

Supplementary Information for “Theoretical study of Nano Onion-Like Fullerenes C₂₀@C₈₀ on XPS and NEXAFS Spectra”

In our calculation, we used ‘INSPUR’ server with the first principles to simulate the C 1s XPS and NEXAFS spectra of NOLFs system. NOLFs C₂₀@C₈₀ is structure with the similar C-C band and C=C band alternating, we first list the bond lengths of two C₂₀@C₈₀ isomers in table 1.

Table 1. The bond lengths(Å) of the two C₂₀@C₈₀(D_{5d}) molecules before and after optimization.

	Outer bond length(Å)	Inner bond length(Å)	Distance between the inner and outer carbon atoms(Å)
C ₂₀ @C ₈₀ (D _{5d}) before optimization	1.41-1.44	1.40	2.1-2.2
C ₂₀ @C ₈₀ (D _{5d}) after optimization	1.41-1.55	1.38,1.43,1.53	1.66,2.49
C ₂₀ @C ₈₀ (D _{5d}) before optimization	1.44-1.49	1.37,1.47-1.49	1.8,2.27
C ₂₀ @C ₈₀ (D _{5d}) after optimization	1.44-1.49	1.37,1.47-1.49	1.8,2.27

For the five structures, i.e., C₂₀@C₈₀(D_{5d}), C₂₀@C₈₀(D_{5d}'), C₂₀(I_h), C₈₀(I_h) and C₁₀₀(D₂), the functional used for structural optimization is B3LYP, the selected base set is 6-31G, and the convergence condition is scf=NoVarAcc. We list the coreness, memory and time used in these five structural optimizations in Table 2.

Table 2. The coreness, memory and time used in the two optimized NOLFs C₂₀@C₈₀ isomers, fullerenes C₂₀(I_h), C₈₀(I_h) and C₁₀₀(D₂).

Molecule	Coreness	Memory(GB)	Time
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$C_{20}@C_{80}(D_{5d})$	6	10	5 days 15 hours 27 minutes 15 seconds
$C_{20}@C_{80}(D_{5d'})$	20	36	11 hours 32 minutes 58 seconds
$C_{20}(I_h)$	6	10	3 hours 40 minutes 11.1 seconds
$C_{80}(I_h)$	2	2	2 days 3 hours 17 minutes 42.9 seconds
$C_{100}(D_2)$	2	2	22 hours 31 minutes 21.3 seconds

We list the three-dimensional coordinates of two NOLFs $C_{20}@C_{80}$ isomers, fullerenes $C_{20}(I_h)$, $C_{80}(I_h)$ and $C_{100}(D_2)$ in Table 3.

Table 3. The three-dimensional coordinates of $C_{20}@C_{80}(D_{5d})$ and $C_{20}@C_{80}(D_{5d'})$, fullerenes $C_{20}(I_h)$, $C_{80}(I_h)$ and $C_{100}(D_2)$.

$C_{20}@C_{80}(D_{5d})$	X	Y	Z
C_1	1.29689300	-3.49943260	1.68528993
C_2	0.86524334	-2.76791579	2.85047371
C_3	1.70187977	-1.72435464	3.32396492
C_4	-0.52693114	-2.66361400	3.08141960
C_5	0.35803367	-4.00269587	0.74958923
C_6	-1.86167535	-3.63588846	-0.24371002
C_7	-1.04694012	-3.79004787	0.92807498

C ₈	-1.47423509	-3.16762230	2.11480330
C ₉	-1.09387619	-1.49102992	3.67647699
C ₁₀	-0.26490988	-0.39464462	4.06036627
C ₁₁	1.14716463	-0.54971199	3.92617815
C ₁₂	-0.80206807	0.91047858	3.94424578
C ₁₃	-2.38698752	-1.27543517	3.09557323
C ₁₄	-3.71892084	0.25839342	1.73242051
C ₁₅	-2.88412273	0.03794121	2.88108315
C ₁₆	-2.10110490	1.12296221	3.34717383
C ₁₇	-2.98873167	-2.78958365	-0.23565361
C ₁₈	-3.36298200	-2.06728448	0.94650871
C ₁₉	-2.62861827	-2.31798782	2.13453186
C ₂₀	-3.94988682	-0.78183127	0.78190637
C ₂₁	0.03121289	2.01731114	3.58813479
C ₂₂	1.41960322	1.84330319	3.34930651
C ₂₃	1.97668967	0.56156126	3.57188582
C ₂₄	2.03589621	2.67772016	2.35133359
C ₂₅	-0.75066013	2.91727487	2.78450735
C ₂₆	-0.95565242	3.92614800	0.56933139
C ₂₇	-0.15581560	3.65409084	1.72575897
C ₂₈	1.25778945	3.56473821	1.56043457
C ₂₉	-3.67901943	1.49600858	1.02855756

C ₃₀	-2.81781034	2.54321506	1.44248064
C ₃₁	-2.06529486	2.35764383	2.63916395
C ₃₂	-2.25397991	3.38722476	0.42935783
C ₃₃	3.10613787	2.18614748	1.54286264
C ₃₄	3.59072230	0.85703849	1.69456183
C ₃₅	3.05468100	0.06878866	2.74926283
C ₃₆	4.06235898	0.17690771	0.52502648
C ₃₇	2.98873167	2.78958365	0.23565361
C ₃₈	2.62861827	2.31798782	-2.13453186
C ₃₉	3.36298200	2.06728448	-0.94650871
C ₄₀	3.94988682	0.78183127	-0.78190637
C ₄₁	-0.35803367	4.00269587	-0.74958923
C ₄₂	1.04694012	3.79004787	-0.92807498
C ₄₃	1.86167535	3.63588846	0.24371002
C ₄₄	1.47423509	3.16762230	-2.11480330
C ₄₅	3.89592669	-1.22068877	0.37737108
C ₄₆	3.25021502	-1.99534477	1.38693658
C ₄₇	2.88489732	-1.33878909	2.59825672
C ₄₈	2.47285909	-3.11468936	0.97154769
C ₄₉	3.67901943	-1.49600858	-1.02855756
C ₅₀	2.06529486	-2.35764383	-2.63916395
C ₅₁	2.81781034	-2.54321506	-1.44248064

C ₅₂	2.25397991	-3.38722476	-0.42935783
C ₅₃	2.38698752	1.27543517	-3.09557323
C ₅₄	2.88412273	-0.03794121	-2.88108315
C ₅₅	3.71892084	-0.25839342	-1.73242051
C ₅₆	2.10110490	-1.12296221	-3.34717383
C ₅₇	0.75066013	-2.91727487	-2.78450735
C ₅₈	0.15581560	-3.65409084	-1.72575897
C ₅₉	0.95565242	-3.92614800	-0.56933139
C ₆₀	-1.25778945	-3.56473821	-1.56043457
C ₆₁	-0.03121289	-2.01731114	-3.58813479
C ₆₂	-1.97668967	-0.56156126	-3.57188582
C ₆₃	-1.41960322	-1.84330319	-3.34930651
C ₆₄	-2.03589621	-2.67772016	-2.35133359
C ₆₅	1.09387619	1.49102992	-3.67647699
C ₆₆	-1.14716463	0.54971199	-3.92617815
C ₆₇	0.26490988	0.39464462	-4.06036627
C ₆₈	0.80206807	-0.91047858	-3.94424578
C ₆₉	-1.29689300	3.49943260	-1.68528993
C ₇₀	-1.70187977	1.72435464	-3.32396492
C ₇₁	-0.86524334	2.76791579	-2.85047371
C ₇₂	0.52693114	2.66361400	-3.08141960
C ₇₃	-3.89592669	1.22068877	-0.37737108

C ₇₄	-2.88489732	1.33878909	-2.59825672
C ₇₅	-3.25021502	1.99534477	-1.38693658
C ₇₆	-2.47285909	3.11468936	-0.97154769
C ₇₇	-3.10613787	-2.18614748	-1.54286264
C ₇₈	-3.05468100	-0.06878866	-2.74926283
C ₇₉	-3.59072230	-0.85703849	-1.69456183
C ₈₀	-4.06235898	-0.17690771	-0.52502648
C ₈₁	-0.70069885	-0.96442923	1.56047870
C ₈₂	-1.13375455	0.36837919	1.56047870
C ₈₃	0.70069885	-0.96442923	1.56047870
C ₈₄	1.13375455	0.36837919	1.56047870
C ₈₅	-0.00000000	1.19210009	1.56047870
C ₈₆	1.13375363	-1.56047881	0.36838156
C ₈₇	1.83445321	-0.59604960	-0.36837845
C ₈₈	1.83445292	0.59604976	0.36837961
C ₈₉	0.00000092	-1.92885849	-0.36837657
C ₉₀	0.00000080	-1.19210014	-1.56047866
C ₉₁	1.13375612	-0.36837922	-1.56047755
C ₉₂	-1.13375306	-1.56047959	0.36837999
C ₉₃	-1.83445345	-0.59604875	-0.36837863
C ₉₄	-1.13375420	-0.36837859	-1.56047910
C ₉₅	-1.83445278	0.59605048	0.36837918

C ₉₆	-1.13375407	1.56047922	-0.36837845
C ₉₇	-0.70069761	0.96443068	-1.56047836
C ₉₈	0.70069885	0.96443066	-1.56047782
C ₉₉	1.13375507	1.56047863	-0.36837787
C ₁₀₀	-0.00000012	1.92885791	0.36837961

C ₂₀ @C ₈₀ (D _{5d})	X	Y	Z
C ₁	1.33794600	-3.66353700	1.75103700
C ₂	0.88245300	-2.90460600	2.89458400
C ₃	1.76649300	-1.83244900	3.39582000
C ₄	-0.57519800	-2.82006200	3.11850400
C ₅	0.36266000	-4.15826500	0.76892900
C ₆	-1.93695500	-3.76583600	-0.27693000
C ₇	-1.09105900	-3.94322300	0.92078300
C ₈	-1.55167500	-3.34937600	2.15631400
C ₉	-1.14935300	-1.62540500	3.68285900
C ₁₀	-0.27397500	-0.43984400	3.88340200
C ₁₁	1.19825600	-0.63550500	3.96122900
C ₁₂	-0.86456900	0.92391100	4.01183600
C ₁₃	-2.44943900	-1.40387400	3.09236800

C ₁₄	-3.83200800	0.22201100	1.67341700
C ₁₅	-2.81158800	-0.00759800	2.73072900
C ₁₆	-2.16442800	1.14536500	3.42087500
C ₁₇	-3.12661500	-2.90229100	-0.27960600
C ₁₈	-3.47691700	-2.16090200	0.91143000
C ₁₉	-2.71763300	-2.45447800	2.14396000
C ₂₀	-4.09721900	-0.83248900	0.72895500
C ₂₁	-0.02289900	2.04871700	3.67441500
C ₂₂	1.36894300	1.75549500	3.22507300
C ₂₃	2.04007500	0.48933600	3.62375600
C ₂₄	2.10845800	2.72768300	2.37656800
C ₂₅	-0.80232700	2.96572800	2.87433900
C ₂₆	-0.97643400	4.03802500	0.52823900
C ₂₇	-0.15266600	3.54722500	1.66460900
C ₂₈	1.32851600	3.64510600	1.57683900
C ₂₉	-3.79355000	1.48441800	0.97030100
C ₃₀	-2.73765100	2.45674200	1.35854300
C ₃₁	-2.12605600	2.40732600	2.71767300
C ₃₂	-2.30089000	3.47955800	0.37159900
C ₃₃	3.22244900	2.25496300	1.59560800
C ₃₄	3.70579900	0.86868700	1.76177000
C ₃₅	3.15406200	0.02190000	2.83919800

C ₃₆	4.22964200	0.20049500	0.59118100
C ₃₇	3.12661500	2.90229100	0.27960600
C ₃₈	2.71763300	2.45447800	-2.14396000
C ₃₉	3.47691700	2.16090200	-0.91143000
C ₄₀	4.09721900	0.83248900	-0.72895500
C ₄₁	-0.36266000	4.15826500	-0.76892900
C ₄₂	1.09105900	3.94322300	-0.92078300
C ₄₃	1.93695500	3.76583600	0.27693000
C ₄₄	1.55167500	3.34937600	-2.15631400
C ₄₅	4.03354700	-1.24746800	0.42989700
C ₄₆	3.34756200	-2.07108200	1.44627000
C ₄₇	2.99438500	-1.43214400	2.69457300
C ₄₈	2.54436000	-3.23802300	1.02711100
C ₄₉	3.79355000	-1.48441800	-0.97030100
C ₅₀	2.12605600	-2.40732600	-2.71767300
C ₅₁	2.73765100	-2.45674200	-1.35854300
C ₅₂	2.30089000	-3.47955800	-0.37159900
C ₅₃	2.44943900	1.40387400	-3.09236800
C ₅₄	2.81158800	0.00759800	-2.73072900
C ₅₅	3.83200800	-0.22201100	-1.67341700
C ₅₆	2.16442800	-1.14536500	-3.42087500
C ₅₇	0.80232700	-2.96572800	-2.87433900

C ₅₈	0.15266600	-3.54722500	-1.66460900
C ₅₉	0.97643400	-4.03802500	-0.52823900
C ₆₀	-1.32851600	-3.64510600	-1.57683900
C ₆₁	0.02289900	-2.04871700	-3.67441500
C ₆₂	-2.04007500	-0.48933600	-3.62375600
C ₆₃	-1.36894300	-1.75549500	-3.22507300
C ₆₄	-2.10845800	-2.72768300	-2.37656800
C ₆₅	1.14935300	1.62540500	-3.68285900
C ₆₆	-1.19825600	0.63550500	-3.96122900
C ₆₇	0.27397500	0.43984400	-3.88340200
C ₆₈	0.86456900	-0.92391100	-4.01183600
C ₆₉	-1.33794600	3.66353700	-1.75103700
C ₇₀	-1.76649300	1.83244900	-3.39582000
C ₇₁	-0.88245300	2.90460600	-2.89458400
C ₇₂	0.57519800	2.82006200	-3.11850400
C ₇₃	-4.03354700	1.24746800	-0.42989700
C ₇₄	-2.99438500	1.43214400	-2.69457300
C ₇₅	-3.34756200	2.07108200	-1.44627000
C ₇₆	-2.54436000	3.23802300	-1.02711100
C ₇₇	-3.22244900	-2.25496300	-1.59560800
C ₇₈	-3.15406200	-0.02190000	-2.83919800
C ₇₉	-3.70579900	-0.86868700	-1.76177000

C ₈₀	-4.22964200	-0.20049500	-0.59118100
C ₈₁	1.53686100	-0.95427400	0.65050600
C ₈₂	1.46076300	-1.32457400	-0.76990500
C ₈₃	0.40010800	-1.32166300	1.33430900
C ₈₄	-0.49504300	-1.81112200	0.41004600
C ₈₅	0.09991000	-1.89832500	-0.93059100
C ₈₆	-0.16381700	-0.20057600	2.10171600
C ₈₇	-1.50050800	0.02744200	1.49318800
C ₈₈	-1.59435600	-0.98216500	0.42823000
C ₈₉	0.70227800	0.95656700	1.75439400
C ₉₀	-0.09991000	1.89832500	0.93059100
C ₉₁	-1.46076300	1.32457400	0.76990500
C ₉₂	1.69160900	0.40382500	0.81674600
C ₉₃	1.59435600	0.98216500	-0.42823000
C ₉₄	0.49504300	1.81112200	-0.41004600
C ₉₅	1.50050800	-0.02744200	-1.49318800
C ₉₆	0.16381700	0.20057600	-2.10171600
C ₉₇	-0.40010800	1.32166300	-1.33430900
C ₉₈	-1.53686100	0.95427400	-0.65050600
C ₉₉	-1.69160900	-0.40382500	-0.81674600
C ₁₀₀	-0.70227800	-0.95656700	-1.75439400

$C_{20}(I_h)$	X	Y	Z
C_1	1.618560	-0.663050	-0.948050
C_2	1.814710	0.662620	-0.477970
C_3	0.489850	-0.664500	-1.809810
C_4	-0.009400	0.663290	-1.876170
C_5	0.808540	1.482680	-1.053920
C_6	-0.509520	-1.485110	-1.222910
C_7	-1.629760	-0.663000	-0.929930
C_8	-1.321090	0.663450	-1.332130
C_9	0.002570	-1.989390	0.001850
C_{10}	-0.807180	-1.483130	1.052850
C_{11}	-1.814460	-0.663680	0.478050
C_{12}	1.317610	-1.481520	0.172760
C_{13}	1.321200	-0.661890	1.332370
C_{14}	0.009340	-0.663250	1.876000
C_{15}	1.629050	0.664640	0.929870
C_{16}	0.506980	1.482420	1.227630
C_{17}	-0.495830	0.662180	1.809000
C_{18}	-1.621670	0.663930	0.943600
C_{19}	-1.312690	1.484360	-0.173470
C_{20}	0.003200	1.988950	0.000400

$C_{80}(I_h)$	X	Y	Z
C_1	1.321660	-2.497670	2.942760
C_2	1.051450	-1.293680	3.688740
C_3	1.976610	-0.223850	3.575970
C_4	-0.301260	-0.979960	3.960990
C_5	0.265490	-3.279670	2.410550
C_6	-2.034050	-3.200320	1.542150
C_7	-1.101390	-2.891160	2.588670
C_8	-1.369270	-1.775530	3.402260
C_9	-0.751260	0.378450	4.012910
C_{10}	0.158480	1.456650	3.797330
C_{11}	1.539630	1.138510	3.632350
C_{12}	-0.335390	2.617540	3.154060
C_{13}	-2.091050	0.425390	3.504160
C_{14}	-3.503100	1.308870	1.712390
C_{15}	-2.555740	1.546890	2.766320
C_{16}	-1.682980	2.655080	2.632780
C_{17}	-3.118380	-2.344390	1.262570
C_{18}	-3.330080	-1.146050	2.023130
C_{19}	-2.479310	-0.909150	3.133810
C_{20}	-3.879510	-0.019860	1.349510
C_{21}	0.497090	3.378590	2.274270

C ₂₂	1.842370	2.999430	2.026470
C ₂₃	2.368760	1.904650	2.752500
C ₂₄	2.377340	3.252690	0.714340
C ₂₅	-0.332210	3.895320	1.219600
C ₂₆	-0.740620	3.838100	-1.188050
C ₂₇	0.170810	4.036410	-0.101290
C ₂₈	1.552670	3.763140	-0.323510
C ₂₉	-3.491740	2.101200	0.528840
C ₃₀	-2.548630	3.145940	0.359380
C ₃₁	-1.676260	3.443310	1.447180
C ₃₂	-2.067050	3.405570	-0.966270
C ₃₃	3.330840	2.365850	0.126940
C ₃₄	3.775480	1.203690	0.816900
C ₃₅	3.328340	1.009840	2.152400
C ₃₆	4.086980	0.040290	0.040820
C ₃₇	3.093350	2.338410	-1.298180
C ₃₈	2.454960	0.904660	-3.168200
C ₃₉	3.305190	1.139860	-2.058300
C ₄₀	3.854420	0.012800	-1.384280
C ₄₁	-0.291420	3.274650	-2.444980
C ₄₂	1.075130	2.886770	-2.623540
C ₄₃	2.009060	3.194940	-1.577450

C ₄₄	1.343900	1.771460	-3.437260
C ₄₅	3.849230	-1.259470	0.547650
C ₄₆	3.288730	-1.451710	1.845780
C ₄₇	3.086490	-0.300030	2.660980
C ₄₈	2.425830	-2.568710	2.039370
C ₄₉	3.465980	-2.108100	-0.562680
C ₅₀	1.651130	-3.448830	-1.482140
C ₅₁	2.523040	-3.152400	-0.393390
C ₅₂	2.041160	-3.411250	0.932040
C ₅₃	2.066910	-0.429790	-3.539110
C ₅₄	2.531510	-1.552050	-2.801640
C ₅₅	3.477700	-1.315310	-1.747120
C ₅₆	1.658630	-2.660200	-2.668500
C ₅₇	0.307890	-3.900330	-1.255360
C ₅₈	-0.195560	-4.041950	0.066000
C ₅₉	0.714190	-3.843460	1.153480
C ₆₀	-1.577390	-3.769050	0.287990
C ₆₁	-0.520630	-3.383640	-2.311340
C ₆₂	-2.392040	-1.909540	-2.788620
C ₆₃	-1.865390	-3.004890	-2.063140
C ₆₄	-2.400700	-3.258880	-0.750540
C ₆₅	0.727670	-0.381930	-4.048660

C ₆₆	-1.563230	-1.142620	-3.667650
C ₆₇	-0.181760	-1.460390	-3.833730
C ₆₈	0.312010	-2.622040	-3.190970
C ₆₉	-1.347980	2.492780	-2.977360
C ₇₀	-2.001450	0.219740	-3.610710
C ₇₁	-1.076620	1.289810	-3.723620
C ₇₂	0.276740	0.976570	-3.996190
C ₇₃	-3.874440	1.252240	-0.581830
C ₇₄	-3.111410	0.294490	-2.695970
C ₇₅	-3.314000	1.445330	-1.879940
C ₇₆	-2.451680	2.562810	-2.073730
C ₇₇	-3.354610	-2.372500	-0.162590
C ₇₈	-3.352430	-1.015790	-2.187860
C ₇₉	-3.799120	-1.210410	-0.852590
C ₈₀	-4.111160	-0.047590	-0.075450

$C_{100}(D_2)$	X	Y	Z
C_1	-0.49318	4.42399	-0.54396
C_2	-1.84017	4.32758	-0.18152
C_3	-2.82527	3.80725	-1.07533
C_4	-0.10056	4.01283	-1.87954
C_5	-1.08144	3.51381	-2.74032
C_6	-2.44514	3.40456	-2.34018
C_7	3.46506	3.22414	-1.08063
C_8	2.23573	3.94985	-1.18109
C_9	1.27978	3.63482	-2.15004
C_{10}	3.74735	2.23304	-2.00020
C_{11}	2.81112	1.94539	-3.03908
C_{12}	1.56800	2.57202	-3.10377
C_{13}	4.22489	1.76271	0.76551
C_{14}	3.77292	3.01095	0.30390
C_{15}	4.33515	0.99973	-1.56665
C_{16}	4.52001	0.71012	-0.21461
C_{17}	-3.92533	0.01200	-2.49114
C_{18}	-3.87030	1.37955	-2.13852
C_{19}	-2.99411	2.18585	-2.88857
C_{20}	-1.98138	1.59028	-3.70807

C ₂₁	-0.59446	-0.41845	-4.01300
C ₂₂	-1.89345	0.20229	-3.86536
C ₂₃	-2.98334	-0.55935	-3.36955
C ₂₄	0.78130	-2.40471	-3.61928
C ₂₅	-0.48003	-1.84964	-3.72165
C ₂₆	0.46217	1.83726	-3.73005
C ₂₇	-0.79868	2.39251	-3.62179
C ₂₈	2.96787	0.54775	-3.38896
C ₂₉	1.87509	-0.21529	-3.87596
C ₃₀	0.57527	0.40519	-4.01760
C ₃₁	1.96355	-1.60297	-3.71495
C ₃₂	-4.22283	1.75930	-0.77061
C ₃₃	-3.77166	3.00900	-0.31277
C ₃₄	-3.46386	3.22577	1.07116
C ₃₅	-4.51741	0.70921	0.21268
C ₃₆	-4.33273	1.00223	1.56392
C ₃₇	-3.74543	2.23697	1.99367
C ₃₈	-3.75520	-2.24084	-1.97145
C ₃₉	-4.34043	-1.00642	-1.53805
C ₄₀	-4.51807	-0.71343	-0.18580
C ₄₁	-3.46812	-3.22966	-1.05068
C ₄₂	-3.76834	-3.01298	0.33495

C ₄₃	-4.21765	-1.76360	0.79564
C ₄₄	-1.58233	-2.58265	-3.08667
C ₄₅	-2.82494	-1.95596	-3.01650
C ₄₆	-2.23949	-3.95557	-1.15623
C ₄₇	-1.28909	-3.64296	-2.13154
C ₄₈	-1.27864	3.63932	2.13881
C ₄₉	-1.56609	2.57904	3.09568
C ₅₀	-2.23481	3.95207	1.16925
C ₅₁	-2.80900	1.95220	3.03323
C ₅₂	-2.96492	0.55551	3.38734
C ₅₃	-1.95997	-1.59402	3.71990
C ₅₄	-1.87182	-0.20594	3.87651
C ₅₅	-0.57217	0.41514	4.01608
C ₅₆	-0.45990	1.84632	3.72392
C ₅₇	0.80058	2.40181	3.61402
C ₅₈	-3.85800	-1.38386	2.16160
C ₅₉	-3.91182	-0.01624	2.51448
C ₆₀	-2.97710	-2.19001	2.90636
C ₆₁	1.08247	3.52073	2.72919
C ₆₂	0.10134	4.01723	1.86705
C ₆₃	0.49370	4.42558	0.53050
C ₆₄	2.44624	3.41116	2.32970

C ₆₅	2.82607	3.81095	1.06392
C ₆₆	1.84081	4.32882	0.16862
C ₆₇	2.99602	2.19439	2.88184
C ₆₈	3.87268	1.38640	2.13443
C ₆₉	3.92850	0.01980	2.49103
C ₇₀	-0.77726	-2.39584	3.62646
C ₇₁	0.48403	-1.84020	3.72709
C ₇₂	0.59796	-0.40808	4.01386
C ₇₃	1.89658	0.21288	3.86446
C ₇₄	1.98362	1.60054	3.70285
C ₇₅	2.98685	-0.54966	3.37104
C ₇₆	1.29355	-3.63738	2.14200
C ₇₇	1.58661	-2.57452	3.09408
C ₇₈	2.82896	-1.94738	3.02201
C ₇₉	2.24409	-3.95233	1.16738
C ₈₀	-1.83719	-4.33122	0.19219
C ₈₁	-2.81739	-3.81119	1.09179
C ₈₂	-2.43041	-3.40842	2.35444
C ₈₃	-0.48808	-4.42747	0.54650
C ₈₄	-0.08810	-4.01590	1.87972
C ₈₅	-1.06423	-3.51714	2.74628
C ₈₆	2.43460	-3.41359	-2.34458

C ₈₇	1.06849	-3.52363	-2.73607
C ₈₈	0.09249	-4.02051	-1.86814
C ₈₉	2.82168	-3.81322	-1.08098
C ₉₀	1.84169	-4.33145	-0.17998
C ₉₁	0.49255	-4.42883	-0.53388
C ₉₂	3.91480	-0.02142	-2.51432
C ₉₃	3.86143	-1.38814	-2.15743
C ₉₄	2.98079	-2.19660	-2.89985
C ₉₅	3.75932	-2.23476	1.97768
C ₉₆	4.34399	-1.00115	1.54089
C ₉₇	4.52135	-0.71153	0.18787
C ₉₈	3.47248	-3.22624	1.05971
C ₉₉	3.77240	-3.01285	-0.32647
C ₁₀₀	4.22122	-1.76441	-0.79055