

Supporting Information Paragraph

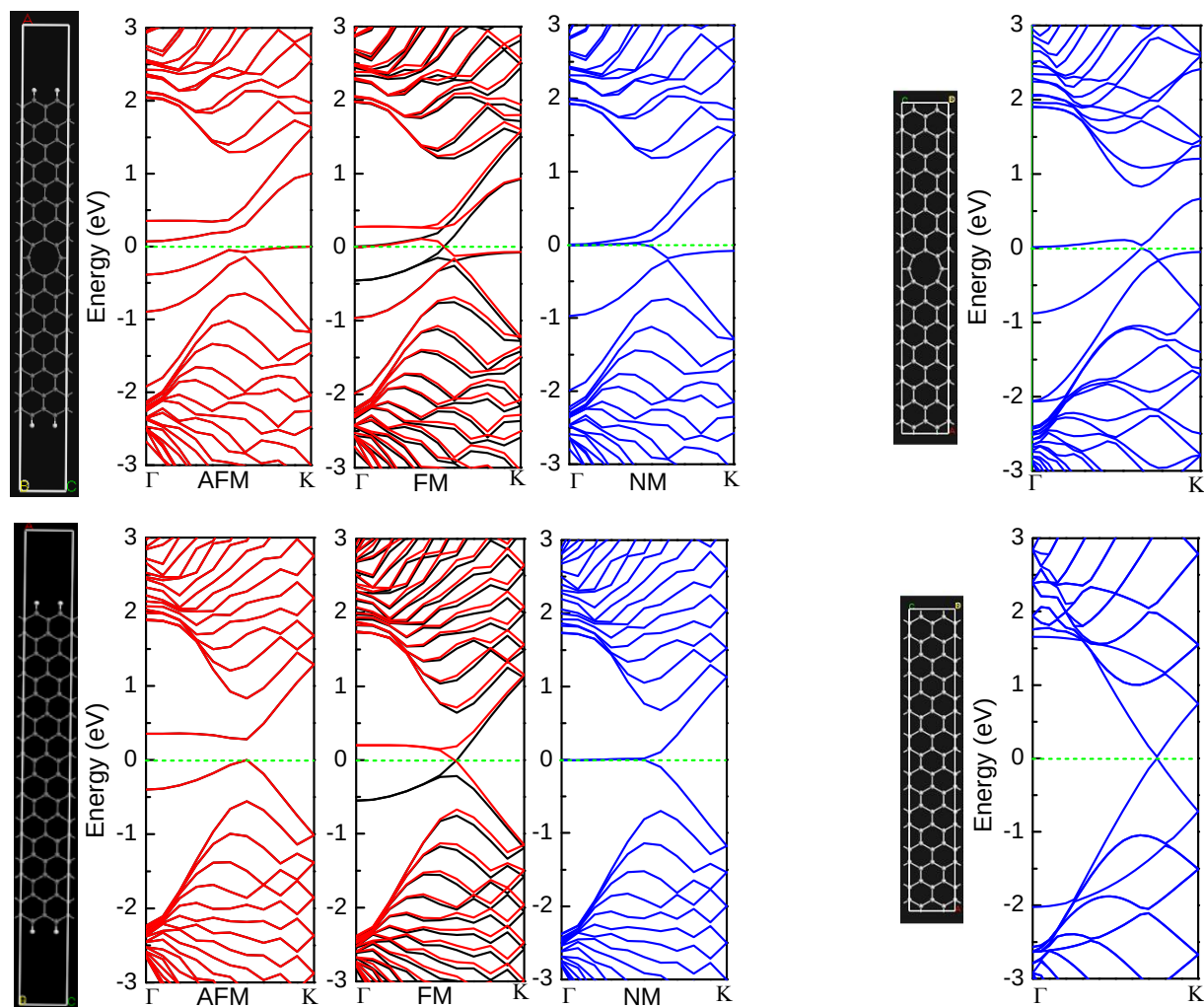


Fig. S1. The electronic structures of GNR-A and normal GNR are compared. Top panel: Left is the unit structure and electronic structures for GNR-A. Right is the geometric and electronic structures for one-dimension GB structure embedded in graphene. Bottom panel: Left is the geometric and electronic structures for normal zigzag-edged GNR. Right is the electronic structure along the width for graphene.

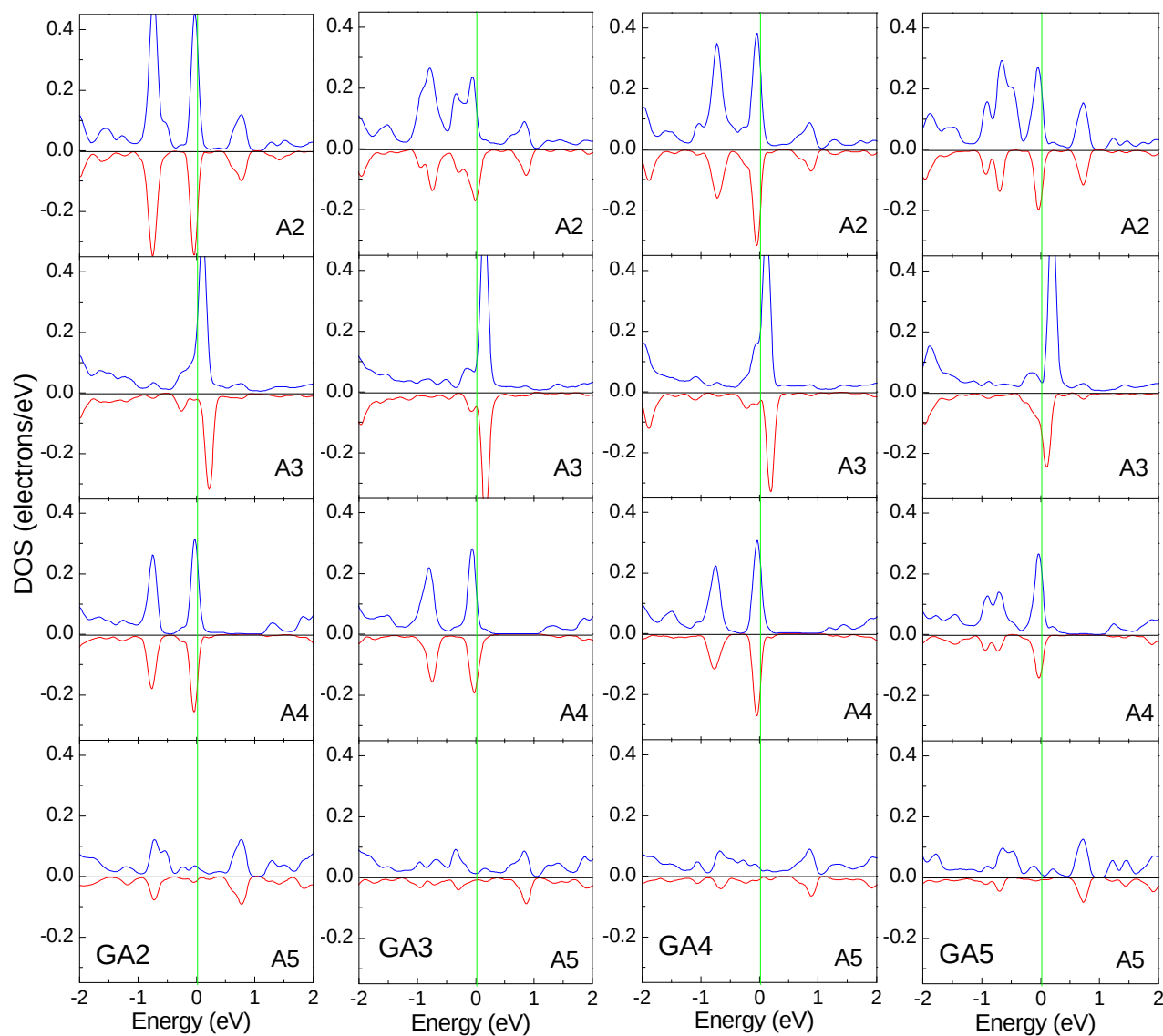


Fig. S2. Calculated local DOS of atoms far away N dopant for N-doped GNR-As are shown. The Fermi level is set as 0 eV.

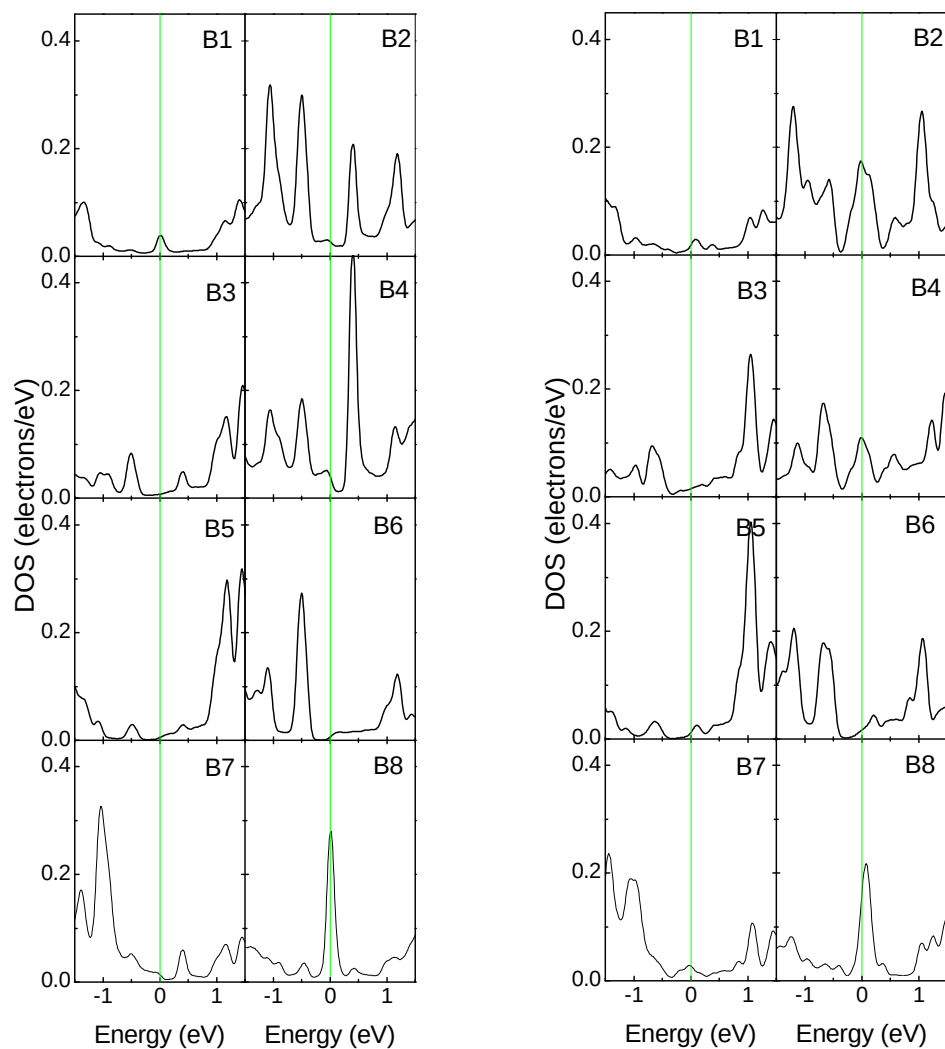


Fig. S3. Calculated local DOS for pristine GNR-B (left) and GB4 (right) are compared. The Fermi level is set as 0 eV.

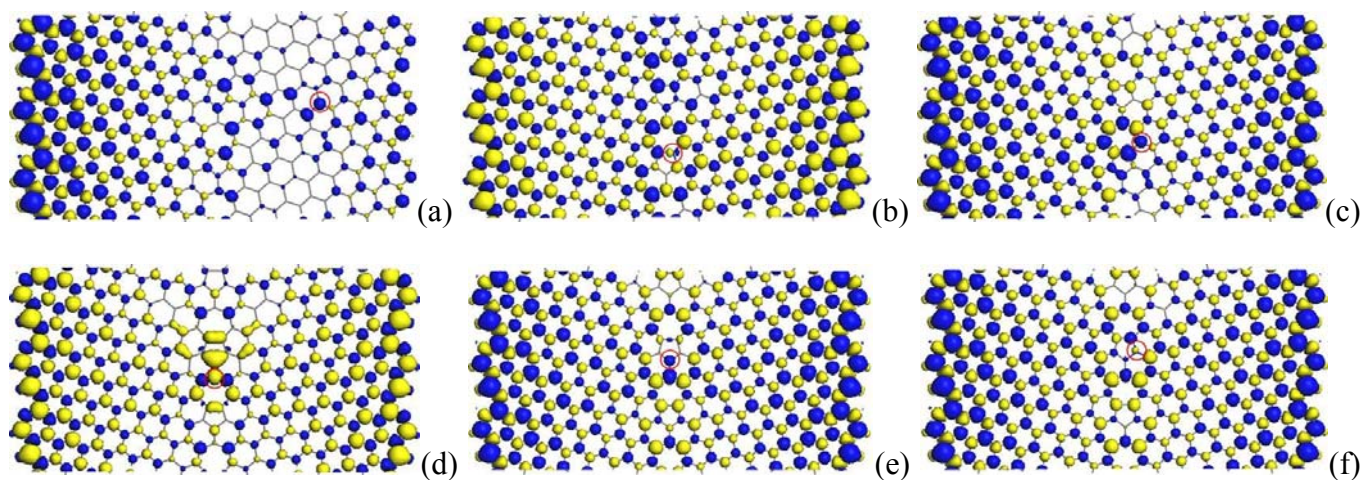


Fig. S4. Isosurface plots of spin density difference are shown at the value of $0.001 \text{ electrons}/a.u.^3$, (a)-(f) corresponding to configuration GB1~GB3, GB5~GB7, where blue and yellow shapes correspond to up and down spin, respectively. The site of N dopant is marked by red circle.

Table S1. The total energy, relative total energy (ΔE) and total spin magnetic moment for the pristine and N-doped hybrid GNRs are listed. For N-doped hybrid GNRs, ΔE is relative to the total energy of GA1 for GNR-A or GB1 for GNR-B.

	Total Energy (Ha)	ΔE (eV)	Magnetic Moment(μ_B)
Pristine GNR-A	-10063.041922		-4.02
GA1	-10079.658375	0	4.95
GA2	-10079.696989	-1.05	-3.01
GA3	-10079.685837	-0.75	5.00
GA4	-10079.695099	-1.00	1.00
GA5	-10079.662842	-0.12	-1.00
GA6	-10079.705707	-1.29	2.99
Pristine GNR-B	-10749.862435		0
GB1	-10766.476196	0	0.99
GB2	-10766.498878	-0.62	-1.00
GB3	-10766.474037	0.06	1.01
GB4	-10766.471404	0.13	0
GB5	-10766.462558	0.37	-0.99
GB6	-10766.506791	-0.83	1.00
GB7	-10766.509801	-0.91	1.00
GB8	-10766.504607	-0.77	0
GB9	-10766.516754	-1.10	1.00

GA2 atomic coordinates using GGA:

Coordinates (Angstroms)			
ATOM	X	Y	Z
1 H	7.757624	4.996293	0.628513
2 C	8.848858	4.996293	0.628597
3 C	11.683651	4.996293	0.628709
4 C	13.114162	4.996293	0.628814
5 C	20.237179	4.996293	0.636151
6 C	17.387992	4.996293	0.627856
7 C	15.963876	4.996293	0.628096
8 C	9.532119	4.996293	4.320579
9 C	10.975706	4.996293	4.320698
10 C	13.826331	4.996293	4.320959
11 C	19.532273	4.996293	4.322150
12 C	18.107315	4.996293	4.321767
13 C	15.252181	4.996293	4.321447
14 C	21.660783	4.996293	0.643071
15 C	24.524578	4.996293	0.589662
16 C	27.239472	4.996293	0.589662
17 C	34.376058	4.996293	0.627856
18 C	31.526871	4.996293	0.636151
19 C	30.103267	4.996293	0.643071
20 C	22.343815	4.996293	4.320320
21 C	23.732939	4.996293	4.319420
22 C	28.031111	4.996293	4.319420
23 C	33.656735	4.996293	4.321767
24 C	32.231777	4.996293	4.322150
25 C	29.420234	4.996293	4.320320
26 C	35.800174	4.996293	0.628096
27 C	42.915192	4.996293	0.628597
28 C	40.080398	4.996293	0.628709
29 C	38.649888	4.996293	0.628814
30 C	36.511868	4.996293	4.321447
31 C	42.231931	4.996293	4.320579
32 C	40.788344	4.996293	4.320698
33 C	37.937719	4.996293	4.320959
34 H	44.006426	4.996293	0.628513
35 H	7.757746	4.996293	3.090300
36 C	8.848979	4.996293	3.090035
37 C	11.683920	4.996293	3.089990
38 C	13.114496	4.996293	3.090159
39 C	20.238763	4.996293	3.083135
40 C	17.389167	4.996293	3.091896
41 C	15.964883	4.996293	3.091179
42 C	9.531688	4.996293	1.859312
43 C	10.975305	4.996293	1.859366
44 C	13.825918	4.996293	1.859497
45 C	19.519221	4.996293	1.859458
46 C	18.097214	4.996293	1.859671
47 C	15.252453	4.996293	1.859683
48 C	21.661243	4.996293	3.075704
49 C	24.523515	4.996293	3.129629
50 C	27.240534	4.996293	3.129629
51 C	34.374882	4.996293	3.091896
52 C	31.525286	4.996293	3.083135
53 C	30.102807	4.996293	3.075704
54 C	22.408380	4.996293	1.859347
55 C	23.869158	4.996293	1.860085
56 C	27.894892	4.996293	1.860085
57 C	33.666836	4.996293	1.859671
58 C	32.244829	4.996293	1.859458
59 C	29.355669	4.996293	1.859347
60 C	35.799166	4.996293	3.091179
61 C	42.915070	4.996293	3.090035
62 C	40.080130	4.996293	3.089990
63 C	38.649553	4.996293	3.090159

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65	C	42.232361	4.996293	1.859312
66	C	40.788745	4.996293	1.859366
67	C	37.938132	4.996293	1.859497
68	H	44.006304	4.996293	3.090300
69	C	25.882025	4.996293	3.597902
70	C	25.882025	4.996293	0.122491
71	H	7.758091	4.996293	5.551430
72	C	8.849319	4.996293	5.551169
73	C	11.684511	4.996293	5.551245
74	C	13.115233	4.996293	5.551611
75	C	20.242942	4.996293	5.559554
76	C	17.391473	4.996293	5.551529
77	C	15.966567	4.996293	5.551261
78	C	9.532929	4.996293	9.242353
79	C	10.976602	4.996293	9.242400
80	C	13.827714	4.996293	9.242495
81	C	19.539339	4.996293	9.243725
82	C	18.111351	4.996293	9.243044
83	C	15.254291	4.996293	9.242735
84	C	21.666900	4.996293	5.565681
85	C	24.526208	4.996293	5.509078
86	C	27.237841	4.996293	5.509078
87	C	34.372577	4.996293	5.551529
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89	C	30.097150	4.996293	5.565681
90	C	22.354111	4.996293	9.245063
91	C	23.755088	4.996293	9.244325
92	C	28.008962	4.996293	9.244325
93	C	33.652699	4.996293	9.243044
94	C	32.224711	4.996293	9.243725
95	C	29.409939	4.996293	9.245063
96	C	35.797483	4.996293	5.551261
97	C	42.914731	4.996293	5.551169
98	C	40.079539	4.996293	5.551245
99	C	38.648816	4.996293	5.551611
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101	C	42.231121	4.996293	9.242353
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103	C	37.936336	4.996293	9.242495
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105	H	7.758500	4.996293	8.012315
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107	C	11.685057	4.996293	8.011984
108	C	13.115880	4.996293	8.012141
109	C	20.248066	4.996293	8.006910
110	C	17.393264	4.996293	8.014327
111	C	15.967948	4.996293	8.013288
112	C	9.532502	4.996293	6.781554
113	C	10.976174	4.996293	6.781650
114	C	13.827785	4.996293	6.781842
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117	C	15.254735	4.996293	6.782283
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122	C	31.515983	4.996293	8.006910
123	C	30.090041	4.996293	8.001950
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146	C	17.394000	4.996293	10.471395
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156	C	27.222376	4.996293	10.417406
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158	C	31.515663	4.996293	10.479512
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179	C	20.250208	4.996293	12.922877
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182	C	9.532856	4.996293	11.703016
183	C	10.976540	4.996293	11.702972
184	C	13.828389	4.996293	11.702872
185	C	19.528046	4.996293	11.701462
186	C	18.104483	4.996293	11.702266
187	C	15.255511	4.996293	11.702644
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210	N	25.882025	4.996293	9.949741
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214	C	13.115349	4.996293	15.393927
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216	C	17.391851	4.996293	15.391481
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220	C	13.825500	4.996293	19.085856
221	C	19.529289	4.996293	19.086108
222	C	18.104922	4.996293	19.085902
223	C	15.251007	4.996293	19.085724
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225	C	24.525926	4.996293	15.358952
226	C	27.238123	4.996293	15.358952
227	C	34.372199	4.996293	15.391481
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229	C	30.099446	4.996293	15.408206
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231	C	23.732719	4.996293	19.087691
232	C	28.031331	4.996293	19.087691
233	C	33.659127	4.996293	19.085902
234	C	32.234760	4.996293	19.086108
235	C	29.421826	4.996293	19.086937
236	C	35.797011	4.996293	15.392576
237	C	42.914628	4.996293	15.394108
238	C	40.079394	4.996293	15.394168
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240	C	36.513043	4.996293	19.085724
241	C	42.232195	4.996293	19.085945
242	C	40.788644	4.996293	19.085898
243	C	37.938550	4.996293	19.085856
244	H	44.005858	4.996293	15.393764
245	H	7.757810	4.996293	17.855064
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247	C	11.684016	4.996293	17.855159
248	C	13.114608	4.996293	17.854829
249	C	20.238087	4.996293	17.848343
250	C	17.388954	4.996293	17.855570
251	C	15.964702	4.996293	17.855513
252	C	9.532118	4.996293	16.624716
253	C	10.975777	4.996293	16.624603
254	C	13.826928	4.996293	16.624331
255	C	19.521320	4.996293	16.624189
256	C	18.099209	4.996293	16.623978
257	C	15.253759	4.996293	16.623866
258	C	21.661476	4.996293	17.842308
259	C	24.524689	4.996293	17.897438
260	C	27.239360	4.996293	17.897438
261	C	34.375096	4.996293	17.855570
262	C	31.525963	4.996293	17.848343
263	C	30.102574	4.996293	17.842308
264	C	22.409882	4.996293	16.626519
265	C	23.868851	4.996293	16.627712
266	C	27.895199	4.996293	16.627712
267	C	33.664841	4.996293	16.623978

268	C	32.242730	4.996293	16.624189
269	C	29.354167	4.996293	16.626519
270	C	35.799348	4.996293	17.855513
271	C	42.915007	4.996293	17.855253
272	C	40.080034	4.996293	17.855159
273	C	38.649442	4.996293	17.854829
274	C	36.510291	4.996293	16.623866
275	C	42.231931	4.996293	16.624716
276	C	40.788272	4.996293	16.624603
277	C	37.937122	4.996293	16.624331
278	H	44.006239	4.996293	17.855064
279	C	25.882025	4.996293	18.364030
280	C	25.882025	4.996293	14.897737

GA6 atomic coordinates using GGA:

Coordinates (Angstroms)				

ATOM		X	Y	Z
1	H	7.749310	4.996293	0.628625
2	C	8.840559	4.996293	0.628672
3	C	11.675661	4.996293	0.628744
4	C	13.106354	4.996293	0.628822
5	C	20.234488	4.996293	0.635828
6	C	17.382331	4.996293	0.627701
7	C	15.957559	4.996293	0.628043
8	C	9.523532	4.996293	4.320172
9	C	10.967138	4.996293	4.320177
10	C	13.817930	4.996293	4.320186
11	C	19.525323	4.996293	4.320189
12	C	18.099855	4.996293	4.320189
13	C	15.243891	4.996293	4.320188
14	C	21.658672	4.996293	0.642443
15	C	24.525329	4.996293	0.588716
16	C	27.241324	4.996293	0.588705
17	C	34.385499	4.996293	0.627635
18	C	31.532525	4.996293	0.635795
19	C	30.108202	4.996293	0.642432
20	C	22.340797	4.996293	4.320169
21	C	23.732578	4.996293	4.320137
22	C	28.033932	4.996293	4.319917
23	C	33.666913	4.996293	4.319336
24	C	32.241417	4.996293	4.319591
25	C	29.425816	4.996293	4.319768
26	C	35.810432	4.996293	0.627973
27	C	42.926857	4.996293	0.628560
28	C	40.091864	4.996293	0.628652
29	C	38.662476	4.996293	0.628731
30	C	36.523741	4.996293	4.319898
31	C	42.242999	4.996293	4.329285
32	C	40.801020	4.996293	4.323108
33	C	37.949826	4.996293	4.319953
34	H	44.018283	4.996293	0.628501
35	H	7.749318	4.996293	3.089741
36	C	8.840567	4.996293	3.089695
37	C	11.675666	4.996293	3.089623
38	C	13.106363	4.996293	3.089549
39	C	20.234503	4.996293	3.082518
40	C	17.382350	4.996293	3.090663
41	C	15.957571	4.996293	3.090326
42	C	9.523419	4.996293	1.859183
43	C	10.967089	4.996293	1.859185
44	C	13.818369	4.996293	1.859187
45	C	19.514857	4.996293	1.859177
46	C	18.092168	4.996293	1.859184
47	C	15.245220	4.996293	1.859188
48	C	21.658691	4.996293	3.075870
49	C	24.525280	4.996293	3.129579
50	C	27.241265	4.996293	3.129446
51	C	34.385224	4.996293	3.090088
52	C	31.532340	4.996293	3.082012
53	C	30.108071	4.996293	3.075541
54	C	22.407765	4.996293	1.859163
55	C	23.867820	4.996293	1.859150
56	C	27.898818	4.996293	1.859083
57	C	33.675286	4.996293	1.858854
58	C	32.252379	4.996293	1.858965
59	C	29.358966	4.996293	1.858998
60	C	35.810152	4.996293	3.089759
61	C	42.925935	4.996293	3.097830
62	C	40.091979	4.996293	3.090028
63	C	38.662394	4.996293	3.089171

64	C	36.523140	4.996293	1.859099
65	C	42.244618	4.996293	1.862145
66	C	40.800881	4.996293	1.860309
67	C	37.950332	4.996293	1.859009
68	H	44.017404	4.996293	3.097680
69	C	25.883215	4.996293	3.596082
70	C	25.883236	4.996293	0.122164
71	H	7.749321	4.996293	5.550578
72	C	8.840572	4.996293	5.550651
73	C	11.675664	4.996293	5.550735
74	C	13.106363	4.996293	5.550817
75	C	20.234525	4.996293	5.557842
76	C	17.382361	4.996293	5.549707
77	C	15.957576	4.996293	5.550046
78	C	9.523510	4.996293	9.242175
79	C	10.967121	4.996293	9.242177
80	C	13.817910	4.996293	9.242183
81	C	19.525321	4.996293	9.242198
82	C	18.099835	4.996293	9.242189
83	C	15.243877	4.996293	9.242185
84	C	21.658735	4.996293	5.564463
85	C	24.525348	4.996293	5.510658
86	C	27.241268	4.996293	5.510453
87	C	34.384037	4.996293	5.548696
88	C	31.531942	4.996293	5.557042
89	C	30.107774	4.996293	5.563934
90	C	22.340776	4.996293	9.242219
91	C	23.732622	4.996293	9.242295
92	C	28.033895	4.996293	9.241899
93	C	33.665832	4.996293	9.241357
94	C	32.240706	4.996293	9.241672
95	C	29.425644	4.996293	9.241912
96	C	35.808870	4.996293	5.548617
97	C	42.924140	4.996293	5.569793
98	C	40.091958	4.996293	5.550797
99	C	38.661243	4.996293	5.550321
100	C	36.519605	4.996293	9.240699
101	C	42.217749	4.996293	9.241294
102	C	40.786022	4.996293	9.243099
103	C	37.943835	4.996293	9.239703
104	H	44.015629	4.996293	5.567969
105	H	7.749317	4.996293	8.011716
106	C	8.840570	4.996293	8.011687
107	C	11.675654	4.996293	8.011622
108	C	13.106352	4.996293	8.011548
109	C	20.234546	4.996293	8.004541
110	C	17.382349	4.996293	8.012672
111	C	15.957573	4.996293	8.012328
112	C	9.523413	4.996293	6.781168
113	C	10.967085	4.996293	6.781172
114	C	13.818373	4.996293	6.781182
115	C	19.514887	4.996293	6.781182
116	C	18.092201	4.996293	6.781185
117	C	15.245224	4.996293	6.781182
118	C	21.658730	4.996293	7.997934
119	C	24.525433	4.996293	8.051660
120	C	27.241314	4.996293	8.051487
121	C	34.382827	4.996293	8.011822
122	C	31.531755	4.996293	8.004002
123	C	30.107628	4.996293	7.997556
124	C	22.407877	4.996293	6.781166
125	C	23.867902	4.996293	6.781125
126	C	27.898662	4.996293	6.780915
127	C	33.673606	4.996293	6.779988
128	C	32.251332	4.996293	6.780382
129	C	29.358665	4.996293	6.780769
130	C	35.807153	4.996293	8.010852
131	C	42.920417	4.996293	8.048762

132	C	40.086783	4.996293	8.008987
133	C	38.656455	4.996293	8.010732
134	C	36.520494	4.996293	6.779961
135	C	42.241103	4.996293	6.794718
136	C	40.801236	4.996293	6.783575
137	C	37.946268	4.996293	6.779706
138	H	44.011980	4.996293	8.056706
139	C	25.883211	4.996293	8.518168
140	C	25.883263	4.996293	5.043952
141	H	7.749307	4.996293	10.472602
142	C	8.840561	4.996293	10.472660
143	C	11.675641	4.996293	10.472739
144	C	13.106340	4.996293	10.472816
145	C	20.234478	4.996293	10.479842
146	C	17.382332	4.996293	10.471700
147	C	15.957550	4.996293	10.472041
148	C	9.523502	4.996293	14.164198
149	C	10.967110	4.996293	14.164194
150	C	13.817893	4.996293	14.164186
151	C	19.525276	4.996293	14.164190
152	C	18.099795	4.996293	14.164185
153	C	15.243855	4.996293	14.164184
154	C	21.658690	4.996293	10.486478
155	C	24.525206	4.996293	10.432734
156	C	27.241054	4.996293	10.432667
157	C	34.383311	4.996293	10.471639
158	C	31.531547	4.996293	10.479776
159	C	30.107723	4.996293	10.486385
160	C	22.340714	4.996293	14.164190
161	C	23.732567	4.996293	14.164180
162	C	28.033848	4.996293	14.164428
163	C	33.665817	4.996293	14.165240
164	C	32.240791	4.996293	14.164861
165	C	29.425549	4.996293	14.164507
166	C	35.806297	4.996293	10.471975
167	N	42.857603	4.996293	10.472573
168	C	40.076300	4.996293	10.472657
169	C	38.653108	4.996293	10.472734
170	C	36.521754	4.996293	14.165245
171	C	42.240873	4.996293	14.150455
172	C	40.801105	4.996293	14.161595
173	C	37.946619	4.996293	14.165486
174	H	43.873060	4.996293	10.472523
175	H	7.749300	4.996293	12.933778
176	C	8.840554	4.996293	12.933711
177	C	11.675634	4.996293	12.933631
178	C	13.106332	4.996293	12.933550
179	C	20.234456	4.996293	12.926544
180	C	17.382314	4.996293	12.934668
181	C	15.957536	4.996293	12.934326
182	C	9.523389	4.996293	11.703187
183	C	10.967064	4.996293	11.703186
184	C	13.818346	4.996293	11.703184
185	C	19.514831	4.996293	11.703191
186	C	18.092151	4.996293	11.703185
187	C	15.245196	4.996293	11.703183
188	C	21.658655	4.996293	12.919930
189	C	24.525231	4.996293	12.973703
190	C	27.241129	4.996293	12.973736
191	C	34.382735	4.996293	12.935342
192	C	31.531639	4.996293	12.926920
193	C	30.107531	4.996293	12.920082
194	C	22.407758	4.996293	11.703201
195	C	23.867793	4.996293	11.703211
196	C	27.898553	4.996293	11.703272
197	C	33.673480	4.996293	11.703883
198	C	32.251073	4.996293	11.703539
199	C	29.358588	4.996293	11.703328

200	C	35.807075	4.996293	12.935652
201	C	42.920329	4.996293	12.896445
202	C	40.086720	4.996293	12.936088
203	C	38.656375	4.996293	12.934178
204	C	36.518203	4.996293	11.704513
205	C	42.217854	4.996293	11.703885
206	C	40.786004	4.996293	11.702088
207	C	37.943379	4.996293	11.705512
208	H	44.011894	4.996293	12.888655
209	C	25.883214	4.996293	13.440325
210	C	25.883302	4.996293	9.966135
211	H	7.749300	4.996293	15.394653
212	C	8.840551	4.996293	15.394683
213	C	11.675638	4.996293	15.394749
214	C	13.106334	4.996293	15.394821
215	C	20.234461	4.996293	15.401835
216	C	17.382312	4.996293	15.393700
217	C	15.957534	4.996293	15.394042
218	C	9.523521	4.996293	19.086194
219	C	10.967127	4.996293	19.086191
220	C	13.817910	4.996293	19.086185
221	C	19.525288	4.996293	19.086168
222	C	18.099815	4.996293	19.086178
223	C	15.243871	4.996293	19.086183
224	C	21.658662	4.996293	15.408457
225	C	24.525258	4.996293	15.354741
226	C	27.241180	4.996293	15.354911
227	C	34.383958	4.996293	15.394576
228	C	31.531857	4.996293	15.402533
229	C	30.107682	4.996293	15.408905
230	C	22.340761	4.996293	19.086170
231	C	23.732576	4.996293	19.086154
232	C	28.034020	4.996293	19.086287
233	C	33.667604	4.996293	19.086394
234	C	32.241878	4.996293	19.086321
235	C	29.425952	4.996293	19.086316
236	C	35.808796	4.996293	15.395330
237	C	42.924054	4.996293	15.375335
238	C	40.091879	4.996293	15.394513
239	C	38.661161	4.996293	15.395151
240	C	36.524443	4.996293	19.086119
241	C	42.244497	4.996293	19.083015
242	C	40.800813	4.996293	19.084867
243	C	37.950763	4.996293	19.086190
244	H	44.015543	4.996293	15.377028
245	H	7.749303	4.996293	17.855785
246	C	8.840553	4.996293	17.855719
247	C	11.675648	4.996293	17.855635
248	C	13.106343	4.996293	17.855555
249	C	20.234469	4.996293	17.848529
250	C	17.382321	4.996293	17.856666
251	C	15.957542	4.996293	17.856326
252	C	9.523400	4.996293	16.625201
253	C	10.967069	4.996293	16.625195
254	C	13.818347	4.996293	16.625186
255	C	19.514830	4.996293	16.625183
256	C	18.092148	4.996293	16.625184
257	C	15.245194	4.996293	16.625184
258	C	21.658678	4.996293	17.841904
259	C	24.525283	4.996293	17.895671
260	C	27.241225	4.996293	17.895790
261	C	34.385168	4.996293	17.857118
262	C	31.532263	4.996293	17.848948
263	C	30.108034	4.996293	17.842213
264	C	22.407772	4.996293	16.625198
265	C	23.867813	4.996293	16.625210
266	C	27.898644	4.996293	16.625357
267	C	33.674496	4.996293	16.625909

268	C	32.251802	4.996293	16.625650
269	C	29.358726	4.996293	16.625500
270	C	35.810081	4.996293	17.856740
271	C	42.925910	4.996293	17.847358
272	C	40.091926	4.996293	17.855032
273	C	38.662355	4.996293	17.855757
274	C	36.522337	4.996293	16.625319
275	C	42.243053	4.996293	16.615885
276	C	40.801007	4.996293	16.622064
277	C	37.949309	4.996293	16.625265
278	H	44.017378	4.996293	17.847591
279	C	25.883261	4.996293	18.362298
280	C	25.883180	4.996293	14.888227

GB2 atomic coordinates using GGA:

Coordinates (Angstroms)			
ATOM	X	Y	Z
1 C	5.393767	4.983450	10.310164
2 C	0.277018	4.983664	10.576899
3 C	5.838855	4.980728	7.870006
4 C	0.741914	4.980968	8.138669
5 H	6.022924	4.978184	5.698989
6 H	1.361136	4.978624	6.065403
7 C	0.744004	4.985222	11.924504
8 C	2.141822	4.985622	12.195755
9 C	1.204583	4.982443	9.497386
10 C	2.598182	4.982783	9.770962
11 C	1.679545	4.979790	7.105666
12 C	3.053137	4.980109	7.352104
13 H	3.620825	4.977701	5.257211
14 C	3.067310	4.984321	11.120906
15 C	4.465932	4.984730	11.385285
16 C	3.529203	4.981586	8.699013
17 C	4.926838	4.981953	8.955538
18 C	3.991127	4.978890	6.284303
19 C	5.334196	4.979189	6.539794
20 C	4.932078	4.986343	12.735308
21 C	6.328104	4.986769	13.002251
22 C	5.419173	5.005765	21.585487
23 C	0.301769	5.007980	21.910256
24 C	5.873325	4.997602	19.187436
25 C	0.754129	4.998471	19.472798
26 C	6.333586	4.992432	16.773063
27 C	1.216962	4.992788	17.046448
28 C	0.283324	4.988341	14.349393
29 C	1.679107	4.988821	14.621346
30 C	0.772289	5.015578	23.284943
31 C	2.170862	5.016714	23.617144
32 C	1.218156	5.002937	20.825604
33 C	2.606419	5.004079	21.109717
34 C	1.682417	4.995609	18.397224
35 C	3.076627	4.996400	18.672964
36 C	2.144317	4.990881	15.969957
37 C	3.541240	4.991464	16.241785
38 C	2.607610	4.987325	13.544663
39 C	4.003866	4.987809	13.813554
40 C	3.062455	5.010046	22.473964
41 C	4.475109	5.011264	22.623508
42 C	3.538535	5.000014	20.024661
43 C	4.947806	5.000721	20.259412
44 C	4.005220	4.993898	17.589330
45 C	5.405280	4.994529	17.846597
46 C	4.469820	4.989690	15.161939
47 C	5.866941	4.990216	15.426079
48 C	4.954845	5.019685	23.903108
49 N	6.288703	5.021011	24.286277
50 C	0.306478	5.038851	28.097528
51 C	0.757302	5.043717	30.536781
52 C	1.220226	5.047897	32.963082
53 C	0.285310	5.051736	35.661129
54 C	0.278367	5.055297	39.434011
55 C	0.742779	5.056986	41.872269
56 H	1.362018	5.058366	43.945403
57 C	0.777735	5.034298	26.720258
58 C	2.173373	5.031794	26.388310
59 C	1.221438	5.040863	29.182637
60 C	2.608666	5.039909	28.898837
61 C	1.686123	5.045683	31.612334
62 C	3.081024	5.045020	31.337045

63	C	2.147303	5.049530	34.040253
64	C	3.543112	5.049001	33.769289
65	C	4.005274	5.052170	36.197001
66	C	3.064577	5.036517	27.536019
67	C	4.474351	5.037269	27.383555
68	C	3.544643	5.042403	29.983755
69	C	4.950710	5.041708	29.749023
70	C	4.007924	5.046887	32.419883
71	C	5.406673	5.046291	32.162635
72	C	4.471126	5.050520	34.848495
73	C	5.868870	5.050127	34.584135
74	C	4.961021	5.034022	26.097558
75	C	6.297671	5.030377	25.708423
76	C	5.424509	5.039030	28.413971
77	C	5.874014	5.043798	30.820260
78	C	6.335384	5.048184	33.236778
79	C	1.681483	5.051270	35.389504
80	C	0.745616	5.054214	38.086180
81	C	2.143083	5.053873	37.815282
82	C	1.205560	5.056121	40.513242
83	C	2.599181	5.055878	40.239773
84	C	1.680346	5.057695	42.905106
85	C	3.054085	5.057519	42.658676
86	H	3.621652	5.059097	44.753511
87	C	2.609195	5.052540	36.465626
88	C	3.068311	5.054850	38.889845
89	C	4.467332	5.054581	38.625521
90	C	3.530207	5.056651	41.311757
91	C	4.927793	5.056438	41.055284
92	C	3.991918	5.058307	43.726401
93	C	5.335062	5.058174	43.470856
94	C	4.933564	5.053344	37.275337
95	C	6.329314	5.053056	37.008460
96	C	5.394829	5.055475	39.700367
97	C	5.839663	5.057193	42.140695
98	H	6.023811	5.058892	44.311647
99	C	4.114383	5.027525	24.997206
100	C	2.711890	5.025598	24.997005
101	C	11.905320	4.983356	10.309436
102	C	6.788845	4.983801	10.577235
103	C	12.350420	4.980621	7.869201
104	C	7.253225	4.981057	8.138763
105	H	12.534162	4.978043	5.698289
106	H	7.872212	4.978641	6.065559
107	C	7.255749	4.985383	11.924735
108	C	8.652910	4.985723	12.195367
109	C	7.715942	4.982532	9.497729
110	C	9.109581	4.982827	9.770853
111	C	8.190728	4.979808	7.105788
112	C	9.564600	4.980087	7.351911
113	H	10.131830	4.977618	5.257024
114	C	9.578365	4.984355	11.120552
115	C	10.977682	4.984689	11.384359
116	C	10.040793	4.981556	8.698611
117	C	11.438338	4.981873	8.954709
118	C	10.502267	4.978809	6.284071
119	C	11.845615	4.979073	6.539266
120	C	11.443619	4.986274	12.733957
121	C	12.839293	4.986619	13.000367
122	C	11.925316	5.006481	21.586371
123	C	6.811127	5.007736	21.926131
124	C	12.381063	4.997625	19.183429
125	C	7.262993	4.998693	19.477866
126	C	12.844580	4.992266	16.769398
127	C	7.728119	4.993067	17.049626
128	C	6.794448	4.988576	14.350180
129	C	8.190988	4.989013	14.621932
130	C	7.278262	5.014691	23.294109

131	C	8.657868	5.016691	23.626912
132	C	7.727197	5.003120	20.834762
133	C	9.110168	5.004368	21.111085
134	C	8.191902	4.995909	18.400226
135	C	9.588147	4.996655	18.672710
136	C	8.655853	4.991087	15.970389
137	C	10.051266	4.991557	16.239654
138	C	9.118662	4.987439	13.544962
139	C	10.514713	4.987815	13.812514
140	C	9.554292	5.010404	22.469094
141	C	10.968207	5.012422	22.622118
142	C	10.049927	5.000316	20.021516
143	C	11.454367	5.001024	20.254572
144	C	10.515610	4.993996	17.588082
145	C	11.914129	4.994505	17.843229
146	C	10.979926	4.989668	15.160269
147	C	12.378238	4.990085	15.423642
148	C	11.460451	5.022063	23.896997
149	C	12.809536	5.023845	24.280764
150	C	6.817596	5.037479	28.081274
151	C	7.266621	5.043209	30.532402
152	C	7.729815	5.047757	32.961478
153	C	6.795893	5.051619	35.659804
154	C	6.789905	5.055254	39.433352
155	C	7.254296	5.056991	41.871994
156	H	7.873068	5.058383	43.945102
157	C	7.296153	5.032644	26.705814
158	C	8.687552	5.031479	26.398344
159	C	7.730414	5.040234	29.176031
160	C	9.115876	5.039905	28.904452
161	C	8.194339	5.045544	31.609697
162	C	9.590810	5.045225	31.339437
163	C	8.657242	5.049575	34.040136
164	C	10.053825	5.049242	33.771771
165	C	10.516227	5.052376	36.198638
166	C	9.570931	5.036864	27.545690
167	C	10.981178	5.038743	27.391947
168	C	10.053231	5.042811	29.990686
169	C	11.460814	5.042619	29.757859
170	C	10.518751	5.047244	32.423484
171	C	11.917154	5.046870	32.168675
172	C	10.982015	5.050807	34.850364
173	C	12.380427	5.050514	34.587228
174	C	11.464093	5.036527	26.114578
175	C	12.813010	5.033287	25.727930
176	C	11.935618	5.040481	28.426651
177	C	12.385397	5.044638	30.827273
178	C	12.847185	5.048689	33.241550
179	C	8.192349	5.051269	35.388652
180	C	7.256789	5.054197	38.085791
181	C	8.654402	5.053922	37.815423
182	C	7.717087	5.056137	40.512924
183	C	9.110610	5.055953	40.239976
184	C	8.191599	5.057719	42.904868
185	C	9.565522	5.057590	42.658818
186	H	10.132671	5.059155	44.753732
187	C	9.120337	5.052643	36.465711
188	C	9.579592	5.054957	38.889966
189	C	10.978922	5.054746	38.626391
190	C	10.041739	5.056738	41.312125
191	C	11.439516	5.056561	41.056174
192	C	10.503192	5.058383	43.726709
193	C	11.846463	5.058269	43.471625
194	C	11.445031	5.053554	37.276852
195	C	12.841178	5.053315	37.010542
196	C	11.906687	5.055623	39.701352
197	C	12.351388	5.057310	42.141537
198	H	12.535007	5.058987	44.312608

199	C	10.610643	5.029594	25.006787
200	C	9.227766	5.026177	25.014614
201	C	18.417792	4.983294	10.309540
202	C	13.300544	4.983658	10.576231
203	C	18.862643	4.980613	7.869594
204	C	13.765313	4.980920	8.137879
205	H	19.046817	4.978075	5.698530
206	H	14.384504	4.978540	6.064838
207	C	13.767258	4.985207	11.923369
208	C	15.165098	4.985536	12.194086
209	C	14.228036	4.982393	9.496758
210	C	15.621501	4.982689	9.770035
211	C	14.702849	4.979704	7.105147
212	C	16.076909	4.979996	7.351474
213	H	16.644696	4.977579	5.256625
214	C	16.090490	4.984198	11.119942
215	C	17.489784	4.984577	11.384445
216	C	16.552913	4.981460	8.698155
217	C	17.950654	4.981823	8.954768
218	C	17.014866	4.978767	6.283770
219	C	18.358052	4.979070	6.539311
220	C	17.955778	4.986150	12.733711
221	C	19.351858	4.986566	13.001124
222	C	18.443526	5.006349	21.584561
223	C	13.320498	5.008286	21.909186
224	C	18.894752	4.997440	19.185108
225	C	13.773975	4.998626	19.468386
226	C	19.356891	4.992140	16.770325
227	C	14.238830	4.992832	17.044096
228	C	13.305875	4.988381	14.348396
229	C	14.702489	4.988774	14.619614
230	C	13.795527	5.016115	23.282597
231	C	15.189456	5.017645	23.610312
232	C	14.236350	5.003201	20.822130
233	C	15.621664	5.004449	21.103123
234	C	14.703464	4.995683	18.394030
235	C	16.099179	4.996432	18.669033
236	C	15.167419	4.990818	15.967008
237	C	16.563844	4.991306	16.238091
238	C	15.631094	4.987217	13.543230
239	C	17.026617	4.987618	13.811785
240	C	16.076702	5.010820	22.464176
241	C	17.488245	5.012541	22.618326
242	C	16.560338	5.000200	20.018784
243	C	17.968939	5.000883	20.253602
244	C	17.028442	4.993752	17.586475
245	C	18.426816	4.994316	17.843551
246	C	17.492345	4.989472	15.159924
247	C	18.890697	4.989954	15.424745
248	C	17.973283	5.022074	23.895377
249	C	19.325088	5.023475	24.279386
250	C	13.327690	5.039306	28.101958
251	C	13.778830	5.044165	30.541950
252	C	14.242480	5.048283	32.966705
253	C	13.308207	5.051925	35.662405
254	C	13.301679	5.055415	39.434638
255	C	13.766240	5.057086	41.872923
256	H	14.385477	5.058442	43.946030
257	C	13.799116	5.034992	26.725287
258	C	15.192585	5.033073	26.398669
259	C	14.242429	5.041532	29.188693
260	C	15.627792	5.040959	28.906997
261	C	14.708003	5.046223	31.616315
262	C	16.103183	5.045746	31.341112
263	C	15.170134	5.049921	34.043056
264	C	16.566807	5.049452	33.772021
265	C	17.028909	5.052436	36.198875
266	C	16.081183	5.037907	27.544532

267	C	17.491876	5.039155	27.390098
268	C	16.565345	5.043390	29.990348
269	C	17.973733	5.042804	29.755063
270	C	17.031913	5.047467	32.423721
271	C	18.430672	5.046849	32.166537
272	C	17.495190	5.050857	34.850273
273	C	18.893117	5.050391	34.585568
274	C	17.976155	5.036670	26.111749
275	C	19.326271	5.032926	25.726674
276	C	18.447825	5.040511	28.423498
277	C	18.899130	5.044514	30.824043
278	C	19.360006	5.048496	33.239108
279	C	14.704550	5.051559	35.391227
280	C	13.768763	5.054377	38.087182
281	C	15.166651	5.054077	37.816523
282	C	14.229109	5.056254	40.514053
283	C	15.622720	5.056021	40.240804
284	C	14.703859	5.057797	42.905727
285	C	16.077723	5.057611	42.659377
286	H	16.645595	5.059146	44.754237
287	C	15.632924	5.052810	36.467374
288	C	16.092003	5.055029	38.890770
289	C	17.491073	5.054742	38.626368
290	C	16.553873	5.056767	41.312577
291	C	17.951660	5.056523	41.055996
292	C	17.015771	5.058372	43.727090
293	C	18.358889	5.058210	43.471570
294	C	17.957400	5.053529	37.276607
295	C	19.353601	5.053179	37.009321
296	C	18.418876	5.055565	39.701241
297	C	18.863616	5.057238	42.141235
298	H	19.047657	5.058903	44.312353
299	C	17.125254	5.029999	25.004060
300	C	15.736530	5.027185	25.004626

GB9 atomic coordinates using GGA:

Coordinates (Angstroms)			
ATOM	X	Y	Z
1 C	5.399532	4.983215	10.308330
2 C	0.287125	4.983656	10.562829
3 C	5.877202	4.980760	7.871401
4 C	0.763601	4.981138	8.124989
5 H	6.057903	4.978433	5.680212
6 H	1.392732	4.978998	6.049774
7 C	0.749625	4.985104	11.912364
8 C	2.145567	4.985395	12.188271
9 C	1.219973	4.982459	9.482093
10 C	2.614481	4.982703	9.761057
11 C	1.711036	4.980044	7.090380
12 C	3.082510	4.980288	7.341005
13 H	3.670374	4.978090	5.246320
14 C	3.075320	4.984086	11.112720
15 C	4.466995	4.984410	11.383745
16 C	3.552072	4.981581	8.691124
17 C	4.947570	4.981865	8.958705
18 C	4.035570	4.979167	6.275022
19 C	5.376713	4.979383	6.532142
20 C	4.932354	4.985959	12.731557
21 C	6.328843	4.986394	13.002926
22 C	5.420655	5.006124	21.580830
23 C	0.301575	5.007822	21.903538
24 C	5.871558	4.997325	19.179713
25 C	0.752185	4.998409	19.462987
26 C	6.332566	4.991962	16.766229
27 C	1.216622	4.992638	17.037087
28 C	0.285330	4.988195	14.337793
29 C	1.678958	4.988577	14.612191
30 C	0.774182	5.015308	23.280994
31 C	2.167622	5.016771	23.608314
32 C	1.215459	5.002881	20.816784
33 C	2.601428	5.004082	21.099251
34 C	1.681387	4.995448	18.387683
35 C	3.075686	4.996220	18.664200
36 C	2.143626	4.990585	15.960499
37 C	3.540085	4.991085	16.233932
38 C	2.608360	4.987006	13.534926
39 C	4.003957	4.987383	13.807395
40 C	3.055525	5.010247	22.461563
41 C	4.466223	5.011984	22.617158
42 C	3.537745	4.999964	20.014809
43 C	4.946249	5.000726	20.250334
44 C	4.004277	4.993568	17.580592
45 C	5.403234	4.994146	17.838060
46 C	4.469728	4.989247	15.155365
47 C	5.865598	4.989744	15.421402
48 C	4.950977	5.020975	23.895164
49 C	6.302259	5.022578	24.281172
50 C	0.301342	5.038679	28.103522
51 C	0.751105	5.044231	30.544818
52 C	1.214281	5.048523	32.970611
53 C	0.279683	5.052077	35.667643
54 C	0.273165	5.055325	39.440560
55 C	0.737620	5.056820	41.878986
56 H	1.356566	5.058057	43.952133
57 C	0.774121	5.033889	26.726145
58 C	2.167509	5.031999	26.399873
59 C	1.215035	5.041275	29.190296
60 C	2.600829	5.040583	28.909012
61 C	1.679684	5.046369	31.619996
62 C	3.075037	5.045870	31.345120

63	C	2.141554	5.050126	34.047916
64	C	3.537945	5.049719	33.777313
65	C	4.000081	5.052608	36.204732
66	C	3.055044	5.037061	27.546418
67	C	4.466105	5.037874	27.391419
68	C	3.537239	5.043320	29.993964
69	C	4.945476	5.042796	29.759374
70	C	4.002876	5.047777	32.428604
71	C	5.401607	5.047258	32.172545
72	C	4.466163	5.051147	34.856140
73	C	5.864065	5.050778	34.592306
74	C	4.950801	5.034580	26.113212
75	C	6.302066	5.031424	25.727377
76	C	5.420155	5.040059	28.427760
77	C	5.869963	5.044894	30.830084
78	C	6.330789	5.048993	33.245555
79	C	1.676094	5.051730	35.396438
80	C	0.740267	5.054359	38.092963
81	C	2.137949	5.054096	37.822355
82	C	1.200438	5.056063	40.519992
83	C	2.594033	5.055886	40.246802
84	C	1.675078	5.057465	42.911846
85	C	3.048872	5.057320	42.665627
86	H	3.616218	5.058715	44.760407
87	C	2.604072	5.052916	36.472854
88	C	3.063201	5.054995	38.896787
89	C	4.462299	5.054757	38.632698
90	C	3.525118	5.056564	41.318799
91	C	4.922837	5.056381	41.062395
92	C	3.986807	5.058013	43.733337
93	C	5.329971	5.057897	43.477854
94	C	4.928545	5.053684	37.282784
95	C	6.324608	5.053401	37.016012
96	C	5.389947	5.055555	39.707557
97	C	5.834775	5.057035	42.147693
98	H	6.018991	5.058527	44.318496
99	C	4.101292	5.028225	25.004074
100	C	2.713030	5.025907	25.003735
101	C	11.909425	4.983515	10.300288
102	C	6.789147	4.983593	10.583719
103	C	12.346023	4.980815	7.851857
104	C	7.259483	4.981073	8.174461
105	H	12.491824	4.978063	5.689398
106	H	7.873678	4.978738	6.208321
107	C	7.259492	4.985094	11.927896
108	C	8.653064	4.985556	12.197388
109	C	7.720220	4.982431	9.512604
110	C	9.117561	4.982845	9.787234
111	N	8.200068	4.979942	7.168585
112	C	9.561962	4.980182	7.374329
113	H	10.079991	4.977546	5.271697
114	C	9.583068	4.984330	11.118566
115	C	10.987519	4.984747	11.377339
116	C	10.043395	4.981675	8.704356
117	C	11.441128	4.982056	8.946951
118	C	10.456539	4.978822	6.296726
119	C	11.820018	4.979146	6.544504
120	C	11.450614	4.986294	12.724692
121	C	12.845630	4.986710	12.988613
122	C	11.932851	5.006233	21.578877
123	C	6.814262	5.007791	21.904878
124	C	12.383739	4.997530	19.175134
125	C	7.263981	4.998378	19.464618
126	C	12.847412	4.992227	16.759324
127	C	7.728838	4.992642	17.040922
128	C	6.795129	4.988148	14.346098
129	C	8.192027	4.988679	14.616696
130	C	7.287033	5.015290	23.281731

131	C	8.679726	5.016792	23.607769
132	C	7.727946	5.002885	20.818423
133	C	9.114085	5.004160	21.099154
134	C	8.193598	4.995510	18.388962
135	C	9.589559	4.996333	18.662768
136	C	8.657634	4.990705	15.963381
137	C	10.053160	4.991288	16.231485
138	C	9.120093	4.987205	13.540974
139	C	10.519620	4.987692	13.805860
140	C	9.567968	5.010304	22.460464
141	C	10.979054	5.012067	22.615354
142	C	10.051280	5.000089	20.013292
143	C	11.458602	5.000863	20.247191
144	C	10.517525	4.993763	17.578939
145	C	11.916945	4.994366	17.834321
146	C	10.983137	4.989551	15.149835
147	C	12.382786	4.990050	15.413140
148	C	11.463322	5.021030	23.893870
149	C	12.813969	5.022615	24.279426
150	C	6.813535	5.038681	28.103758
151	C	7.263059	5.044246	30.544969
152	C	7.726169	5.048529	32.970672
153	C	6.791500	5.052091	35.667723
154	C	6.784972	5.055336	39.440611
155	C	7.249412	5.056836	41.879031
156	H	7.868409	5.058076	43.952157
157	C	7.286478	5.033902	26.726591
158	C	8.679609	5.032032	26.399987
159	C	7.727152	5.041296	29.190438
160	C	9.112935	5.040613	28.909007
161	C	8.191631	5.046380	31.620142
162	C	9.587001	5.045877	31.345212
163	C	8.653458	5.050131	34.047995
164	C	10.049779	5.049716	33.777371
165	C	10.511914	5.052609	36.204730
166	C	9.567248	5.037087	27.546493
167	C	10.978159	5.037901	27.391083
168	C	10.049296	5.043330	29.994007
169	C	11.457290	5.042798	29.759268
170	C	10.514748	5.047768	32.428600
171	C	11.913449	5.047250	32.172425
172	C	10.977990	5.051159	34.856174
173	C	12.375913	5.050770	34.592260
174	C	11.462953	5.034606	26.112540
175	C	12.813919	5.031449	25.726690
176	C	11.931955	5.040061	28.427405
177	C	12.381734	5.044885	30.829971
178	C	12.842633	5.048983	33.245489
179	C	8.187950	5.051734	35.396519
180	C	7.252094	5.054371	38.093013
181	C	8.649753	5.054115	37.822411
182	C	7.712237	5.056078	40.520020
183	C	9.105850	5.055894	40.246827
184	C	8.186910	5.057467	42.911857
185	C	9.560721	5.057322	42.665658
186	H	10.128176	5.058711	44.760421
187	C	9.115894	5.052925	36.472884
188	C	9.575013	5.055004	38.896828
189	C	10.974135	5.054763	38.632716
190	C	10.036958	5.056574	41.318822
191	C	11.434666	5.056375	41.062405
192	C	10.498690	5.058018	43.733318
193	C	11.841867	5.057877	43.477845
194	C	11.440388	5.053678	37.282796
195	C	12.836412	5.053390	37.015987
196	C	11.901766	5.055541	39.707549
197	C	12.346623	5.057027	42.147687
198	H	12.530888	5.058513	44.318481

199	C	10.613318	5.028287	25.003371
200	C	9.225561	5.025941	25.003874
201	C	18.429354	4.983394	10.294074
202	C	13.308912	4.983857	10.562568
203	C	18.881513	4.980829	7.854705
204	C	13.773357	4.981185	8.118094
205	H	19.062709	4.978314	5.683908
206	H	14.390713	4.978814	6.047357
207	C	13.773357	4.985354	11.907561
208	C	15.172911	4.985706	12.179870
209	C	14.235561	4.982613	9.477598
210	C	15.629946	4.982908	9.753053
211	C	14.709030	4.979982	7.088692
212	C	16.089148	4.980267	7.335814
213	H	16.661471	4.977861	5.241888
214	C	16.097901	4.984361	11.104259
215	C	17.497550	4.984647	11.370423
216	C	16.564606	4.981694	8.680823
217	C	17.965219	4.981998	8.939483
218	C	17.029441	4.979050	6.269951
219	C	18.374566	4.979330	6.525618
220	C	17.960134	4.986187	12.719359
221	C	19.356357	4.986493	12.989030
222	C	18.444331	5.006196	21.578965
223	C	13.326178	5.007915	21.902954
224	C	18.894584	4.997427	19.176533
225	C	13.777283	4.998551	19.460691
226	C	19.356676	4.992049	16.760011
227	C	14.241636	4.992860	17.034345
228	C	13.310411	4.988442	14.337103
229	C	14.707010	4.988887	14.608533
230	C	13.798112	5.015343	23.279402
231	C	15.191613	5.016827	23.606436
232	C	14.240233	5.003014	20.815252
233	C	15.625230	5.004228	21.097067
234	C	14.705821	4.995678	18.385288
235	C	16.101127	4.996438	18.661044
236	C	15.169817	4.990885	15.955429
237	C	16.566584	4.991351	16.227519
238	C	15.636155	4.987327	13.529107
239	C	17.030476	4.987663	13.798779
240	C	16.079023	5.010352	22.459773
241	C	17.490077	5.012063	22.615427
242	C	16.562099	5.000145	20.011180
243	C	17.970337	5.000866	20.246935
244	C	17.029798	4.993783	17.576253
245	C	18.426999	4.994296	17.833727
246	C	17.494591	4.989496	15.148366
247	C	18.891801	4.989883	15.414465
248	C	17.974209	5.021005	23.893639
249	C	19.325545	5.022591	24.279789
250	C	13.325219	5.038680	28.103310
251	C	13.774838	5.044234	30.544740
252	C	14.237926	5.048519	32.970544
253	C	13.303303	5.052078	35.667660
254	C	13.296800	5.055320	39.440578
255	C	13.761274	5.056831	41.879016
256	H	14.380303	5.058039	43.952151
257	C	13.797946	5.033922	26.726058
258	C	15.191236	5.032021	26.399331
259	C	14.238831	5.041282	29.190145
260	C	15.624493	5.040590	28.908657
261	C	14.703341	5.046368	31.619933
262	C	16.098698	5.045863	31.344979
263	C	15.165218	5.050131	34.047915
264	C	16.561549	5.049712	33.777297
265	C	17.023672	5.052599	36.204692
266	C	16.078644	5.037074	27.545929

267	C	17.489668	5.037889	27.390848
268	C	16.560882	5.043319	29.993777
269	C	17.968949	5.042789	29.759224
270	C	17.026490	5.047755	32.428473
271	C	18.425106	5.047238	32.172422
272	C	17.489731	5.051139	34.856082
273	C	18.887657	5.050762	34.592220
274	C	17.974234	5.034587	26.112365
275	C	19.325434	5.031445	25.726889
276	C	18.443548	5.040051	28.427271
277	C	18.893355	5.044883	30.829867
278	C	19.354328	5.048986	33.245479
279	C	14.699749	5.051724	35.396417
280	C	13.763901	5.054357	38.092993
281	C	15.161572	5.054103	37.822372
282	C	14.224076	5.056063	40.519995
283	C	15.617658	5.055882	40.246797
284	C	14.698740	5.057452	42.911840
285	C	16.072555	5.057296	42.665624
286	H	16.639994	5.058664	44.760435
287	C	15.627710	5.052916	36.472829
288	C	16.086809	5.054984	38.896776
289	C	17.485927	5.054743	38.632665
290	C	16.548757	5.056554	41.318793
291	C	17.946461	5.056351	41.062381
292	C	17.010469	5.057971	43.733333
293	C	18.353632	5.057853	43.477850
294	C	17.952159	5.053670	37.282764
295	C	19.348199	5.053391	37.015975
296	C	18.413566	5.055525	39.707524
297	C	18.858377	5.057008	42.147678
298	H	19.042581	5.058477	44.318536
299	C	17.124674	5.028243	25.002952
300	C	15.736674	5.025930	25.002803
