E-03 0.2600233391E-02
Hamiltonian kinetic energy K(r): -0.1159851240E-02
Potential energy density V(r): -0.2760577632E-02
Energy density E(r) or H(r): 0.1159851240E-02
Laplacian of electron density: 0.2032112045E-01

---------- **CP 316, Type (3,-1)** ----------

Position (Bohr): 0.40335535286536 11.96419894609708 2.52852396604999
Density of all electrons: 0.6065819337E-02
Density of Alpha electrons: 0.3032909669E-02
Density of Beta electrons: 0.3032909669E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.4112331623E-02
G(r) in X,Y,Z: 0.1511007747E-02 0.1033653047E-02 0.1567670828E-02
Hamiltonian kinetic energy K(r): -0.9004889262E-03
Potential energy density V(r): -0.3211842696E-02
Energy density E(r) or H(r): 0.9004889262E-03
Laplacian of electron density: 0.2005128220E-01

---------- **CP 343, Type (3,-1)** ----------

Position (Bohr): -2.96621860392586 15.41095019684567 -0.73600360365183
Density of all electrons: 0.7866128192E-02
Density of Alpha electrons: 0.3933064096E-02
Density of Beta electrons: 0.3933064096E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.7142660663E-02
G(r) in X,Y,Z: 0.2246604644E-02 0.6035523091E-03 0.4292503710E-02
Hamiltonian kinetic energy K(r): -0.1058113316E-02
Potential energy density V(r): -0.6084547347E-02
Energy density E(r) or H(r): 0.1058113316E-02
Laplacian of electron density: 0.3280309591E-01

Site-C

---------- **CP 242, Type (3,-1)** ----------

Position (Bohr): 19.45887867564022 -2.73171956051977 -1.49936983420961
Density of all electrons: 0.6547064631E-02
Density of Alpha electrons: 0.3273532315E-02
Density of Beta electrons: 0.3273532315E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.5650758807E-02
G(r) in X,Y,Z: 0.2286231186E-02 0.1979280479E-02 0.1385247141E-02
Hamiltonian kinetic energy K(r): -0.1260854038E-02
Potential energy density V(r): -0.4389904769E-02
Energy density E(r) or H(r): 0.1260854038E-02
Laplacian of electron density: 0.2764645138E-01

---------- **CP 252, Type (3,-1)** ----------

Position (Bohr): 21.52098866898213 -1.70816946350324 -0.07894044601608

Density of all electrons: 0.5186052234E-02
Density of Alpha electrons: 0.2593026117E-02
Density of Beta electrons: 0.2593026117E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.5714278685E-02
G(r) in X,Y,Z: 0.4034523572E-03 0.5401168618E-03 0.4770709466E-02
Hamiltonian kinetic energy K(r): -0.1061277623E-02
Potential energy density V(r): -0.4653001062E-02
Energy density E(r) or H(r): 0.1061277623E-02
Laplacian of electron density: 0.2710222523E-01

---------- **CP 258, Type (3,-1)** ----------

Position (Bohr): 17.56859617890165 -0.92379986484257 -0.70139884353928
Density of all electrons: 0.6057749264E-02
Density of Alpha electrons: 0.3028874632E-02
Density of Beta electrons: 0.3028874632E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.4009047513E-02
G(r) in X,Y,Z: 0.2627674544E-03 0.2043417845E-02 0.1702862214E-02
Hamiltonian kinetic energy K(r): -0.1098358921E-02
Potential energy density V(r): -0.2910688592E-02
Energy density E(r) or H(r): 0.1098358921E-02
Laplacian of electron density: 0.2042962574E-01

---------- **CP 273, Type (3,-1)** ----------

Position (Bohr): 20.67274453967661 0.80622125661345 1.52152644798349
Density of all electrons: 0.4567786469E-02
Density of Alpha electrons: 0.2283893235E-02
Density of Beta electrons: 0.2283893235E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.3256027478E-02
G(r) in X,Y,Z: 0.8464567764E-03 0.1294725928E-02 0.1114844773E-02
Hamiltonian kinetic energy K(r): -0.8410582983E-03
Potential energy density V(r): -0.2414969180E-02
Energy density E(r) or H(r): 0.8410582983E-03
Laplacian of electron density: 0.1638834311E-01

---------- **CP 277, Type (3,-1)** ----------

Position (Bohr): 22.75129497228982 1.06934003951298 2.07049396467219
Density of all electrons: 0.5482537941E-02
Density of Alpha electrons: 0.2741268970E-02
Density of Beta electrons: 0.2741268970E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.3644510020E-02
G(r) in X,Y,Z: 0.3420643315E-03 0.1177959132E-02 0.2124486557E-02
Hamiltonian kinetic energy K(r): -0.9272617464E-03
Potential energy density V(r): -0.2717248274E-02
Energy density E(r) or H(r): 0.9272617464E-03
Laplacian of electron density: 0.1828708707E-01

---------- **CP 280, Type (3,-1)** ----------

Position (Bohr): 14.52343362394382 1.18786818070334 -2.13229145031576
Density of all electrons: 0.8830702683E-02

Density of Alpha electrons: 0.4415351342E-02
Density of Beta electrons: 0.4415351342E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.6578544370E-02
G(r) in X,Y,Z: 0.5364755242E-02 0.4593561068E-03 0.7544330217E-03
Hamiltonian kinetic energy K(r): -0.1243059428E-02
Potential energy density V(r): -0.5335484942E-02
Energy density E(r) or H(r): 0.1243059428E-02
Laplacian of electron density: 0.3128641519E-01

---------- **CP 301, Type (3,-1)** ----------

Position (Bohr): 14.80949154221511 3.48221659390179 -3.16047896778359
Density of all electrons: 0.6683525373E-02
Density of Alpha electrons: 0.3341762687E-02
Density of Beta electrons: 0.3341762687E-02
Spin density of electrons: 0.0000000000E+00
Lagrangian kinetic energy G(r): 0.4831286534E-02
G(r) in X,Y,Z: 0.3159493407E-02 0.1335635301E-02 0.3361578254E-03
Hamiltonian kinetic energy K(r): -0.1029766805E-02
Potential energy density V(r): -0.3801519729E-02
Energy density E(r) or H(r): 0.1029766805E-02
Laplacian of electron density: 0.2344421335E-01

E. DOS data representing the contributions of Hz, df and CFC-11 towards HOMO and LUMO. (in %)

Hz-df:

	Hz (%)	**Df (%)**
LUMO	100	0
HOMO	8	92

Site-A

	Hz (%)	**Df (%)**	**CFC-11 (%)**
LUMO	100	0	0
HOMO	7	93	0

Site-B

	Hz (%)	**Df (%)**	**CFC-11 (%)**
LUMO	100	0	0

HOMO	8	92	0

Site-C

	Hz (%)	**Df (%)**	**CFC-11 (%)**
LUMO	99	1	0
HOMO	8	99	0

F. Coordinates of Hz-df at 1 fs, 29 fs and 45.5 fs of the dynamic simulations:

1 fs:

C	9.4231786922	9.6997238175	16.2965084616
C	7.4374378169	10.2370596343	15.4090124704
C	9.1497638364	11.8962562817	16.0863768489
C	7.1783163204	12.6298177125	14.7688579233
C	8.8425540224	13.9630172818	15.3847219393
N	9.9485539524	10.9406559710	16.6164849883
N	8.2119575730	9.2060608688	15.8263633172
N	7.9294238817	11.5876806172	15.4086085148
N	9.6038178004	13.1630209090	16.2101089100
N	7.6968246423	13.8739492652	14.6260629790
N	6.2145197711	9.9233555372	14.9329477175
C	5.5954465926	11.0707443508	14.4196056762
N	5.9618799953	12.4116390041	14.2326967877
C	8.5954466268	16.2919557545	15.1941665808
C	6.7047626701	17.2473694544	15.8571320579
C	8.4530360929	18.3831029949	14.5104432214
C	6.4488918599	19.6462271240	15.2409889140
C	8.2595863249	20.5898662446	14.3214375131
N	9.1574590219	17.2385975587	14.3651806118
N	7.4708745109	16.1347417605	15.9725221424

N	7.2107070115	18.4278637627	15.2172322887
N	9.0240942656	19.4877462265	13.9766407501
N	6.9834547208	20.8176162115	14.8215164772
N	5.4801886078	17.2039810454	16.4164300645
N	5.1988261566	19.6961080530	15.7453769934
C	14.7781005530	13.6202396687	14.7973259415
C	12.6959366968	14.3926926198	14.7877773423
C	14.6677041391	15.7890240354	15.2086699267
C	12.4465013492	16.6892342810	15.7477209079
C	14.3009050805	17.9062269244	15.7104262542
N	15.4983029734	14.7464938526	15.1155171078
N	13.4649773455	13.3329893910	14.4439053953
N	13.2578213497	15.6221605405	15.2538711157
N	15.2364222622	17.0028684238	15.2611558493
N	12.9743750286	17.8797171422	16.1161140177
N	11.3563026282	14.2608311371	14.6606358838
C	10.7527851857	15.3423213732	15.2755947860
N	11.1129530383	16.5252123656	15.8947811265
C	18.4438756173	11.7169225592	16.4795728922
C	20.4415567466	13.1464086934	16.8495736791
C	18.6737572644	13.8655179151	15.2617064228
C	20.3731101650	15.1428914765	15.8875078561
N	21.0253745208	12.2159102855	17.6289811948
N	18.9433205417	10.7197701871	17.2352268929
N	19.1709936197	12.9231825346	16.2198534594
N	21.0921461734	14.3281674548	16.7353837711
N	19.2881627612	15.0439388689	15.0295915172
N	17.1735728156	11.5678280904	16.0340468841
C	16.8857298940	12.5846882517	15.1424899863
N	17.5402706927	13.6395647493	14.5581890622
C	13.2126025552	7.7113683257	15.0114024777
C	15.0610018637	9.1739338609	14.2104179141

C	13.3394383896	10.0697488263	15.7562641018
C	14.9828601693	11.2731713117	14.9159493900
N	15.6626011408	8.1578568562	13.5672764725
N	13.7558950572	6.6225169509	14.4301456805
N	13.8631732773	8.9935655225	14.9770094534
N	15.6158057806	10.4054799710	14.0619177627
N	13.9710706469	11.2672890917	15.8454333019
N	11.9902773648	7.5569871279	15.5709883675
C	11.5818754665	8.7590989424	16.1332496166
N	12.1657328988	9.9829917040	16.4195843339
C	14.0480382073	20.2501436005	15.6467440407
C	12.1725051620	21.0609716458	14.8185051947
C	13.7103033665	22.3468582607	16.2792173783
C	11.5719315527	23.3644990031	15.5019924477
C	13.1476046486	24.4925647774	16.6458603426
N	14.5113816532	21.2650751073	16.4487253624
N	13.0363089196	20.0199025355	14.7435748694
N	12.4789810088	22.2491398418	15.5488472920
N	14.1020536472	23.4893728469	16.8718427589
N	11.8880532473	24.5607669849	16.0377598032
N	10.9945246582	20.8805257460	14.1838122518
C	10.1742549180	21.9658036039	14.4493094598
N	10.3313695861	23.2426966482	14.9733864356
C	20.1713807449	17.4625767297	15.5660687100
C	18.1758630264	18.3910698846	15.8349168563
C	20.0084897687	19.3872754298	14.4831612707
C	17.7418366488	20.4083204631	14.4559782039
C	19.5290849984	21.3255265510	13.4463195928
N	20.8489210548	18.3660372395	14.7770331840
N	18.9605529810	17.3675020323	16.2331593554
N	18.6339714649	19.3784468550	14.9026371068
N	20.5211618667	20.3804358823	13.7301630999

N	18.1554231168	21.4460973546	13.7042124722
N	16.9233215512	18.4127355522	16.3443238249
C	16.1883465371	19.3190823694	15.6170454084
N	16.4107452787	20.3318326022	14.7087692460
N	14.8422755235	19.1459923487	15.8195298478
N	9.3999193557	15.1983884183	15.2764465407
N	15.5643174257	12.5171326170	14.7750183205
N	8.8473755471	21.8176934326	14.1255843053
N	20.9401581241	16.3751512782	15.8226294673
N	10.2599338248	8.6221629888	16.4829533729
N	4.3485574490	10.8184771117	13.9693037854
N	3.5791607886	18.4274142251	16.7355769876
H	3.2801435790	17.5429982725	17.1674928899
H	3.0775264566	19.3246869610	16.6967066584
N	15.5537644136	5.9045628273	13.2230092502
H	16.4150892113	6.1109551575	12.7004109163
H	15.0509341782	5.0111419857	13.3069485106
N	20.7846685113	10.0934999434	18.4308783876
H	21.6953135290	10.3250678019	18.8515303803
H	20.2047431978	9.2553758374	18.5746002154
C	4.8409943426	18.4426020700	16.2566352461
C	14.9499334927	6.9695086356	13.7884768965
C	20.2125864912	11.0788666800	17.7084286528
H	4.0426011558	9.8378605257	14.0286970787
H	3.8637948100	11.6171403341	13.5384548892
H	9.8497405295	7.7444232898	16.1201591022
H	8.2664399037	22.5930521654	14.4876988977
N	13.5286907555	25.6786792116	17.1626357404
N	20.0085521593	22.3697316274	12.7392577079
H	12.8465187830	26.4438251645	17.0723901007
H	14.4293269891	25.6756675940	17.6598571713
H	19.3081951098	23.0634592084	12.4458007334

H	20.9980901389	22.3011324720	12.4659106269
C	22.2839292653	16.5040083936	15.9760460854
C	23.0276467918	17.2512930781	16.8325756863
O	23.0008504424	15.7497899400	15.0542208006
C	24.3575397334	16.9786357410	16.4854131454
H	22.6312982819	17.8870623920	17.6117954382
C	24.2974149293	16.0813063756	15.4463970357
H	25.2545551203	17.3674586747	16.9401028788
C	25.2900720944	15.4423563712	14.7223056841
C	25.2218515120	14.5420659044	13.6912996047
O	26.5991275622	15.7694533218	15.1048624073
C	26.5683340029	14.2550082081	13.3724654624
H	24.3158798323	14.1528818875	13.2387333564
C	27.3582721067	14.9900924113	14.2182318279
H	26.9263938467	13.5829547398	12.6048586819
H	28.4276009892	15.1108997244	14.3589102116

29 fs:

C	9.3376825870	9.6040537977	16.4023338682
C	7.3773052631	10.2628712933	15.3885489429
C	9.0545056651	11.8219955642	16.1115109529
C	7.1404547845	12.5323129241	14.7590625435
C	8.7989408913	13.9136558676	15.3917415802
N	9.8099982229	10.8608210416	16.6898298281
N	8.1359157029	9.2383807352	15.8492905637
N	7.8805037481	11.5489071105	15.4055390824
N	9.4867751076	13.0908392451	16.2403526786
N	7.6861737932	13.7565875954	14.6235789681
N	6.1553607110	9.9722003271	14.8913035886
C	5.4447664947	11.0300146598	14.3562479187
N	5.9169927769	12.3236456369	14.2229616684

C	8.5417362421	16.3288799335	15.1824091367
C	6.6471205145	17.3322667424	15.8675724848
C	8.3447907246	18.4359562197	14.4903254512
C	6.3961016325	19.6073671429	15.2634371150
C	8.1529844691	20.6653048910	14.2162467624
N	9.0267119348	17.2844770453	14.3340509451
N	7.4384574010	16.2462238283	15.9755013026
N	7.1545076808	18.4547711446	15.2223503332
N	8.8696069803	19.5366761142	13.9057672510
N	6.9149057622	20.7697529508	14.7985741600
N	5.4187038355	17.2793223576	16.4309564767
N	5.1519137417	19.6353948282	15.7882322997
C	14.7931034383	13.6290725590	14.7062461743
C	12.7184684500	14.4486042925	14.7548871643
C	14.6136796188	15.7909176851	15.1941303993
C	12.4798549309	16.6358538846	15.7788663280
C	14.3069612483	17.9088254750	15.7790894600
N	15.4348161238	14.7506701283	15.1025822579
N	13.4891160005	13.4296698782	14.3458230459
N	13.2515274081	15.6212090651	15.2515907379
N	15.1606220233	17.0054624507	15.2431007180
N	13.0151682201	17.7905143939	16.2021591321
N	11.3924094752	14.3301915597	14.6292132976
C	10.7490587350	15.3399829721	15.2759063542
N	11.1638841475	16.4605535365	15.9264842265
C	18.5104932350	11.7157892812	16.5172597483
C	20.4187690894	13.0583324576	16.8722520616
C	18.7502984008	13.7790768605	15.2630971124
C	20.4171030620	15.1096991551	15.8989278095
N	20.9958785672	12.1229993970	17.6613465464
N	19.0153229792	10.7202211232	17.2823892781
N	19.2008791315	12.8805638982	16.2385653602

N	21.0546783447	14.2361652689	16.7290225529
N	19.3559453004	14.9556101407	15.0420864071
N	17.2546537484	11.6052138758	16.0327426525
C	16.9449843616	12.5354018715	15.0760847597
N	17.6683444109	13.5235750042	14.4953171462
C	13.2715396997	7.6895079670	14.9825842132
C	15.0197057906	9.0723116908	14.2002940957
C	13.3619899282	9.9651876536	15.7679066354
C	14.9644873468	11.2179092115	14.8623185944
N	15.6335501287	8.0565599077	13.5558188838
N	13.8280635156	6.6135686368	14.3804612210
N	13.8718965626	8.9347471950	14.9721946891
N	15.5380672551	10.3047487806	14.0419790279
N	14.0055808807	11.1544207015	15.8329654659
N	12.0683101245	7.5275378491	15.5843587520
C	11.5864843024	8.6365665133	16.2336604931
N	12.2168155755	9.8357150151	16.4769719396
C	14.0137666763	20.3067147422	15.6905350878
C	12.1692723968	21.1743515360	14.7998276560
C	13.6498495074	22.4405590820	16.2857208659
C	11.6266612510	23.4002645963	15.5309592855
C	13.1865995404	24.6480771402	16.7171699548
N	14.4153382170	21.3489743782	16.4607282165
N	13.0416981608	20.1428780219	14.7437861658
N	12.4739320395	22.3101720619	15.5555789902
N	14.0531230003	23.5832020763	16.8819641909
N	11.9582782440	24.5866678001	16.0867954281
N	11.0063339715	21.0366509018	14.1239621965
C	10.1484619751	22.0880062058	14.3501900068
N	10.4041808964	23.2904144086	14.9575912389
C	20.1987773091	17.5126092794	15.5820769562
C	18.2280952334	18.4907103238	15.8301535032

C	19.9719849162	19.4650898958	14.4524825121
C	17.8147027312	20.4214631989	14.4248783676
C	19.5821851594	21.4569755547	13.3478027951
N	20.7892052127	18.4476248438	14.7851184750
N	19.0001581204	17.4731275222	16.2322992268
N	18.6588970502	19.4285305201	14.8860802516
N	20.4759552387	20.4594707021	13.6861248557
N	18.2332123362	21.4598773144	13.6666727696
N	17.0110439336	18.5439074394	16.4012990608
C	16.2262546119	19.3788837969	15.6774864522
N	16.5008590467	20.3110866056	14.7194937682
N	14.8449905996	19.1898459259	15.9304139023
N	9.3599919654	15.1930889780	15.2718010376
N	15.5881610132	12.4823024823	14.6593744876
N	8.7798225210	21.9276774590	13.9579086903
N	20.9889964376	16.3897747407	15.8600839574
N	10.2210772369	8.5029251831	16.6503112119
N	4.1669410785	10.7803141958	13.9100552059
N	3.3952334345	18.4263516013	16.7984670624
H	3.0388387303	17.5931793549	17.2916555996
H	2.8345823681	19.2918792395	16.8278589394
N	15.6432223323	5.7423043420	13.1437159569
H	16.4862343888	5.8755835533	12.5646740314
H	15.1929520697	4.8142350371	13.1511484443
N	20.8674976857	9.9418787526	18.5337517186
H	21.7593510020	10.1142284270	19.0255196525
H	20.3372576802	9.0875461104	18.7683023223
C	4.6868117006	18.4491059720	16.3235189237
C	15.0181637887	6.8278279889	13.7124116096
C	20.2773968293	10.9518339450	17.8062653051
H	3.7937081327	9.8182192882	13.9042008841
H	3.6348017274	11.5179907269	13.4231651001

H	9.8146447729	7.6065478197	16.3232011976
H	8.1979097054	22.7214782110	14.2837230231
N	13.5835711637	25.8597436825	17.2334199303
N	20.0749491340	22.5309779873	12.6391560843
H	12.9459412079	26.6710099003	17.2188831554
H	14.4520668972	25.9268378140	17.7866208153
H	19.4323060741	23.2448440879	12.2627097815
H	21.0448983112	22.5145554885	12.2864449655
C	22.3459011190	16.5647821690	16.0537861122
C	23.1024106187	17.3115502837	16.9102199838
O	23.0929566531	15.8365982906	15.1503366869
C	24.4478804452	17.0347848574	16.5444152596
H	22.7362619005	17.9548798237	17.7092301094
C	24.4108053943	16.1249352872	15.4858501759
H	25.3321176871	17.4502682606	17.0276584753
C	25.3646061250	15.4119793743	14.6837531605
C	25.3274875926	14.4957184320	13.6378284800
O	26.6917608434	15.6964415747	15.0234775700
C	26.6869692003	14.1989148835	13.3099876491
H	24.4472139104	14.0785342800	13.1485866064
C	27.4768874964	14.9384391161	14.1608497139
H	27.0320230168	13.5166797798	12.5302564148
H	28.5484175081	15.0641925281	14.3120424651

45.5 fs:

C	9.2832938162	9.5045592731	16.4553773594
C	7.2587347139	10.1084146332	15.3976744470
C	9.0085863287	11.7739577518	16.1929454581
C	7.0360273263	12.5233238165	14.7027466997
C	8.7451033672	13.9086936095	15.3859215589
N	9.7155136109	10.7560410513	16.7976259182

N	8.0806093806	9.0913590086	15.8960334739
N	7.7836146389	11.4615553603	15.3985311877
N	9.4195764142	13.0880277579	16.2617653628
N	7.6508691910	13.7443200050	14.5880878847
N	6.0109421689	9.8677847110	14.8447659346
C	5.3696712026	10.9896195104	14.3233030285
N	5.7953824434	12.3008623218	14.1573353606
C	8.4893961025	16.3213542469	15.1869298118
C	6.5461201156	17.3178475760	15.9267015018
C	8.2851905434	18.4729352226	14.4064765211
C	6.2485643362	19.7325531470	15.2597123116
C	8.0767145398	20.7514339875	14.1631686895
N	8.9592039148	17.2742072392	14.3115772177
N	7.4015689327	16.2471332553	16.0069855611
N	7.0436515521	18.5172711782	15.2327966188
N	8.7530645807	19.6199248355	13.7992624280
N	6.8278139027	20.9007737340	14.7538226397
N	5.2986403127	17.2746179374	16.4987810797
N	4.9910243534	19.7058868519	15.8400911847
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