

## Alteration of the central core of DF-PCIC chromophore to boost the photovoltaic applications of non-fullerene acceptor based organic solar cells

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**TableS1:** Frontier molecular orbitals (HOMO-LUMO) and bandgap of the reference attained from all four functionals, along with the experimental values.

Compounds	HOMO energy (eV)	LUMO energy (eV)	E <sub>g</sub> (eV)
Experimental [1, 2]	5.49	3.77	1.72
B3LYP	5.45	3.34	2.11
CAMB3LYP	6.57	2.27	4.30
MPW1PW91	5.71	3.30	2.41
WB97XD	7.18	1.74	5.44

**Table S2:** Ground state energies of the molecules at MPW1PW91 functional

Compounds	Energies (hartree fock)
R	-5336.32
M1	-7343.97
M2	-7190.35
M3	-7622.23
M4	-5366.97
M5	-6655.13

**Table S3:** Values of absorption profile of all the molecules at TD-DFT/MPW1PW91/6-31G+(d,p) in chloroform solvent.

Compounds	Experimental $\lambda_{\max}$ (nm)	Computed $\lambda_{\max}$ (nm)	Excitation energies $E_x$ (eV)	Oscillator strength ( $f$ )	Major transition character
<b>R</b>	671	659	1.88	3.34	HOMO→LUMO
<b>M1</b>	-	646	1.91	3.30	HOMO→LUMO
<b>M2</b>	-	692	1.79	3.52	HOMO→LUMO
<b>M3</b>	-	693	1.79	3.52	HOMO→LUMO
<b>M4</b>	-	704	1.76	3.13	HOMO→LUMO
<b>M5</b>	-	728	1.70	3.80	HOMO→LUMO

**Table S4:** Computed results of  $\lambda_{\max}$ , first excitation energy and oscillator strength along with experimental  $\lambda_{\max}$  in gas phase at three different functionals.

Compounds	Functional	Computed $\lambda_{\max}$ (nm)	Excitation energies ( $E_x$ ) (eV)	Oscillator strength ( $f$ )	Major transition character
<b>R</b>	MPW1PW91	613	2.02	3.06	HOMO→LUMO
	B3LYP	656	1.88	2.40	HOMO→LUMO
	$\omega$ B97XD	479	2.58	3.20	HOMO→LUMO
<b>M1</b>	MPW1PW91	603	2.05	2.96	HOMO→LUMO
	B3LYP	653	1.89	2.40	HOMO→LUMO
	$\omega$ B97XD	472	2.62	3.60	HOMO→LUMO
<b>M2</b>	MPW1PW91	640	1.94	3.22	HOMO→LUMO
	B3LYP	689	1.79	2.95	HOMO→LUMO
	$\omega$ B97XD	486	2.54	3.89	HOMO→LUMO
<b>M3</b>	MPW1PW91	640	1.94	3.24	HOMO→LUMO
	B3LYP	691	1.79	3.01	HOMO→LUMO
	$\omega$ B97XD	483	2.56	3.84	HOMO→LUMO
<b>M4</b>	MPW1PW91	644	1.92	2.90	HOMO→LUMO

	B3LYP	685	1.80	2.71	HOMO→LUMO
	$\omega$ B97XD	489	2.59	3.80	HOMO→LUMO
<b>M5</b>	MPW1PW91	681	1.82	3.49	HOMO→LUMO
	B3LYP	736	1.68	3.16	HOMO→LUMO
	$\omega$ B97XD	500	2.47	4.33	HOMO→LUMO

**Table S5:** Values of vertical excitation energy ( $E_x$ ) according to different methodologies.

Compounds	$E_x$ (eV)	$E_x$ (eV)	$E_x$ (eV)	$E_x$ (eV) by CIS method
	MPW1PW91/6- 31G (d,p)	MPW1PW91/6- 31G+ (d,p)	B3LYP/6- 31G (d,p)	
<b>R</b>	1.90	1.88	1.77	2.72
<b>M1</b>	1.94	1.91	1.78	2.77
<b>M2</b>	1.82	1.79	1.68	2.69
<b>M3</b>	1.82	1.79	1.67	2.68
<b>M4</b>	1.78	1.76	1.66	2.65
<b>M5</b>	1.72	1.71	1.58	2.61

**Table S6:** Frontier molecular orbitals according to three different basis sets.

Compounds	Basis set	HOMO energy (eV)	LUMO energy (eV)	$E_g$ (eV)
<b>R</b>	6-31G	-5.70	-3.29	2.41
	6-311G	-5.90	-3.47	2.43
	LanL2DZ	-5.92	-3.60	2.32
<b>M1</b>	6-31G	-5.57	-3.15	2.42
	6-311G	-5.76	-3.31	2.45
	LanL2DZ	-5.76	-3.42	2.34
<b>M2</b>	6-31G	-5.50	-3.20	2.30
	6-311G	-5.68	-3.38	2.30
	LanL2DZ	-5.71	-3.48	2.23
<b>M3</b>	6-31G	-5.52	-3.23	2.29
	6-311G	-5.70	-3.31	2.39

	LanL2DZ	-5.75	-3.53	2.22
<b>M4</b>	6-31G	-5.48	-3.18	2.30
	6-311G	-5.66	-3.34	2.32
<b>M5</b>	LanL2DZ	-5.64	-3.44	2.20
	6-31G	-5.44	-3.26	2.18
	6-311G	-5.61	-3.42	2.19
	LanL2DZ	-5.69	-3.53	2.16

**Table S7:** Dipole moment of **R** and **M1-M6** in gas phase and solvent and their difference.

Molecule	$\mu_g$ (Debye)	$\mu_s$ (Debye)	$\Delta\mu$ (Debye)
<b>R</b>	0.365837	0.386188	0.020351
<b>M1</b>	0.917760	1.135922	0.218162
<b>M2</b>	1.302373	1.695221	0.392848
<b>M3</b>	2.174931	2.621592	0.446661
<b>M4</b>	0.175986	0.244109	0.068123
<b>M5</b>	0.726893	0.922841	0.195948

Supporting information, Cartesian coordinates of internally optimized geometries of all molecules (reference **R**, and investigated molecules **M1**, **M2**, **M3**, **M4**, and **M5** along X, Y and Z axis at MPW1PW91/6-31G (d, p) level of density functional theory (DFT).

#### Cartesian coordinates of Reference Molecule **R**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.972644	-1.031361	0.221152
2	6	0	-0.397988	-1.172764	0.235103
3	6	0	-1.283752	-0.091669	0.099283
4	6	0	-0.676351	1.164883	-0.060681

5	6	0	0.693555	1.304776	-0.081212
6	6	0	1.577691	0.224511	0.058053
7	1	0	1.573310	-1.922963	0.356476
8	1	0	-1.273948	2.062890	-0.162881
9	9	0	1.185898	2.543082	-0.254600
10	9	0	-0.884924	-2.414028	0.392866
11	6	0	-2.728933	-0.247035	0.111398
12	6	0	-3.491757	-1.326011	0.529290
13	6	0	-4.871017	-1.094841	0.397245
14	6	0	-5.158140	0.161489	-0.110741
15	16	0	-3.744068	1.067552	-0.457979
16	1	0	-3.049130	-2.230794	0.917344
17	6	0	-6.352148	-3.503566	-1.403479
18	6	0	-7.788290	-3.248687	-1.915786
19	6	0	-5.287351	-2.776442	-2.236045
20	6	0	-5.232095	-3.179232	-3.705763
21	6	0	-8.335622	-4.289898	-2.909939
22	6	0	-9.126226	-5.436363	-2.272994
23	6	0	-8.331345	-6.336659	-1.333694
24	6	0	-7.466608	-2.548921	2.933947
25	6	0	-7.102322	-3.755756	3.821066
26	6	0	-8.219624	-1.407132	3.646565
27	6	0	-9.723109	-1.589343	3.836828
28	6	0	-8.252095	-4.542326	4.473357
29	6	0	-8.518054	-4.203861	5.944393
30	6	0	-7.446766	-4.735113	6.891651
31	6	0	-6.570919	0.317970	-0.199055
32	6	0	-7.181159	-0.853045	0.268744
33	6	0	-8.564170	-0.742580	0.227107
34	6	0	-9.021664	0.489160	-0.274232

35	16	0	-7.664584	1.533605	-0.698744
36	6	0	3.022554	0.382995	0.030000
37	6	0	3.781833	1.508989	0.300373
38	6	0	5.161610	1.272500	0.166255
39	6	0	5.448283	-0.035301	-0.190794
40	16	0	4.034204	-0.984522	-0.397998
41	1	0	3.336650	2.451995	0.581775
42	6	0	7.715717	2.907618	2.615925
43	6	0	7.345466	4.142807	3.456458
44	6	0	8.435194	1.798433	3.411115
45	6	0	9.947191	1.945726	3.561751
46	6	0	8.471883	4.868904	4.185787
47	6	0	8.011296	6.186092	4.807253
48	6	0	9.116264	6.904688	5.572133
49	6	0	5.534361	3.609045	-2.749525
50	6	0	8.081070	3.152949	-2.421308
51	6	0	8.097718	1.811871	-3.149959
52	6	0	4.831805	2.281362	-3.035398
53	6	0	3.743412	2.401492	-4.106957
54	6	0	2.575642	3.306558	-3.723907
55	6	0	6.861614	-0.208701	-0.237829
56	6	0	7.471217	1.005848	0.099697
57	6	0	8.854206	0.893442	0.079584
58	6	0	9.313219	-0.387603	-0.275956
59	16	0	7.957764	-1.473648	-0.586208
60	6	0	-10.408258	0.742378	-0.362779
61	6	0	-11.160550	1.811981	-0.791267
62	6	0	-10.624252	3.066458	-1.348483
63	6	0	-12.616265	1.905464	-0.799315
64	6	0	-11.786588	3.902272	-1.708479

65	6	0	-12.968512	3.218799	-1.389504
66	6	0	-14.196320	3.827965	-1.651216
67	6	0	-14.197923	5.099551	-2.223373
68	6	0	-13.011743	5.766723	-2.533709
69	6	0	-11.783432	5.164806	-2.275033
70	1	0	-15.136903	3.345632	-1.425977
71	1	0	-15.148606	5.578464	-2.430466
72	1	0	-13.051544	6.755393	-2.977455
73	1	0	-10.842195	5.652167	-2.502849
74	6	0	-13.533978	0.981949	-0.342286
75	6	0	-14.943610	1.180282	-0.402915
76	6	0	-13.180449	-0.266074	0.247622
77	7	0	-16.099662	1.299493	-0.433516
78	7	0	-12.922220	-1.290253	0.734871
79	8	0	-9.450900	3.370622	-1.496275
80	6	0	10.700225	-0.648857	-0.334257
81	6	0	11.453177	-1.756949	-0.647824
82	6	0	10.918283	-3.063271	-1.071744
83	6	0	12.909304	-1.847036	-0.654105
84	6	0	12.081647	-3.925031	-1.360305
85	6	0	13.262893	-3.209125	-1.119427
86	6	0	14.491440	-3.834833	-1.334398
87	6	0	14.494528	-5.154930	-1.783236
88	6	0	13.309053	-5.853977	-2.016820
89	6	0	12.080011	-5.235884	-1.803821
90	1	0	15.431505	-3.328902	-1.165911
91	1	0	15.445801	-5.646882	-1.953843
92	1	0	13.349919	-6.880107	-2.365180
93	1	0	11.139293	-5.746961	-1.974700
94	6	0	13.825900	-0.882707	-0.288736

95	6	0	15.235938	-1.081798	-0.337104
96	6	0	13.470545	0.413012	0.185936
97	7	0	16.392208	-1.200116	-0.361918
98	7	0	13.210811	1.476818	0.578162
99	8	0	9.745294	-3.386299	-1.175211
100	1	0	9.554326	1.688622	0.303852
101	1	0	-9.267010	-1.505160	0.538514
102	6	0	-6.139068	-1.858607	0.741266
103	6	0	-6.188169	-3.277568	0.114236
104	6	0	6.429440	2.060987	0.434210
105	6	0	6.419472	2.358402	1.971071
106	6	0	6.540486	3.424870	-0.302019
107	6	0	6.761594	3.687321	-1.817619
108	6	0	-6.165034	-2.003130	2.294746
109	1	0	-10.968354	-0.113897	-0.004637
110	1	0	-5.929620	-1.025053	2.726728
111	1	0	-5.321942	-2.654005	2.553426
112	1	0	-8.123692	-2.926004	2.137331
113	1	0	-7.736590	-1.215612	4.613767
114	1	0	-8.072666	-0.493109	3.060324
115	1	0	-9.973649	-2.412840	4.505868
116	1	0	-10.164500	-0.682890	4.259713
117	1	0	-10.227231	-1.778048	2.883994
118	1	0	-6.521110	-4.440358	3.192559
119	1	0	-6.402604	-3.412772	4.595063
120	1	0	-9.166847	-4.407113	3.886729
121	1	0	-8.026602	-5.613784	4.414678
122	1	0	-8.605933	-3.118900	6.069597
123	1	0	-9.487939	-4.621912	6.236606
124	1	0	-7.383160	-5.826329	6.838920



125	1	0	-6.456358	-4.337299	6.651545
126	1	0	-7.664199	-4.464550	7.928152
127	1	0	-5.259804	-3.768043	0.432998
128	1	0	-6.995032	-3.826244	0.612358
129	1	0	-6.158934	-4.578484	-1.524279
130	1	0	-8.478505	-3.206161	-1.065248
131	1	0	-7.830442	-2.253007	-2.370349
132	1	0	-8.997083	-3.785755	-3.623006
133	1	0	-7.515738	-4.706320	-3.505547
134	1	0	-9.982971	-5.016282	-1.731350
135	1	0	-9.551419	-6.050169	-3.075316
136	1	0	-7.960880	-5.790804	-0.461526
137	1	0	-8.950631	-7.157333	-0.961804
138	1	0	-7.467463	-6.778274	-1.840492
139	1	0	5.641405	3.985477	-0.014984
140	1	0	7.368072	3.944580	0.193815
141	1	0	6.939736	4.771522	-1.778360
142	1	0	5.851728	4.038863	-3.710381
143	1	0	4.789897	4.311013	-2.353841
144	1	0	5.551684	1.525842	-3.355300
145	1	0	4.374888	1.898732	-2.120273
146	1	0	4.190680	2.759147	-5.043281
147	1	0	3.359197	1.397780	-4.320818
148	1	0	2.139205	3.004236	-2.767190
149	1	0	2.881825	4.351901	-3.630433
150	1	0	1.784998	3.268313	-4.478062
151	1	0	8.836215	3.141722	-1.627109
152	1	0	8.432011	3.907621	-3.135331
153	1	0	7.548672	1.862810	-4.093245
154	1	0	9.127523	1.536570	-3.394206

155	1	0	7.672875	0.999969	-2.558131
156	1	0	6.126522	1.438733	2.487822
157	1	0	5.597251	3.065000	2.133578
158	1	0	8.399429	3.244938	1.824161
159	1	0	6.847962	4.860129	2.789835
160	1	0	6.583538	3.843786	4.189999
161	1	0	8.879531	4.230590	4.977355
162	1	0	9.299556	5.066960	3.492488
163	1	0	7.624538	6.841715	4.017232
164	1	0	7.165650	5.992269	5.478759
165	1	0	9.963699	7.134717	4.919368
166	1	0	8.761292	7.846115	5.999213
167	1	0	9.492894	6.288691	6.394240
168	1	0	7.965980	1.717380	4.400660
169	1	0	8.243287	0.840700	2.915359
170	1	0	10.361689	1.090071	4.101438
171	1	0	10.444562	1.983202	2.588047
172	1	0	10.236161	2.845741	4.105424
173	1	0	11.259631	0.241713	-0.071210
174	1	0	-5.456028	-1.695940	-2.171455
175	1	0	-4.304460	-2.955710	-1.784844
176	1	0	-5.065021	-4.254873	-3.820912
177	1	0	-6.154907	-2.926995	-4.234274
178	1	0	-4.414232	-2.662583	-4.214899

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**Cartesian coordinates of Designed Molecule M1**  
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

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1	6	0	-6.044489	0.718290	0.258699
2	6	0	-7.445556	0.646980	0.206029
3	6	0	-7.906914	-0.633429	-0.061940
4	16	0	-6.629458	-1.770711	-0.224375
5	1	0	-5.471124	1.609011	0.481385
6	6	0	-8.906314	1.830484	3.000422
7	6	0	-10.407741	1.525517	3.193880
8	6	0	-8.011191	0.632370	3.338139
9	6	0	-8.122514	0.130077	4.773275
10	6	0	-10.956432	1.755057	4.616054
11	6	0	-11.586233	3.131855	4.844474
12	6	0	-10.611387	4.302251	4.778160
13	6	0	-9.611437	3.588055	-1.176329
14	6	0	-9.032301	5.013514	-1.281856
15	6	0	-10.405338	3.097013	-2.402406
16	6	0	-11.881899	3.477874	-2.455323
17	6	0	-9.996639	6.197384	-1.449693
18	6	0	-10.238610	6.645489	-2.894907
19	6	0	-9.027928	7.309303	-3.542214
20	6	0	-9.329316	-0.613345	-0.121389
21	6	0	-9.768990	0.697901	0.106521
22	6	0	-11.151240	0.780810	0.029820
23	6	0	-11.781764	-0.450943	-0.225296
24	16	0	-10.586214	-1.737883	-0.403301
25	6	0	6.379814	-1.026499	-0.472436
26	6	0	7.757601	-0.879161	-0.239617
27	6	0	8.131407	0.447418	-0.076308
28	16	0	6.793272	1.521241	-0.139305
29	1	0	5.875323	-1.965289	-0.662023
30	6	0	10.320045	-3.045077	-2.219152

31	6	0	9.923481	-4.414010	-2.800987
32	6	0	11.102062	-2.142429	-3.195147
33	6	0	12.616816	-2.330537	-3.232283
34	6	0	11.033154	-5.331625	-3.302126
35	6	0	10.510894	-6.707942	-3.710891
36	6	0	11.604795	-7.629160	-4.237099
37	6	0	7.660422	-2.950686	3.011015
38	6	0	10.152249	-2.221097	2.887590
39	6	0	9.924345	-0.773235	3.314506
40	6	0	6.754119	-1.720937	2.956644
41	6	0	5.614153	-1.781704	3.976766
42	6	0	4.585315	-2.877962	3.719781
43	6	0	9.548378	0.525759	0.029551
44	6	0	10.073957	-0.769972	-0.057095
45	6	0	11.457971	-0.754903	0.027611
46	6	0	12.003331	0.533296	0.180203
47	16	0	10.725455	1.749844	0.228705
48	6	0	-13.188206	-0.515529	-0.318710
49	6	0	-14.089048	-1.529110	-0.558596
50	6	0	-13.744989	-2.945049	-0.776933
51	6	0	-15.539565	-1.405188	-0.636264
52	6	0	-15.020866	-3.674748	-0.922418
53	6	0	-16.086918	-2.767214	-0.840135
54	6	0	-17.587047	-4.608378	-1.161948
55	6	0	-16.514621	-5.498004	-1.245467
56	6	0	-15.208457	-5.031520	-1.118241
57	1	0	-18.600272	-4.984599	-1.251009
58	1	0	-16.703203	-6.554448	-1.401476
59	1	0	-14.351080	-5.692867	-1.172638
60	6	0	-16.309169	-0.263353	-0.545660

61	6	0	-17.731292	-0.269077	-0.632660
62	6	0	-15.777073	1.045731	-0.362378
63	7	0	-18.891594	-0.234731	-0.697869
64	7	0	-15.374743	2.127133	-0.214633
65	8	0	-12.628435	-3.435800	-0.846896
66	6	0	13.403173	0.700995	0.247783
67	6	0	14.235344	1.789451	0.383183
68	6	0	13.798377	3.187317	0.550993
69	6	0	15.692672	1.770548	0.418543
70	6	0	15.023119	4.000742	0.695497
71	6	0	16.146720	3.165573	0.622031
72	6	0	17.418943	3.725474	0.738770
73	6	0	17.522618	5.103492	0.925017
74	6	0	16.393782	5.921899	0.994340
75	6	0	15.121156	5.368936	0.878732
76	1	0	18.317296	3.125888	0.690850
77	1	0	18.508373	5.545866	1.018195
78	1	0	16.512847	6.989978	1.139138
79	1	0	14.222068	5.972810	0.926907
80	6	0	16.540550	0.692560	0.268001
81	6	0	17.960101	0.802143	0.319762
82	6	0	16.100552	-0.642006	0.032112
83	7	0	19.120656	0.858955	0.359480
84	7	0	15.769758	-1.740347	-0.161034
85	8	0	12.651917	3.605959	0.601893
86	1	0	12.102877	-1.623755	-0.017967
87	1	0	-11.736874	1.681886	0.163837
88	6	0	-8.591684	1.638640	0.315170
89	6	0	-8.573861	2.460818	1.630580
90	6	0	8.970508	-1.789877	-0.275288

91	6	0	9.024694	-2.339605	-1.743253
92	6	0	8.945001	-3.011953	0.683620
93	6	0	8.995981	-3.012212	2.236679
94	6	0	-8.434837	2.624184	-0.886006
95	1	0	-13.617512	0.468046	-0.165616
96	1	0	-8.221795	2.033820	-1.783457
97	1	0	-7.523997	3.199361	-0.683435
98	1	0	-10.296940	3.578375	-0.316516
99	1	0	-9.892130	3.427830	-3.314957
100	1	0	-10.350155	2.002982	-2.418694
101	1	0	-12.043230	4.551746	-2.548041
102	1	0	-12.367257	3.001072	-3.311057
103	1	0	-12.412662	3.144968	-1.557761
104	1	0	-8.444983	5.173358	-0.369716
105	1	0	-8.297984	5.021344	-2.098683
106	1	0	-10.952067	5.968544	-0.965223
107	1	0	-9.592282	7.056459	-0.900564
108	1	0	-10.551193	5.792958	-3.507674
109	1	0	-11.078333	7.349546	-2.908500
110	1	0	-8.723686	8.204202	-2.989941
111	1	0	-8.164392	6.638602	-3.579647
112	1	0	-9.247443	7.612387	-4.569212
113	1	0	-7.568650	2.897260	1.691488
114	1	0	-9.252130	3.310013	1.492717
115	1	0	-8.650263	2.622282	3.718817
116	1	0	-10.995504	2.140342	2.502597
117	1	0	-10.601720	0.490452	2.893019
118	1	0	-11.716848	0.996579	4.830993
119	1	0	-10.164144	1.599298	5.356982
120	1	0	-12.389381	3.283472	4.112622

121	1	0	-12.072049	3.133392	5.826959
122	1	0	-10.144649	4.388061	3.792761
123	1	0	-11.118334	5.249698	4.979329
124	1	0	-9.809901	4.192323	5.515440
125	1	0	8.068043	-3.606237	0.396017
126	1	0	9.807616	-3.613993	0.378537
127	1	0	9.293814	-4.057668	2.400798
128	1	0	7.914205	-3.138850	4.064222
129	1	0	7.072349	-3.824783	2.701662
130	1	0	7.327517	-0.809447	3.134892
131	1	0	6.327312	-1.618866	1.956655
132	1	0	6.040469	-1.913398	4.979760
133	1	0	5.104102	-0.812035	3.990801
134	1	0	4.112490	-2.750197	2.740538
135	1	0	5.033420	-3.874907	3.745269
136	1	0	3.791740	-2.857057	4.471168
137	1	0	11.018698	-2.266669	2.218606
138	1	0	10.454510	-2.778832	3.782163
139	1	0	9.230317	-0.706599	4.155904
140	1	0	10.868354	-0.330572	3.643709
141	1	0	9.533774	-0.151111	2.508068
142	1	0	8.808681	-1.503996	-2.416599
143	1	0	8.174378	-3.025053	-1.838252
144	1	0	10.966483	-3.231556	-1.350112
145	1	0	9.359307	-4.950126	-2.025816
146	1	0	9.209202	-4.243540	-3.619085
147	1	0	11.535998	-4.878445	-4.163236
148	1	0	11.799042	-5.453056	-2.524965
149	1	0	10.016820	-7.177576	-2.851368
150	1	0	9.733611	-6.586272	-4.475529

151	1	0	12.380447	-7.792508	-3.482898
152	1	0	11.205100	-8.606651	-4.518914
153	1	0	12.090135	-7.202278	-5.119903
154	1	0	10.681947	-2.263824	-4.202677
155	1	0	10.910967	-1.098984	-2.922820
156	1	0	13.070597	-1.617041	-3.925403
157	1	0	13.064868	-2.152804	-2.250245
158	1	0	12.918277	-3.329231	-3.548853
159	1	0	13.897733	-0.260666	0.170908
160	1	0	-8.242195	-0.192441	2.655282
161	1	0	-6.967715	0.904244	3.139648
162	1	0	-7.888296	0.919181	5.494712
163	1	0	-9.125033	-0.241596	5.000714
164	1	0	-7.423300	-0.692311	4.945835
165	6	0	-17.393064	-3.242291	-0.956733
166	1	0	-18.250817	-2.587373	-0.894385
167	6	0	-5.443688	-0.509817	0.038129
168	6	0	5.705434	0.183290	-0.443583
169	6	0	1.975566	0.030590	-0.506613
170	6	0	2.010788	1.358720	-0.960644
171	6	0	0.834376	2.111345	-1.202441
172	6	0	-0.371605	1.480910	-0.953696
173	6	0	-0.462335	0.149230	-0.489336
174	6	0	0.717906	-0.608414	-0.265430
175	6	0	3.282291	-0.489005	-0.280831
176	6	0	4.284949	0.397470	-0.575472
177	1	0	-1.285340	2.030734	-1.146515
178	1	0	3.484254	-1.468603	0.131604
179	6	0	-1.724016	-0.478853	-0.237595
180	6	0	-1.759765	-1.815163	0.186025



181	6	0	-0.582086	-2.579934	0.389862
182	6	0	0.627214	-1.951133	0.168959
183	6	0	-3.028581	0.082404	-0.334978
184	6	0	-4.027800	-0.789479	0.010616
185	1	0	1.533221	-2.526825	0.314908
186	1	0	-3.238229	1.088293	-0.673616
187	16	0	3.644830	1.923833	-1.138609
188	16	0	-3.388628	-2.348258	0.477921
189	6	0	0.880118	3.494849	-1.677913
190	6	0	1.718897	4.071515	-2.601739
191	16	0	-0.248184	4.672476	-1.075201
192	6	0	1.445126	5.445981	-2.829215
193	1	0	2.484409	3.519171	-3.131117
194	6	0	0.402115	5.906638	-2.078571
195	1	0	1.994857	6.063345	-3.527861
196	1	0	-0.014338	6.902683	-2.049021
197	6	0	-0.640932	-3.973204	0.847177
198	6	0	-1.489335	-4.977239	0.447905
199	16	0	0.484799	-4.561918	2.027546
200	6	0	-1.227001	-6.216477	1.089595
201	1	0	-2.255690	-4.829533	-0.301821
202	6	0	-0.187445	-6.143340	1.971906
203	1	0	-1.784040	-7.125599	0.902810
204	1	0	0.213822	-6.926025	2.598601

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**Cartesian coordinates of Designed Molecule M2**

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

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1	6	0	5.570483	-1.287020	0.155457
2	6	0	6.948567	-1.036717	0.092568
3	6	0	7.244645	0.316906	0.013990
4	16	0	5.836458	1.298649	0.028432
5	1	0	5.119771	-2.268302	0.227780
6	6	0	8.610193	-2.496539	2.617693
7	6	0	10.070052	-2.056445	2.866091
8	6	0	7.582803	-1.487400	3.148783
9	6	0	7.633186	-1.234939	4.652026
10	6	0	10.701365	-2.551501	4.181589
11	6	0	11.520369	-3.838537	4.052159
12	6	0	10.726969	-5.070743	3.631132
13	6	0	9.388824	-3.430391	-1.801430
14	6	0	8.977833	-4.882239	-2.116354
15	6	0	10.080388	-2.671625	-2.952384
16	6	0	11.572111	-2.931375	-3.145673
17	6	0	10.082285	-5.876059	-2.511491
18	6	0	10.240382	-6.103230	-4.019492
19	6	0	9.113193	-6.931820	-4.628068
20	6	0	8.655171	0.481920	-0.069515
21	6	0	9.257094	-0.783963	-0.052792
22	6	0	10.636202	-0.680644	-0.154691
23	6	0	11.103498	0.643768	-0.240315
24	16	0	9.757198	1.784399	-0.195364
25	6	0	-5.815223	1.389526	0.214644
26	6	0	-7.195738	1.142374	0.193235
27	6	0	-7.497978	-0.207517	0.080772
28	16	0	-6.092218	-1.191408	0.029772
29	1	0	-5.361752	2.368963	0.292697
30	6	0	-9.630957	3.553923	-1.666152

31	6	0	-9.214173	4.991576	-2.024797
32	6	0	-10.324101	2.797265	-2.818932
33	6	0	-11.828658	3.015281	-2.960291
34	6	0	-10.302434	5.946388	-2.506314
35	6	0	-9.800060	7.382482	-2.642252
36	6	0	-10.867532	8.343837	-3.150711
37	6	0	-7.690034	2.319774	3.694719
38	6	0	-10.231889	2.102028	3.134962
39	6	0	-10.314680	0.593943	3.358436
40	6	0	-7.047814	0.937828	3.560071
41	6	0	-5.998212	0.663219	4.642345
42	6	0	-4.758040	1.549127	4.565120
43	6	0	-8.909982	-0.364704	-0.000294
44	6	0	-9.504967	0.902782	0.062653
45	6	0	-10.885823	0.812290	-0.018967
46	6	0	-11.361947	-0.506390	-0.140736
47	16	0	-10.022113	-1.655267	-0.154254
48	6	0	12.487489	0.894036	-0.351885
49	6	0	13.251033	2.035793	-0.448430
50	6	0	12.733844	3.415198	-0.431088
51	6	0	14.702503	2.103101	-0.563119
52	6	0	13.906437	4.309012	-0.518148
53	6	0	15.074940	3.537803	-0.590686
54	6	0	16.331898	5.576197	-0.680934
55	6	0	15.158776	6.329562	-0.610400
56	6	0	13.923451	5.692876	-0.527506
57	1	0	17.288136	6.083841	-0.744000
58	1	0	15.214371	7.412527	-0.619952
59	1	0	12.991960	6.244624	-0.470232
60	6	0	15.602539	1.060118	-0.648463

61	6	0	17.011067	1.245363	-0.755476
62	6	0	15.229017	-0.314855	-0.648329
63	7	0	18.165786	1.349092	-0.842542
64	7	0	14.954669	-1.445327	-0.652544
65	8	0	11.567496	3.769916	-0.358617
66	6	0	-12.748849	-0.747018	-0.240966
67	6	0	-13.518417	-1.881747	-0.366007
68	6	0	-13.006586	-3.262892	-0.404082
69	6	0	-14.971800	-1.940042	-0.463404
70	6	0	-14.183632	-4.149034	-0.506225
71	6	0	-15.350003	-3.371596	-0.536523
72	6	0	-16.588249	-4.008088	-0.625993
73	6	0	-16.615832	-5.401119	-0.683557
74	6	0	-15.445008	-6.160437	-0.654805
75	6	0	-14.206215	-5.531417	-0.564750
76	1	0	-17.517404	-3.456570	-0.650624
77	1	0	-17.574829	-5.902729	-0.752651
78	1	0	-15.504772	-7.242164	-0.702481
79	1	0	-13.276350	-6.088231	-0.539278
80	6	0	-15.869031	-0.891834	-0.499953
81	6	0	-17.279419	-1.068781	-0.595999
82	6	0	-15.490740	0.481051	-0.454941
83	7	0	-18.435451	-1.165838	-0.672557
84	7	0	-15.212409	1.609998	-0.421599
85	8	0	-11.840913	-3.623920	-0.356728
86	1	0	-11.575107	1.646823	0.011068
87	1	0	11.331630	-1.510460	-0.167605
88	6	0	8.206587	-1.885545	0.008640
89	6	0	8.334288	-2.918608	1.159029
90	6	0	-8.449815	1.993069	0.148973

91	6	0	-8.368878	2.790746	-1.194450
92	6	0	-8.591507	3.027298	1.298925
93	6	0	-8.871508	2.759047	2.803326
94	6	0	8.125262	-2.658984	-1.344443
95	1	0	13.036264	-0.040767	-0.359608
96	1	0	7.834109	-1.945792	-2.122504
97	1	0	7.282341	-3.352856	-1.246232
98	1	0	10.101802	-3.474848	-0.965820
99	1	0	9.536725	-2.871315	-3.885050
100	1	0	9.956157	-1.599133	-2.766197
101	1	0	11.793385	-3.955303	-3.448189
102	1	0	11.974860	-2.270811	-3.918127
103	1	0	12.134700	-2.733392	-2.228172
104	1	0	8.469003	-5.261437	-1.222480
105	1	0	8.206947	-4.858127	-2.898234
106	1	0	11.035077	-5.555635	-2.077220
107	1	0	9.865214	-6.846971	-2.050473
108	1	0	10.302019	-5.140740	-4.539151
109	1	0	11.193479	-6.610425	-4.206845
110	1	0	9.069067	-7.927040	-4.175072
111	1	0	8.136349	-6.461448	-4.481751
112	1	0	9.253883	-7.062451	-5.704118
113	1	0	7.398350	-3.491484	1.142389
114	1	0	9.117500	-3.629392	0.873220
115	1	0	8.459590	-3.424357	3.187432
116	1	0	10.700490	-2.411584	2.042714
117	1	0	10.124628	-0.963607	2.820480
118	1	0	11.362304	-1.772239	4.576278
119	1	0	9.924965	-2.697558	4.940408
120	1	0	12.334377	-3.670569	3.335989

121	1	0	12.004878	-4.040620	5.014274
122	1	0	10.286545	-4.952090	2.636871
123	1	0	11.366850	-5.956554	3.597535
124	1	0	9.912460	-5.277492	4.332523
125	1	0	-7.681834	3.640424	1.253831
126	1	0	-9.398918	3.696228	0.980697
127	1	0	-9.021271	3.796675	3.134908
128	1	0	-8.036728	2.428834	4.732238
129	1	0	-6.904868	3.076854	3.574330
130	1	0	-7.807243	0.155969	3.611541
131	1	0	-6.573020	0.838235	2.581610
132	1	0	-6.460561	0.768446	5.632144
133	1	0	-5.687564	-0.384496	4.564517
134	1	0	-4.274843	1.459176	3.586751
135	1	0	-4.996355	2.604259	4.724400
136	1	0	-4.023949	1.264340	5.323548
137	1	0	-10.944005	2.391431	2.353861
138	1	0	-10.603599	2.581324	4.048512
139	1	0	-9.824414	0.301832	4.290357
140	1	0	-11.361280	0.287421	3.437433
141	1	0	-9.865053	0.019411	2.547667
142	1	0	-8.058898	2.093506	-1.979475
143	1	0	-7.535937	3.493501	-1.075346
144	1	0	-10.347488	3.618669	-0.835407
145	1	0	-8.738805	5.430903	-1.137365
146	1	0	-8.424951	4.940345	-2.788001
147	1	0	-10.689891	5.616598	-3.476627
148	1	0	-11.152120	5.925049	-1.811636
149	1	0	-9.426941	7.727965	-1.670156
150	1	0	-8.937273	7.400114	-3.319744

151	1	0	-11.728784	8.370843	-2.476409
152	1	0	-10.481392	9.362759	-3.236486
153	1	0	-11.232495	8.043179	-4.137354
154	1	0	-9.818785	3.053474	-3.759580
155	1	0	-10.156099	1.724298	-2.677354
156	1	0	-12.227426	2.408001	-3.777159
157	1	0	-12.362811	2.722613	-2.051586
158	1	0	-12.090620	4.053436	-3.166736
159	1	0	-13.293502	0.189645	-0.208615
160	1	0	7.712103	-0.533384	2.626611
161	1	0	6.578488	-1.840112	2.886110
162	1	0	7.514186	-2.163092	5.219937
163	1	0	8.575620	-0.774626	4.958853
164	1	0	6.828679	-0.558846	4.953170
165	6	0	16.309850	4.181973	-0.673078
166	1	0	17.240378	3.635072	-0.729213
167	6	0	4.817857	-0.121688	0.136204
168	6	0	-5.066564	0.223357	0.145138
169	6	0	1.117765	-0.598009	0.138251
170	6	0	1.014776	0.814599	0.270560
171	6	0	-0.202324	1.488482	0.340404
172	6	0	-1.365847	0.692641	0.246400
173	6	0	-1.262886	-0.720304	0.118270
174	6	0	-0.045782	-1.396474	0.073199
175	6	0	2.474072	-1.029151	0.075119
176	6	0	3.381752	-0.009932	0.181126
177	1	0	2.751160	-2.064352	-0.069680
178	6	0	-2.722500	1.126967	0.258769
179	6	0	-3.630166	0.105943	0.170588
180	16	0	-2.844200	-1.459997	0.064513

181	16	0	2.596922	1.548964	0.367116
182	6	0	0.054465	-2.858032	-0.020366
183	6	0	0.709113	-3.706487	0.838443
184	16	0	-0.657221	-3.756008	-1.328878
185	6	0	0.630734	-5.070476	0.451688
186	1	0	1.205685	-3.352684	1.733672
187	6	0	-0.078645	-5.247157	-0.701471
188	1	0	1.072806	-5.885370	1.010354
189	1	0	-0.298906	-6.170294	-1.217259
190	6	0	-0.301958	2.942269	0.518303
191	6	0	-0.963378	3.618243	1.514173
192	6	0	-0.880556	5.030069	1.388540
193	6	0	-0.159831	5.415913	0.294877
194	16	0	0.422467	4.065839	-0.593827
195	1	0	-1.326632	5.727936	2.085352
196	1	0	0.065570	6.418079	-0.039262
197	1	0	-2.999905	2.170134	0.321056
198	1	0	-1.470771	3.107094	2.323099

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**Cartesian coordinates of Designed Molecule M3**

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.671294	-1.291266	0.361499
2	6	0	7.045391	-1.016309	0.285454
3	6	0	7.309641	0.317161	0.008921
4	16	0	5.878462	1.251182	-0.157446
5	1	0	5.238359	-2.256456	0.591110
6	6	0	8.660019	-2.015074	3.057545



7	6	0	10.109774	-1.525780	3.279071
8	6	0	7.615667	-0.942161	3.394640
9	6	0	7.624100	-0.466439	4.843545
10	6	0	10.715790	-1.839274	4.659928
11	6	0	11.521804	-3.139028	4.730107
12	6	0	10.725249	-4.415804	4.484714
13	6	0	9.617584	-3.593352	-1.135748
14	6	0	9.269280	-5.092060	-1.227910
15	6	0	10.317245	-3.001689	-2.376372
16	6	0	11.823053	-3.226976	-2.489521
17	6	0	10.423079	-6.090543	-1.416661
18	6	0	10.639347	-6.571931	-2.855667
19	6	0	9.557953	-7.530962	-3.343844
20	6	0	8.718717	0.509039	-0.056028
21	6	0	9.350623	-0.720563	0.175192
22	6	0	10.729818	-0.592319	0.099582
23	6	0	11.165922	0.716401	-0.175832
24	16	0	9.790984	1.809365	-0.346704
25	6	0	-5.760314	1.067754	-0.341321
26	6	0	-7.136714	0.805577	-0.263251
27	6	0	-7.412504	-0.528032	0.007178
28	16	0	-5.988415	-1.466011	0.210057
29	1	0	-5.318592	2.025926	-0.582638
30	6	0	-9.686858	2.595829	-2.619581
31	6	0	-9.323946	3.844862	-3.442525
32	6	0	-10.410869	1.502215	-3.431881
33	6	0	-11.926438	1.640787	-3.550440
34	6	0	-10.456448	4.573523	-4.159648
35	6	0	-10.003616	5.896559	-4.774322
36	6	0	-11.116144	6.618491	-5.525034

37	6	0	-9.418498	3.962071	2.501037
38	6	0	-7.688494	2.054939	2.702305
39	6	0	-6.408728	2.873629	2.846926
40	6	0	-8.727067	5.282928	2.149749
41	6	0	-9.282517	6.484203	2.919980
42	6	0	-10.740188	6.814155	2.614149
43	6	0	-8.824140	-0.716178	0.038828
44	6	0	-9.442826	0.510349	-0.235480
45	6	0	-10.823344	0.404476	-0.162655
46	6	0	-11.276162	-0.892860	0.141820
47	16	0	-9.914060	-1.995234	0.354659
48	6	0	12.546212	0.987231	-0.291779
49	6	0	13.282243	2.121683	-0.548953
50	6	0	12.729124	3.471886	-0.753281
51	6	0	14.734003	2.212926	-0.647146
52	6	0	13.879362	4.375737	-0.954518
53	6	0	15.069000	3.636553	-0.888957
54	6	0	16.273162	5.673269	-1.270344
55	6	0	15.079651	6.394135	-1.334230
56	6	0	13.860121	5.741781	-1.174802
57	1	0	17.216929	6.192727	-1.395008
58	1	0	15.106715	7.464175	-1.508170
59	1	0	12.913482	6.268464	-1.217856
60	6	0	15.662613	1.195959	-0.555076
61	6	0	17.067666	1.403334	-0.667748
62	6	0	15.325575	-0.172736	-0.346888
63	7	0	18.220672	1.526217	-0.752604
64	7	0	15.081056	-1.297620	-0.179488
65	8	0	11.552692	3.799356	-0.754429
66	6	0	-12.660837	-1.153624	0.227739

67	6	0	-13.409506	-2.276623	0.498036
68	6	0	-12.867727	-3.607737	0.822968
69	6	0	-14.864478	-2.363254	0.540389
70	6	0	-14.025964	-4.485647	1.083251
71	6	0	-15.210643	-3.753162	0.922029
72	6	0	-16.435254	-4.390264	1.124869
73	6	0	-16.431215	-5.738354	1.481338
74	6	0	-15.242560	-6.453518	1.636211
75	6	0	-14.017235	-5.823844	1.435473
76	1	0	-17.377685	-3.872654	1.015411
77	1	0	-17.379499	-6.239595	1.641300
78	1	0	-15.277901	-7.501272	1.913601
79	1	0	-13.074072	-6.346757	1.546678
80	6	0	-15.787502	-1.373708	0.269298
81	6	0	-17.196298	-1.572057	0.345951
82	6	0	-15.440869	-0.049222	-0.125491
83	7	0	-18.351946	-1.688556	0.396991
84	7	0	-15.188475	1.038452	-0.451686
85	8	0	-11.693200	-3.937497	0.876639
86	1	0	-11.525761	1.214900	-0.315429
87	1	0	11.445541	-1.393501	0.234871
88	6	0	8.326374	-1.829837	0.373845
89	6	0	8.430566	-2.665646	1.677405
90	6	0	-8.413005	1.595724	-0.505219
91	6	0	-8.384260	2.036871	-2.000515
92	6	0	-8.567639	2.850213	0.389577
93	6	0	-8.845888	2.663204	1.889176
94	6	0	8.314308	-2.809492	-0.840660
95	1	0	13.118728	0.079246	-0.140766
96	1	0	8.023747	-2.239621	-1.729335

97	1	0	7.492745	-3.511373	-0.655627
98	1	0	10.304215	-3.475957	-0.285165
99	1	0	9.810970	-3.373119	-3.276997
100	1	0	10.148572	-1.919333	-2.371405
101	1	0	12.093698	-4.276059	-2.613482
102	1	0	12.223256	-2.685788	-3.351064
103	1	0	12.350654	-2.857358	-1.604947
104	1	0	8.733711	-5.345232	-0.305420
105	1	0	8.532424	-5.221550	-2.032196
106	1	0	11.348841	-5.656526	-1.024814
107	1	0	10.232124	-6.974221	-0.796188
108	1	0	10.695293	-5.713716	-3.534348
109	1	0	11.611684	-7.073100	-2.920723
110	1	0	9.520347	-8.429405	-2.720133
111	1	0	8.564618	-7.073193	-3.319458
112	1	0	9.745037	-7.848282	-4.372991
113	1	0	7.500374	-3.246179	1.725228
114	1	0	9.226725	-3.403673	1.529804
115	1	0	8.494682	-2.842119	3.761918
116	1	0	10.766215	-1.968493	2.521096
117	1	0	10.150469	-0.446236	3.099217
118	1	0	11.382167	-1.019133	4.948850
119	1	0	9.927191	-1.864841	5.420138
120	1	0	12.346513	-3.082916	4.008656
121	1	0	11.992540	-3.200924	5.717981
122	1	0	10.307157	-4.449469	3.474555
123	1	0	11.357306	-5.300121	4.602035
124	1	0	9.893814	-4.507797	5.190846
125	1	0	-7.675276	3.469139	0.240383
126	1	0	-9.398187	3.431701	-0.026970

127	1	0	-9.655656	1.926757	1.965586
128	1	0	-9.432940	3.847942	3.592928
129	1	0	-10.469416	4.037268	2.197843
130	1	0	-7.652915	5.212420	2.343129
131	1	0	-8.828184	5.480151	1.075117
132	1	0	-9.166398	6.305605	3.996272
133	1	0	-8.664669	7.360176	2.692015
134	1	0	-10.888563	6.987903	1.543495
135	1	0	-11.415437	6.009012	2.914699
136	1	0	-11.057080	7.717436	3.141791
137	1	0	-7.437549	1.082336	2.269047
138	1	0	-8.075139	1.836752	3.704932
139	1	0	-6.559603	3.765443	3.459378
140	1	0	-5.631828	2.276631	3.331992
141	1	0	-6.009846	3.196097	1.880738
142	1	0	-8.043382	1.187005	-2.601240
143	1	0	-7.589869	2.789426	-2.070905
144	1	0	-10.361889	2.919448	-1.814574
145	1	0	-8.829624	4.556209	-2.767107
146	1	0	-8.562187	3.560132	-4.182085
147	1	0	-10.867632	3.939722	-4.953059
148	1	0	-11.279975	4.764387	-3.459464
149	1	0	-9.612439	6.547009	-3.982105
150	1	0	-9.162745	5.709958	-5.453888
151	1	0	-11.958994	6.841183	-4.863873
152	1	0	-10.766930	7.564147	-5.947544
153	1	0	-11.497604	6.007909	-6.348903
154	1	0	-9.959543	1.455332	-4.431940
155	1	0	-10.200616	0.532128	-2.969248
156	1	0	-12.343899	0.801159	-4.112502

157	1	0	-12.406330	1.640001	-2.567329
158	1	0	-12.231915	2.557168	-4.056755
159	1	0	-13.224080	-0.247779	0.034494
160	1	0	7.762552	-0.078242	2.737092
161	1	0	6.619122	-1.334193	3.159884
162	1	0	7.478240	-1.298685	5.539551
163	1	0	8.562577	0.027540	5.107673
164	1	0	6.818853	0.252438	5.016102
165	6	0	16.287761	4.296450	-1.049531
166	1	0	17.233654	3.775312	-1.006608
167	6	0	4.893834	-0.163717	0.148443
168	6	0	-4.992001	-0.060683	-0.100549
169	6	0	1.207900	-0.734585	0.014140
170	6	0	1.063197	0.663688	0.234865
171	6	0	-0.168536	1.311383	0.261656
172	6	0	-1.306419	0.501278	0.064937
173	6	0	-1.162501	-0.897005	-0.158070
174	6	0	0.069542	-1.544105	-0.182642
175	6	0	2.579923	-1.123291	-0.042409
176	6	0	3.453782	-0.087941	0.145186
177	1	0	2.901419	-2.132861	-0.259534
178	6	0	-2.678124	0.891707	0.117689
179	6	0	-3.552588	-0.141308	-0.078095
180	16	0	-2.722956	-1.667333	-0.331998
181	16	0	2.622947	1.436705	0.400834
182	1	0	-2.998873	1.900728	0.338468
183	6	0	0.187490	-3.005302	-0.392196
184	6	0	0.831841	-3.814818	0.550609
185	6	0	-0.349109	-3.604914	-1.535922
186	6	0	0.948396	-5.183598	0.346257

187	1	0	1.236363	-3.366996	1.451275
188	6	0	-0.241032	-4.973865	-1.707606
189	1	0	-0.849156	-3.020294	-2.299046
190	6	0	0.415563	-5.797387	-0.791226
191	1	0	1.456444	-5.802602	1.077181
192	6	0	-0.284258	2.771964	0.471888
193	6	0	0.252773	3.373539	1.616825
194	6	0	-0.922888	3.586113	-0.467595
195	6	0	0.138933	4.737774	1.787577
196	1	0	0.743192	2.790552	2.387273
197	6	0	-1.025565	4.960379	-0.278500
198	1	0	-1.327757	3.141477	-1.369924
199	6	0	-0.493990	5.570507	0.860045
200	1	0	-1.518102	5.558622	-1.034786
201	16	0	-0.544963	7.290095	1.239536
202	16	0	0.495570	-7.556787	-0.968570
203	6	0	-1.392084	7.974172	-0.199797
204	6	0	1.284417	-7.741037	-2.594682
205	1	0	-0.831689	7.799847	-1.119918
206	1	0	-2.408605	7.588449	-0.294970
207	1	0	-1.443492	9.048872	-0.022111
208	1	0	2.270657	-7.276235	-2.603270
209	1	0	1.395739	-8.814538	-2.753074
210	1	0	0.660091	-7.324199	-3.382724
211	9	0	0.647298	5.298928	2.893497
212	9	0	-0.782601	-5.515479	-2.806635

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**Cartesian coordinates of Designed Molecule M4**

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Center	Atomic	Atomic	Coordinates (Angstroms)
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Number	Number	Type	X	Y	Z
1	6	0	-0.973252	0.933188	0.201076
2	6	0	0.398490	1.138391	0.206241
3	6	0	1.276086	0.033577	0.151838
4	6	0	0.696475	-1.241062	0.068972
5	6	0	-0.675885	-1.445539	0.026079
6	6	0	-1.555201	-0.339424	0.098148
7	1	0	-1.621300	1.795446	0.316052
8	1	0	1.355347	-2.100112	0.052253
9	6	0	2.720218	0.195011	0.159060
10	6	0	3.480957	1.252791	0.626705
11	6	0	4.859956	1.039247	0.468873
12	6	0	5.152803	-0.186561	-0.107975
13	16	0	3.740194	-1.078007	-0.502119
14	1	0	3.027228	2.128183	1.068328
15	6	0	6.286033	3.540963	-1.233258
16	6	0	7.714785	3.316805	-1.780835
17	6	0	5.207256	2.846507	-2.078039
18	6	0	5.111664	3.319786	-3.524709
19	6	0	8.243260	4.405867	-2.732713
20	6	0	9.039673	5.523306	-2.053805
21	6	0	8.256790	6.378141	-1.063434
22	6	0	7.481539	2.403709	3.027192
23	6	0	7.130476	3.590214	3.947016
24	6	0	8.245829	1.246706	3.701262
25	6	0	9.751469	1.426753	3.874219
26	6	0	8.290706	4.364822	4.595431
27	6	0	8.566922	4.010780	6.060796
28	6	0	7.507905	4.540809	7.022363



29	6	0	6.564966	-0.326066	-0.212681
30	6	0	7.171781	0.826372	0.307128
31	6	0	8.553687	0.728673	0.251425
32	6	0	9.018825	-0.474526	-0.312466
33	16	0	7.664711	-1.506798	-0.779077
34	6	0	-3.004233	-0.482619	0.059697
35	6	0	-3.795702	-1.574640	0.376104
36	6	0	-5.168211	-1.315991	0.215704
37	6	0	-5.426465	-0.022417	-0.207660
38	16	0	-3.988952	0.880420	-0.458427
39	1	0	-3.369542	-2.510181	0.705012
40	6	0	-7.766560	-2.850845	2.690757
41	6	0	-7.404965	-4.085543	3.534425
42	6	0	-8.486390	-1.735773	3.477749
43	6	0	-9.998007	-1.883869	3.632920
44	6	0	-8.538858	-4.813918	4.249930
45	6	0	-8.086703	-6.137006	4.865064
46	6	0	-9.199820	-6.859267	5.614466
47	6	0	-5.563507	-3.694002	-2.635456
48	6	0	-8.117438	-3.287206	-2.313360
49	6	0	-8.151964	-1.995938	-3.125874
50	6	0	-4.892567	-2.359670	-2.962842
51	6	0	-3.858719	-2.475856	-4.086583
52	6	0	-2.662977	-3.361236	-3.747587
53	6	0	-6.834030	0.177013	-0.269519
54	6	0	-7.472764	-1.009529	0.117406
55	6	0	-8.851338	-0.863137	0.099066
56	6	0	-9.282247	0.414439	-0.306184
57	16	0	-7.901047	1.451870	-0.669841
58	6	0	10.404712	-0.711004	-0.420988

59	6	0	11.167919	-1.751646	-0.903224
60	6	0	10.647210	-2.985401	-1.515276
61	6	0	12.622395	-1.822566	-0.917825
62	6	0	11.820282	-3.790067	-1.911800
63	6	0	12.993818	-3.105140	-1.565085
64	6	0	14.228302	-3.688057	-1.854046
65	6	0	14.244814	-4.934895	-2.478704
66	6	0	13.067008	-5.603394	-2.815410
67	6	0	11.831921	-5.027701	-2.530474
68	1	0	15.163572	-3.205167	-1.610263
69	1	0	15.201205	-5.392718	-2.706331
70	1	0	13.118310	-6.572149	-3.300106
71	1	0	10.896232	-5.516497	-2.777394
72	6	0	13.520440	-0.899926	-0.419973
73	6	0	14.934934	-1.057877	-0.483016
74	6	0	13.135031	0.312682	0.221557
75	7	0	16.094735	-1.135520	-0.509110
76	7	0	12.842731	1.307063	0.749848
77	8	0	9.477734	-3.300413	-1.673758
78	6	0	-10.659794	0.709528	-0.366111
79	6	0	-11.384537	1.827210	-0.717010
80	6	0	-10.813900	3.099698	-1.190394
81	6	0	-12.836025	1.959716	-0.717017
82	6	0	-11.953251	3.985425	-1.503755
83	6	0	-13.153285	3.314804	-1.228831
84	6	0	-14.364087	3.969169	-1.457675
85	6	0	-14.331298	5.271609	-1.954988
86	6	0	-13.127492	5.925306	-2.222413
87	6	0	-11.915802	5.278224	-1.995379
88	1	0	-15.317436	3.498315	-1.263951

89	1	0	-15.268819	5.785478	-2.136902
90	1	0	-13.140329	6.938799	-2.608032
91	1	0	-10.961472	5.753846	-2.191436
92	6	0	-13.780690	1.037581	-0.312742
93	6	0	-15.183746	1.279856	-0.360333
94	6	0	-13.464661	-0.251172	0.206083
95	7	0	-16.335942	1.434084	-0.382848
96	7	0	-13.239735	-1.308819	0.635088
97	8	0	-9.632478	3.383806	-1.314459
98	1	0	-9.570512	-1.629297	0.360487
99	1	0	9.253384	1.480716	0.594420
100	6	0	6.125108	1.798270	0.835203
101	6	0	6.151751	3.244835	0.274765
102	6	0	-6.452219	-2.070871	0.501415
103	6	0	-6.465336	-2.310806	2.046771
104	6	0	-6.565004	-3.458434	-0.188384
105	6	0	-6.783158	-3.772003	-1.694298
106	6	0	6.173019	1.870540	2.391743
107	1	0	10.959773	0.132550	-0.025543
108	1	0	5.957346	0.870424	2.781544
109	1	0	5.326790	2.497202	2.696218
110	1	0	8.127266	2.797628	2.229327
111	1	0	7.776152	1.029728	4.669732
112	1	0	8.092654	0.347850	3.093518
113	1	0	10.011152	2.231039	4.562881
114	1	0	10.200407	0.509151	4.263863
115	1	0	10.240183	1.643468	2.919143
116	1	0	6.535342	4.286475	3.345103
117	1	0	6.446565	3.227772	4.726473
118	1	0	9.199734	4.228331	4.000348

119	1	0	8.072186	5.438303	4.548576
120	1	0	8.647234	2.923918	6.174625
121	1	0	9.542402	4.418705	6.348765
122	1	0	7.452607	5.633013	6.981005
123	1	0	6.512430	4.153171	6.786512
124	1	0	7.731760	4.258116	8.054278
125	1	0	5.224469	3.710298	0.631977
126	1	0	6.962548	3.778865	0.782838
127	1	0	6.087985	4.619635	-1.301916
128	1	0	8.418603	3.239454	-0.944183
129	1	0	7.754410	2.342674	-2.280428
130	1	0	8.896303	3.939297	-3.478532
131	1	0	7.413634	4.846564	-3.296162
132	1	0	9.903780	5.080417	-1.543004
133	1	0	9.454124	6.174091	-2.832382
134	1	0	7.898432	5.792731	-0.211930
135	1	0	8.880910	7.181582	-0.662913
136	1	0	7.386019	6.841879	-1.537783
137	1	0	-5.662268	-4.005362	0.113940
138	1	0	-7.388422	-3.967175	0.325182
139	1	0	-6.934678	-4.858135	-1.620002
140	1	0	-5.878674	-4.156366	-3.582026
141	1	0	-4.801064	-4.369157	-2.227500
142	1	0	-5.636301	-1.613042	-3.248012
143	1	0	-4.392177	-1.970046	-2.073738
144	1	0	-4.346625	-2.851047	-4.995434
145	1	0	-3.497514	-1.470525	-4.330341
146	1	0	-2.183671	-3.026015	-2.822316
147	1	0	-2.954428	-4.406489	-3.611475
148	1	0	-1.913432	-3.334381	-4.543125

149	1	0	-8.865901	-3.231918	-1.515275
150	1	0	-8.468881	-4.086990	-2.976237
151	1	0	-7.575494	-2.090553	-4.049897
152	1	0	-9.182711	-1.769271	-3.412466
153	1	0	-7.768346	-1.135147	-2.576798
154	1	0	-6.186924	-1.369637	2.531649
155	1	0	-5.640437	-3.004011	2.248635
156	1	0	-8.449714	-3.187964	1.898434
157	1	0	-6.900130	-4.801274	2.871429
158	1	0	-6.650516	-3.787727	4.276114
159	1	0	-8.951243	-4.180546	5.042969
160	1	0	-9.361695	-5.004357	3.548782
161	1	0	-7.694702	-6.787386	4.073217
162	1	0	-7.246410	-5.950547	5.545356
163	1	0	-10.041989	-7.081876	4.952383
164	1	0	-8.850807	-7.804997	6.036986
165	1	0	-9.582353	-6.249075	6.438174
166	1	0	-8.015574	-1.643086	4.465538
167	1	0	-8.297950	-0.783041	2.970964
168	1	0	-10.412631	-1.021510	4.161721
169	1	0	-10.496944	-1.934698	2.660650
170	1	0	-10.285240	-2.776658	4.189397
171	1	0	-11.241752	-0.154178	-0.065309
172	1	0	5.385114	1.765705	-2.070600
173	1	0	4.233743	2.992857	-1.595448
174	1	0	4.930930	4.398037	-3.583259
175	1	0	6.023436	3.104728	-4.087293
176	1	0	4.287352	2.818862	-4.039371
177	8	0	0.929618	2.372793	0.303893
178	8	0	-1.231450	-2.678059	-0.082906

179	6	0	0.158356	3.458968	-0.159866
180	6	0	-0.373877	-3.784671	-0.270143
181	1	0	0.864094	4.249546	-0.416185
182	1	0	-0.402462	3.181609	-1.060894
183	1	0	-0.535348	3.820843	0.606170
184	1	0	-1.021957	-4.648290	-0.413538
185	1	0	0.254242	-3.656781	-1.158354
186	1	0	0.263330	-3.954476	0.604517

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**Cartesian coordinates of Designed Molecule M5**

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

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1	6	0	6.594239	0.475630	0.017251
2	6	0	7.221081	-0.753511	-0.117304
3	6	0	8.620455	-0.648250	-0.103117
4	6	0	9.056597	0.662122	0.022863
5	16	0	7.758031	1.779238	0.158106
6	1	0	6.668539	-1.678956	-0.225919
7	6	0	10.015461	-2.604062	2.236430
8	6	0	11.507968	-2.391934	2.576298
9	6	0	9.102962	-1.548539	2.875213
10	6	0	9.126896	-1.508643	4.399432
11	6	0	12.026572	-3.150942	3.812583
12	6	0	12.672904	-4.505324	3.509214
13	6	0	11.740674	-5.550903	2.907311
14	6	0	10.880139	-3.016998	-2.242271
15	6	0	10.321746	-4.354947	-2.772330
16	6	0	11.709512	-2.185634	-3.242195

17	6	0	13.178423	-2.570540	-3.403268
18	6	0	11.313083	-5.429213	-3.248826
19	6	0	11.524075	-5.499596	-4.766308
20	6	0	10.330541	-6.082081	-5.517195
21	6	0	10.478873	0.685045	0.002384
22	6	0	10.946318	-0.627860	-0.145549
23	6	0	12.332517	-0.659314	-0.191218
24	6	0	12.935129	0.606142	-0.070502
25	16	0	11.711588	1.866502	0.100716
26	6	0	-6.773361	-0.378302	0.118923
27	6	0	-7.407495	0.848575	-0.001117
28	6	0	-8.806664	0.737455	0.052459
29	6	0	-9.235347	-0.575625	0.169558
30	16	0	-7.929872	-1.686247	0.280441
31	1	0	-6.861451	1.777118	-0.115222
32	6	0	-11.044065	3.001718	-2.164108
33	6	0	-10.510814	4.334627	-2.727375
34	6	0	-11.806726	2.119859	-3.175254
35	6	0	-13.287077	2.432241	-3.385417
36	6	0	-11.502769	5.324403	-3.331456
37	6	0	-10.859347	6.673408	-3.647388
38	6	0	-11.830828	7.667231	-4.272745
39	6	0	-9.355572	2.950813	3.459598
40	6	0	-11.821595	2.974499	2.749880
41	6	0	-12.181299	1.728325	3.555073
42	6	0	-8.933129	1.550969	3.906635
43	6	0	-8.366900	1.530932	5.329151
44	6	0	-7.093202	2.350805	5.511247
45	6	0	-10.656619	-0.611121	0.114418
46	6	0	-11.130036	0.697440	-0.044376

47	6	0	-12.512136	0.719696	-0.160686
48	6	0	-13.109133	-0.551249	-0.072114
49	16	0	-11.883947	-1.801330	0.157216
50	6	0	14.341220	0.723447	-0.107148
51	6	0	15.216087	1.782357	-0.016793
52	6	0	14.835079	3.190626	0.188934
53	6	0	16.671280	1.717841	-0.084587
54	6	0	16.090687	3.963384	0.265279
55	6	0	17.181361	3.096428	0.108042
56	6	0	18.474604	3.618582	0.150814
57	6	0	18.630595	4.990083	0.348843
58	6	0	17.533667	5.839541	0.501868
59	6	0	16.240733	5.325063	0.460462
60	1	0	19.350212	2.995375	0.036765
61	1	0	19.632933	5.402571	0.384146
62	1	0	17.693262	6.901416	0.653268
63	1	0	15.365078	5.953785	0.575799
64	6	0	17.468192	0.611779	-0.299747
65	6	0	18.891102	0.666584	-0.346067
66	6	0	16.962901	-0.704298	-0.507012
67	7	0	20.052867	0.664658	-0.390706
68	7	0	16.579666	-1.788831	-0.680274
69	8	0	13.706640	3.647776	0.284765
70	6	0	-14.511396	-0.679667	-0.177618
71	6	0	-15.384245	-1.743113	-0.130530
72	6	0	-15.010708	-3.150087	0.098129
73	6	0	-16.834616	-1.683144	-0.269524
74	6	0	-16.266844	-3.925231	0.119224
75	6	0	-17.350713	-3.061573	-0.093216
76	6	0	-18.643544	-3.586456	-0.106840



77	6	0	-18.805907	-4.956928	0.092930
78	6	0	-17.715549	-5.803084	0.301453
79	6	0	-16.423060	-5.286045	0.315753
80	1	0	-19.514293	-2.966087	-0.264813
81	1	0	-19.808088	-5.371199	0.084999
82	1	0	-17.879859	-6.864248	0.452748
83	1	0	-15.552430	-5.912147	0.475093
84	6	0	-17.620588	-0.579840	-0.531863
85	6	0	-19.039552	-0.635626	-0.647720
86	6	0	-17.104664	0.734086	-0.726261
87	7	0	-20.197713	-0.634528	-0.749261
88	7	0	-16.710333	1.815992	-0.890687
89	8	0	-13.887415	-3.605147	0.247968
90	1	0	-13.118702	1.606065	-0.299561
91	1	0	12.939041	-1.548935	-0.305466
92	6	0	9.787152	-1.607770	-0.272162
93	6	0	9.747307	-2.793003	0.728909
94	6	0	-9.977942	1.683711	-0.119868
95	6	0	-9.843998	2.216741	-1.582186
96	6	0	-10.017672	2.949597	0.800683
97	6	0	-10.357009	3.216483	2.308823
98	6	0	9.687890	-2.175555	-1.722632
99	1	0	14.795043	-0.252675	-0.235238
100	1	0	9.516584	-1.334407	-2.402471
101	1	0	8.769303	-2.773111	-1.751530
102	1	0	11.541288	-3.259020	-1.397661
103	1	0	11.201354	-2.193446	-4.215486
104	1	0	11.686334	-1.142211	-2.908820
105	1	0	13.320917	-3.564508	-3.825700
106	1	0	13.685910	-1.862154	-4.063548

107	1	0	13.704328	-2.547724	-2.443752
108	1	0	9.719019	-4.774813	-1.958742
109	1	0	9.606318	-4.136057	-3.576364
110	1	0	12.271822	-5.292872	-2.736719
111	1	0	10.948801	-6.411983	-2.926692
112	1	0	11.748233	-4.504922	-5.164789
113	1	0	12.406554	-6.115289	-4.974143
114	1	0	10.120085	-7.104087	-5.187303
115	1	0	9.422033	-5.493460	-5.359828
116	1	0	10.516374	-6.112131	-6.593944
117	1	0	8.750187	-3.236805	0.614241
118	1	0	10.447683	-3.553388	0.367289
119	1	0	9.726894	-3.570444	2.672658
120	1	0	12.122924	-2.695407	1.720951
121	1	0	11.695298	-1.319941	2.700126
122	1	0	12.773011	-2.532171	4.322560
123	1	0	11.215471	-3.295903	4.534921
124	1	0	13.523953	-4.348376	2.834748
125	1	0	13.097237	-4.902494	4.438475
126	1	0	11.353428	-5.240701	1.932428
127	1	0	12.261012	-6.501097	2.760186
128	1	0	10.882329	-5.741891	3.559269
129	1	0	-9.044811	3.430491	0.634430
130	1	0	-10.734362	3.596442	0.282265
131	1	0	-10.312012	4.313164	2.250670
132	1	0	-9.810065	3.432451	4.337066
133	1	0	-8.453415	3.538900	3.250756
134	1	0	-9.775829	0.857932	3.859240
135	1	0	-8.174908	1.160714	3.231453
136	1	0	-9.132982	1.887426	6.030054

137	1	0	-8.163586	0.490732	5.607762
138	1	0	-6.309616	2.017508	4.823131
139	1	0	-7.262914	3.415335	5.328380
140	1	0	-6.702984	2.253878	6.527875
141	1	0	-12.467839	3.055407	1.867386
142	1	0	-12.097015	3.826593	3.382723
143	1	0	-11.681969	1.727791	4.527440
144	1	0	-13.257734	1.713466	3.748508
145	1	0	-11.927604	0.798903	3.050651
146	1	0	-9.623610	1.362813	-2.230873
147	1	0	-8.944509	2.843153	-1.598296
148	1	0	-11.741667	3.244175	-1.349797
149	1	0	-9.982428	4.844195	-1.910336
150	1	0	-9.741139	4.105000	-3.477715
151	1	0	-11.929242	4.917904	-4.253981
152	1	0	-12.343602	5.478743	-2.642689
153	1	0	-10.440943	7.098454	-2.726642
154	1	0	-10.008008	6.517919	-4.321561
155	1	0	-12.676388	7.865270	-3.607180
156	1	0	-11.345053	8.623026	-4.485214
157	1	0	-12.236572	7.284897	-5.214227
158	1	0	-11.272952	2.146211	-4.134699
159	1	0	-11.743050	1.081538	-2.831471
160	1	0	-13.732228	1.712060	-4.077129
161	1	0	-13.846196	2.363911	-2.447115
162	1	0	-13.464425	3.426292	-3.793220
163	1	0	-14.965016	0.293622	-0.327339
164	1	0	9.373739	-0.558994	2.490773
165	1	0	8.073084	-1.728827	2.545006
166	1	0	8.866335	-2.480435	4.830468

167	1	0	10.108442	-1.224382	4.787133
168	1	0	8.405414	-0.778144	4.774785
169	6	0	-3.324392	-1.777333	0.136168
170	6	0	-2.876732	-0.465475	0.131862
171	6	0	-1.485320	-0.150040	0.125235
172	6	0	-0.587780	-1.250113	0.131817
173	6	0	-1.059761	-2.654034	0.141111
174	6	0	-0.959322	1.145596	0.109531
175	6	0	0.782153	-1.040286	0.125754
176	6	0	1.308121	0.255275	0.109544
177	6	0	0.410749	1.355365	0.100229
178	6	0	0.883478	2.758862	0.076224
179	6	0	3.148078	1.881232	0.071107
180	6	0	2.699434	0.569918	0.095223
181	1	0	-1.601281	2.019833	0.100642
182	1	0	1.424128	-1.914532	0.130528
183	7	0	2.261349	2.942504	0.069307
184	7	0	-2.437371	-2.838266	0.139023
185	8	0	0.114059	3.710004	0.064734
186	6	0	-2.946555	-4.198441	0.144216
187	6	0	2.770601	4.302519	0.049159
188	1	0	3.433497	4.472630	0.900754
189	1	0	3.314722	4.496447	-0.879017
190	1	0	1.913637	4.968564	0.112129
191	1	0	-2.086954	-4.864058	0.147956
192	1	0	-3.552293	-4.376499	1.036340
193	1	0	-3.550499	-4.384379	-0.747494
194	8	0	-0.290076	-3.604960	0.148107
195	6	0	-4.736015	-1.883900	0.130789
196	6	0	-5.362612	-0.656421	0.129059

197	16	0	-4.204518	0.645684	0.137711
198	6	0	4.559636	1.986013	0.039539
199	6	0	5.184829	0.757635	0.047524
200	16	0	4.025980	-0.542553	0.097901
201	1	0	5.101698	2.920816	-0.003569
202	1	0	-5.277044	-2.820208	0.118857

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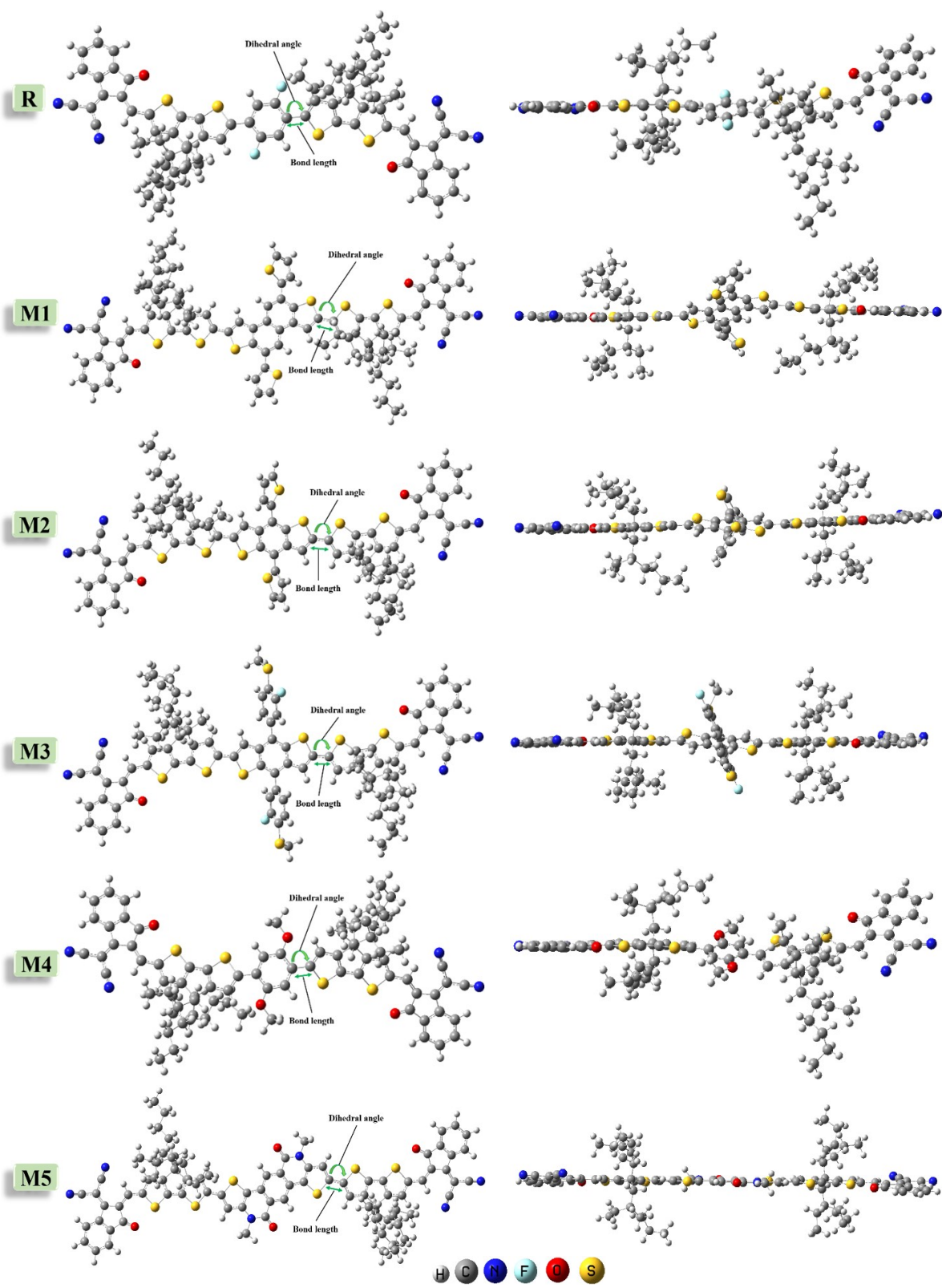
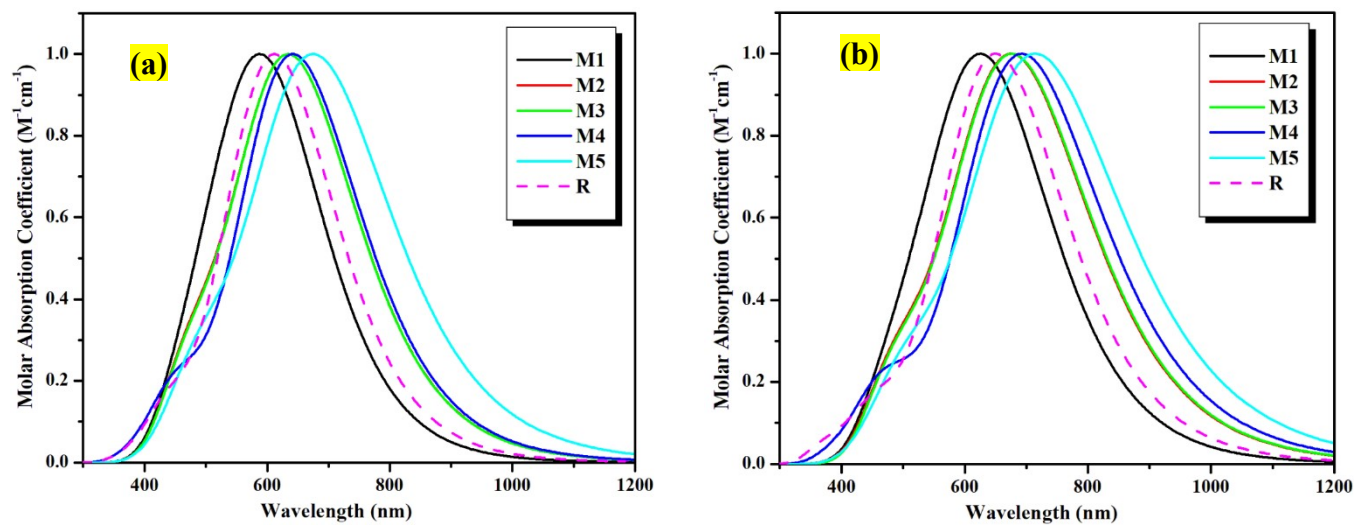


Fig. S1. Optimized molecular structures of reference and modified molecules.



**Fig. S2.** Graphs representing absorption of **R** and **M1-M5** in **(a)** gas phase and **(b)** solvent phase (chloroform).

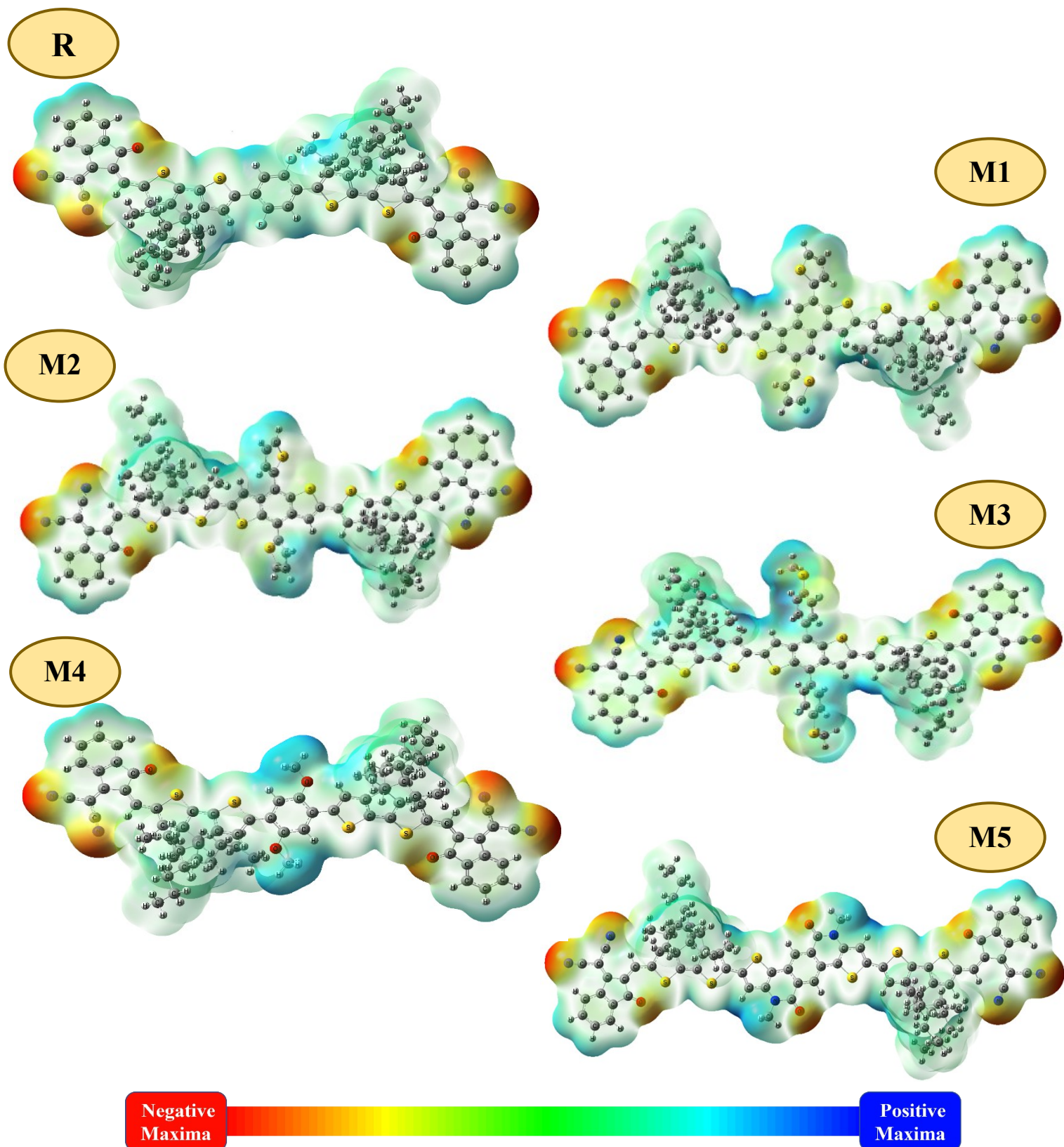
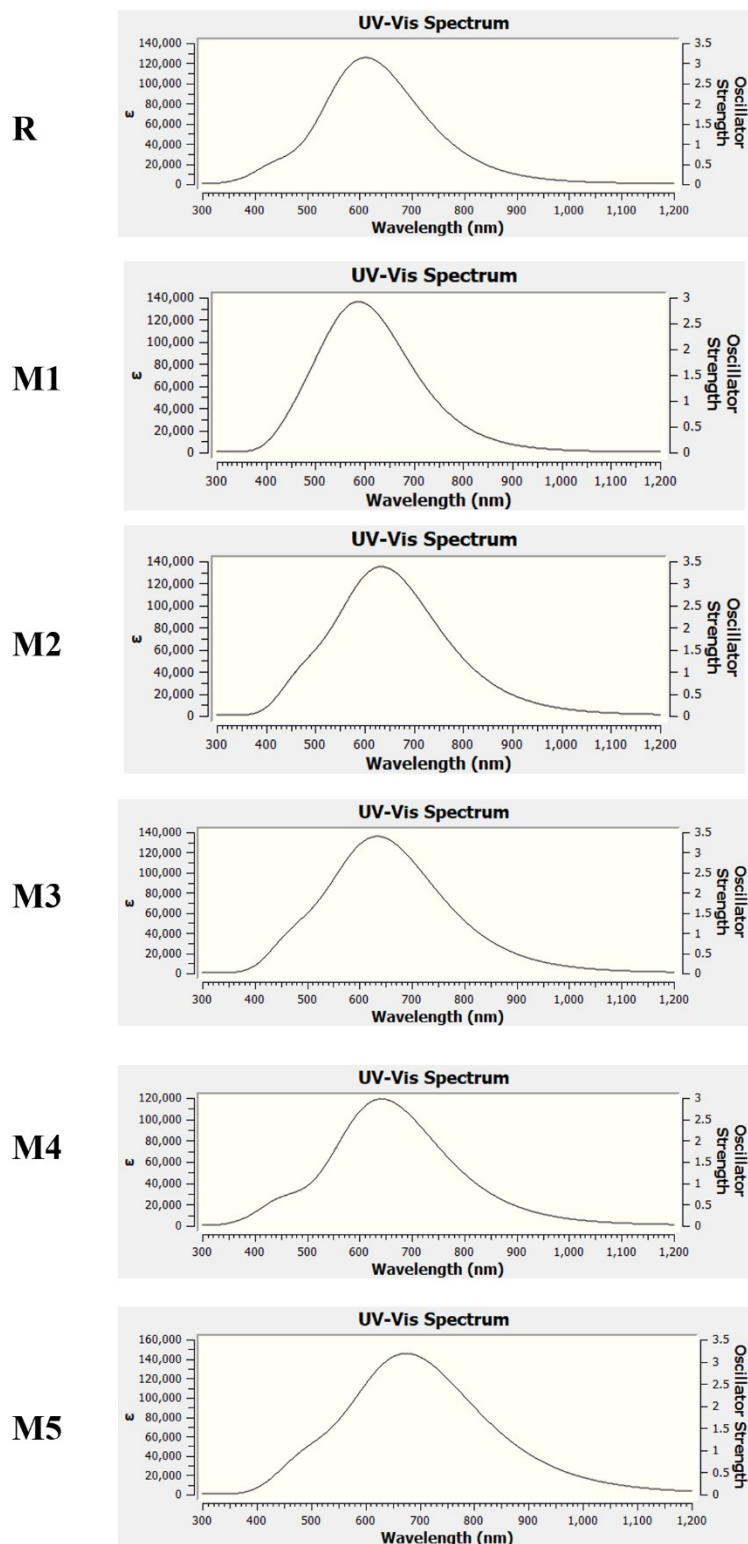
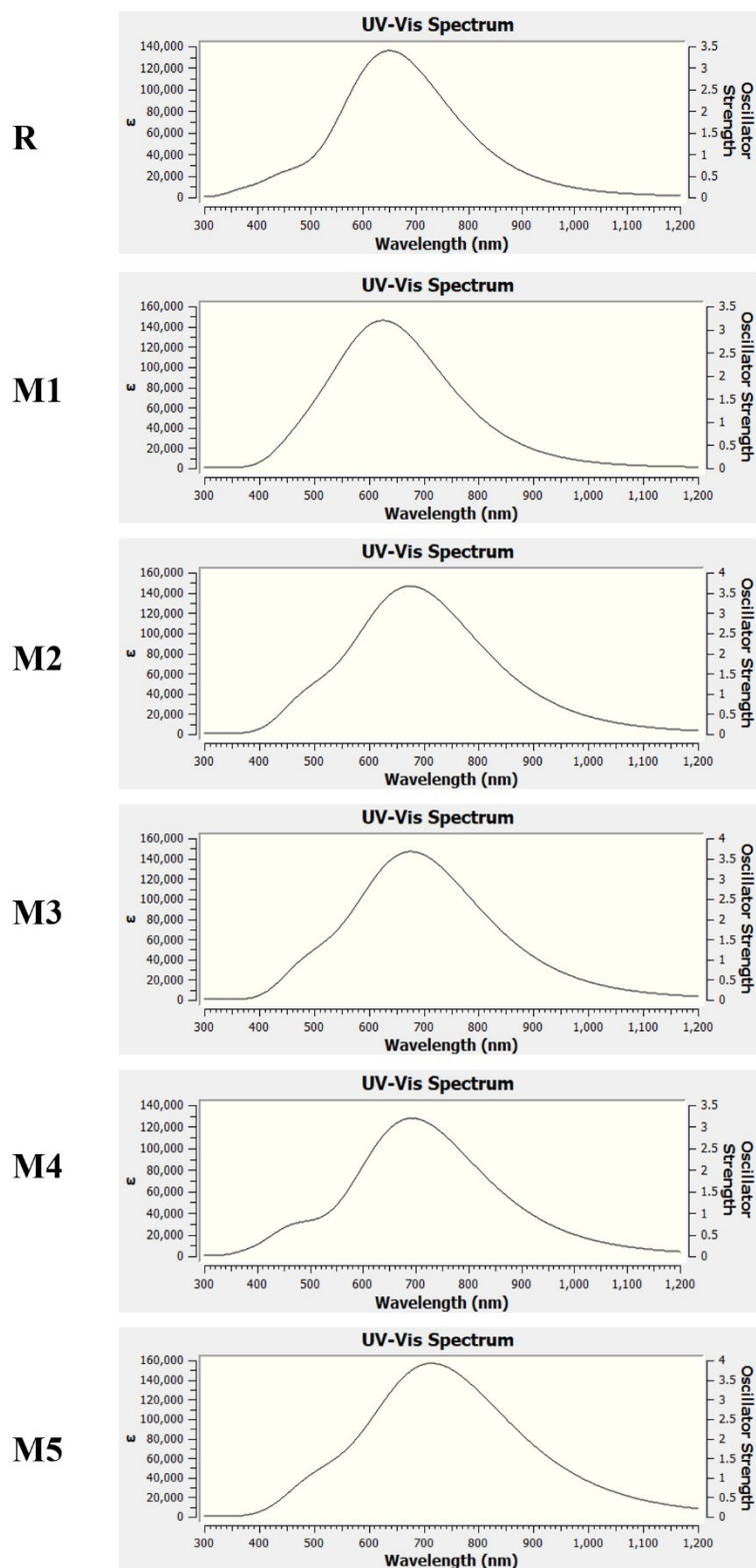


Fig. S3. Shaded maps of MEP for R and M1-M5.





**Figure S4:** Guassview absorption curves of all the molecules in the gas phase phase at MPW1PW91/6-31G (d, p) showing their oscillator strength (right y-axis), molar absorptivity (left y-axis) and wavelength (x-axis).



**Figure S5:** Guassview absorption curves of all the molecules in the solvent phase at MPW1PW91/6-31G (d, p) showing their oscillator strength (right y-axis), molar absorptivity (left y-axis) and wavelength (x-axis).

## References

1. Wang, N., et al., *Enhancement of intra-and inter-molecular  $\pi$ -conjugated effects for a non-fullerene acceptor to achieve high-efficiency organic solar cells with an extended photoresponse range and optimized morphology*. Materials Chemistry Frontiers, 2018. **2**(11): p. 2006-2012.
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