Supplementary Materials

Theoretical Study on the Diels–Alder Reaction of Fullerenes: Analysis of Isomerism, Aromaticity, and Solvation

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Table S1. Electronic energies obtained (in vacuum) for the various species studied at different theoretical levels. M06-2X/6-311++G(2d,p), B3LYP/6-31+G(d), and MP2/cc-pVDZ are single point energy calculations on the optimized M06-2X/6-31+G(d) geometries.

Species	E_{el} / Hartree			
	M06-2X/ 6-31+G(d)	M06-2X/ 6-311++G(2d,p)	B3LYP/ 6-31+G(d)	MP2/ cc-pVDZ [1]
anthracene	-539.308194	-539.444350	-539.548294	-537.848034 (-536.038262)
indene	-347.614828	-347.704859	-347.775603	-
C_{60}	-2285.492704	-2285.994963	-2286.220335	-2279.675979 (-2271.964664)
$AC_{60}MA$	-2824.837241	-2825.471834	-2825.765670	-2817.587061 (-2808.014434)
C_{70}	-2666.503092	-2667.089136	-2667.356359	-
$AIC_{70}MA$ *a*	-3205.848078	-3206.566391	-3206.901523	-
$AIC_{70}MA$ *b*	-3205.846171	-3206.564118	-3206.896679	-
$AIC_{70}MA$ *c*	-3205.818709	-	-	-
$AIC_{70}MA$ *d*	-3205.774922	-	-	-
ICMA	-2633.151952	-2633.740334	-2634.007738	-
AICBA *trans*-1	-3172.494885	-3173.215574	-3173.550477	-
AICBA *trans*-2 *a*	-3172.495132	-	-	-
AICBA *trans*-2 *b*	-3172.495216	-	-	-
AICBA *trans*-3 a	-3172.496658	-	-	-
AICBA *trans*-3 *b*	-3172.496348	-3173.217473	-3173.552751	-
AICBA *trans*-4 *a*	-3172.494920	-	-	-
AICBA *trans*-4 *b*	-3172.494882	-	-	-
AICBA *e*-face *a*	-3172.496894	-3173.217558	-3173.552494	-
AICBA *e*-face *b*	-3172.496743	-	-	-
AICBA *e*-edge	-3172.496762	-	-	-
AICBA *cis*-3 *a*	-3172.490488	-	-	-
AICBA *cis*-3 *b*	-3172.490574	-	-	-
AICBA *cis*-2 *a*	-3172.489805	-	-	-
AICBA *cis*-2 *b*	-3172.484859	-3173.210505	-3173.543610	-

[1] The calculated Hartree-Fock energy is shown in parenthesis.

Table S2. Electronic energies obtained for the species in *m*-xylene, simulated using SMD – Solvent Model based on Density. The energies were obtained through single point calculations on the optimized geometries obtained in vacuum, at the M06-2X/6-31+G(d) level. For a few representative molecules the geometries were reoptimized in solution using the same level of theory.

Species	$E_{el}^{m-\text{xylene}}(\text{single point})$ / Hartree	$E_{el}^{m-\text{xylene}}(\text{opt in } m-\text{xylene})$ / Hartree
anthracene	-539.324296	-539.324302
indene	-347.626159	-347.626165
C_{60}	-2285.548057	-2285.548311
$AC_{60}MA$	-2824.900524	-2824.900552
C_{70}	-2666.565639	-2666.565789
$AIC_{70}MA$ *a*	-3205.919287	-3205.919317
$AIC_{70}MA$ *b*	-3205.917180	-
ICMA	-2633.211855	-2633.211890
AICBA *trans*-1	-3172.563408	-
AICBA *trans*-2 *a*	-3172.564002	-
AICBA *trans*-2 *b*	-3172.563872	-
AICBA *trans*-3 a	-3172.565535	-
AICBA *trans*-3 *b*	-3172.565046	-
AICBA *trans*-4 *a*	-3172.563268	-
AICBA *trans*-4 *b*	-3172.565046	-
AICBA *e*-face *a*	-3172.565521	-3172.565551
AICBA *e*-face *b*	-3172.565133	-
AICBA *e*-edge	-3172.565868	-
AICBA *cis*-3 *a*	-3172.559316	-
AICBA *cis*-3 *b*	-3172.558671	-
AICBA *cis*-2 *a*	-3172.558345	-
AICBA *cis*-2 *b*	-3172.552854	-

Table S3 Thermal corrections to enthalpy (including ZPE) from T = 0 to 298.15 K, $\Delta H_{thermal}$, and absolute enthalpies, at T = 298.15 K, obtained from optimization and frequencies calculations for the various species using M06-2X/6-31+G(d).

Species	$\Delta H_{\text{thermal}}$ / Hartree	$H(T = 298.15\,\text{K})$ / Hartree
Indene	0.150539	-347.4642888
Anthracene	0.206977	-539.1012174
C_{60}	0.399011	-2285.093693
C_{70}	0.465784	-2666.037308
$IC_{60}MA$	0.553810	-2632.598142
$AC_{60}MA$	0.609736	-2824.227505
$AC_{70}MA$ *a*	0.678131	-3205.169947
AIC60BA *e*-face *a*	0.766103	-3171.730791

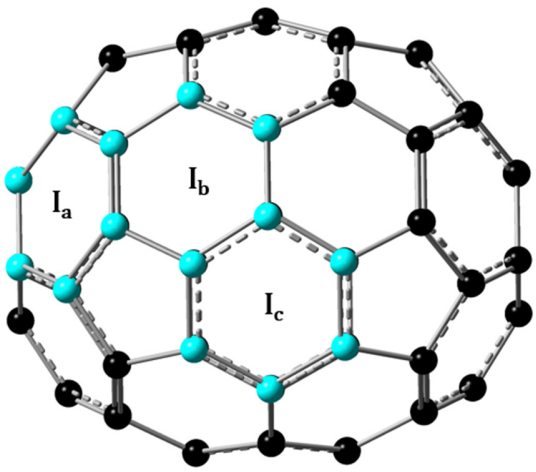

Figure S1. Designated types of hexagons in C_{70}. The same logic applies to Type-II hexagons, except they are adjacent to an addend.

Table S4. HOMA analysis, decomposed in EN and GEO values, for the hexagon rings in C_{60} and C_{70}, and hexagons adjacent to the addends in the respective adducts.

Species	EN	GEO	HOMA	Ring Type
C_{60} [1]	0.267	0.529	0.204	I
$AC_{60}MA$ [2]	0.158	0.368	0.474	II
$IC_{60}MA$	0.162	0.363	0.475	II
	0.162	0.363	0.475	II
	0.163	0.369	0.468	II
	0.163	0.369	0.468	II
AICBA *trans*-1	0.161	0.349	0.490	II
	0.161	0.349	0.490	II
	0.158	0.355	0.488	II
	0.158	0.355	0.488	II
	0.165	0.364	0.470	II
	0.165	0.364	0.470	II
	0.156	0.349	0.495	II
	0.156	0.349	0.495	II
AICBA *trans*-2 *a*	0.159	0.351	0.490	II
	0.174	0.382	0.444	II
	0.155	0.353	0.492	II
	0.165	0.373	0.462	II
	0.159	0.349	0.492	II
	0.166	0.359	0.475	II
	0.165	0.366	0.469	II
	0.162	0.371	0.467	II
AICBA *trans*-2 *b*	0.162	0.366	0.472	II
	0.169	0.379	0.453	II
	0.170	0.370	0.460	II
	0.164	0.347	0.489	II
	0.160	0.369	0.472	II
	0.155	0.352	0.493	II
	0.164	0.373	0.463	II
	0.160	0.349	0.491	II
AICBA *trans*-3 *a*	0.170	0.371	0.459	II
	0.176	0.388	0.436	II
	0.170	0.375	0.455	II
	0.163	0.346	0.491	II
	0.182	0.392	0.426	II
	0.160	0.357	0.483	II
	0.157	0.345	0.498	II
	0.164	0.367	0.469	II
AICBA *trans*-3 *b*	0.167	0.365	0.469	II
	0.167	0.361	0.472	II
	0.164	0.356	0.479	II
	0.187	0.403	0.410	II
	0.162	0.366	0.471	II
	0.161	0.358	0.481	II
	0.154	0.344	0.502	II
	0.176	0.387	0.437	II
AICBA *trans*-4 *a*	0.080	0.217	0.703	III
	0.160	0.363	0.477	II

	0.173	0.377	0.449	II
	0.168	0.377	0.454	II
	0.160	0.363	0.477	II
	0.152	0.353	0.495	II
	0.163	0.381	0.456	II
AICBA *trans*-4 *b*	0.083	0.228	0.690	III
	0.165	0.378	0.457	II
	0.163	0.384	0.454	II
	0.165	0.378	0.457	II
	0.175	0.391	0.434	II
	0.157	0.351	0.492	II
	0.169	0.384	0.448	II
AICBA *e*-face *a*	0.084	0.222	0.694	III
	0.084	0.222	0.694	III
	0.161	0.365	0.474	II
	0.161	0.365	0.474	II
	0.156	0.347	0.497	II
	0.156	0.347	0.497	II
AICBA *e*-face *b*	0.086	0.232	0.682	III
	0.086	0.232	0.682	III
	0.159	0.354	0.487	II
	0.159	0.354	0.487	II
	0.160	0.359	0.481	II
	0.160	0.359	0.481	II
AICBA *e*-edge	0.084	0.220	0.696	III
	0.086	0.232	0.682	III
	0.164	0.362	0.474	II
	0.165	0.353	0.483	II
	0.155	0.361	0.484	II
	0.154	0.357	0.489	II
C_{70} [3]	0.219	0.462	0.319	Ia
	0.473	0.705	-0.177	Ib
	0.253	0.259	0.489	Ic
$AIC_{70}MA$ *a*	0.126	0.299	0.575	IIa
	0.126	0.299	0.575	IIa
	0.330	0.585	0.085	IIb
	0.330	0.585	0.085	IIb
$AIC_{70}MA$ *b*	0.118	0.306	0.576	IIa
	0.118	0.306	0.576	IIa
	0.178	0.199	0.624	IIc
	0.178	0.199	0.624	IIc

[1] All 20 hexagons are equivalent.

[2] All 4 four hexagons adjacent to the addend are equivalent.

[3] Ia and Ib hexagons exist in 10 equivalent unities and Ic rings in 5 equivalent unities.

Table S5. M06-2X/6-31+G(d) optimized geometries.

Anthracene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.652663	0.714593	-0.000019
2	6	0	2.475821	1.405672	0.000041
3	6	0	1.219600	0.718406	0.000033
4	6	0	1.219602	-0.718405	0.000018
5	6	0	2.475822	-1.405671	-0.000018
6	6	0	3.652664	-0.714592	-0.000058
7	6	0	0.000000	1.400640	0.000026
8	6	0	0.000001	-1.400641	0.000027
9	6	0	-1.219601	-0.718406	0.000022
10	6	0	-1.219602	0.718405	0.000010
11	6	0	-2.475821	1.405671	-0.000025
12	1	0	-2.470912	2.493147	-0.000062
13	6	0	-3.652663	0.714592	-0.000054
14	6	0	-3.652663	-0.714592	-0.000008
15	6	0	-2.475821	-1.405672	0.000027
16	1	0	-0.000005	2.489468	0.000039
17	1	0	4.598900	1.247714	-0.000049
18	1	0	2.470909	2.493147	0.000087
19	1	0	2.470910	-2.493147	-0.000025
20	1	0	4.598897	-1.247719	-0.000116
21	1	0	-0.000003	-2.489468	0.000042
22	1	0	-4.598898	1.247718	-0.000086
23	1	0	-4.598898	-1.247718	-0.000025
24	1	0	-2.470913	-2.493147	0.000064

Indene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.229273	-0.686185	0.000045
2	6	0	-1.663420	-1.156195	0.000032
3	6	0	-0.211136	0.720159	-0.000036
4	6	0	-2.436045	0.140941	0.000024
5	6	0	-1.601730	1.194800	-0.000163
6	6	0	0.955768	-1.408064	0.000094
7	6	0	0.997046	1.414277	-0.000058
8	6	0	2.168267	-0.712014	0.000067
9	6	0	2.186769	0.684998	-0.000008
10	1	0	-1.896160	-1.768092	-0.881467
11	1	0	-1.896149	-1.767921	0.881654
12	1	0	-3.519346	0.186958	0.000044
13	1	0	-1.890978	2.240588	-0.000263
14	1	0	0.946677	-2.495516	0.000143
15	1	0	1.014951	2.501053	-0.000137
16	1	0	3.104918	-1.261990	0.000090
17	1	0	3.138628	1.208614	-0.000040

C_{60}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.922830	-1.753120	-0.959790
2	6	0	3.240993	-0.397478	-1.370838
3	6	0	3.468725	0.582444	-0.414105
4	6	0	3.388865	0.251837	0.997712
5	6	0	3.085783	-1.044804	1.390662
6	6	0	2.847166	-2.069469	0.389655
7	6	0	1.939362	-2.283939	-1.886619
8	6	0	1.649904	-1.256635	-2.870820
9	6	0	2.453940	-0.090174	-2.551636
10	6	0	1.928901	1.183238	-2.723839
11	6	0	2.919433	1.914396	-0.594194
12	6	0	2.789966	1.379089	1.689995
13	6	0	1.913369	1.160776	2.744289
14	6	0	1.595928	-0.195325	3.154159
15	6	0	2.169032	-1.273392	2.493286
16	6	0	1.364526	-2.439438	2.174214
17	6	0	1.784002	-2.931546	0.874419
18	6	0	0.843336	-3.439273	-0.011656
19	6	0	0.922899	-3.108257	-1.423087
20	6	0	0.355759	-1.098126	-3.347041
21	6	0	-0.707340	-1.960557	-2.863109
22	6	0	-0.430401	-2.943371	-1.922390
23	6	0	-1.346698	-3.170435	-0.819052
24	6	0	-0.559372	-3.477467	0.361486
25	6	0	-0.960482	-3.007300	1.604720
26	6	0	0.023023	-2.476014	2.530920
27	6	0	-0.575293	-1.348865	3.222907
28	6	0	0.193480	-0.233921	3.526741
29	6	0	2.499845	2.406197	0.705620
30	6	0	-1.939363	2.283939	1.886618
31	6	0	-0.922900	3.108256	1.423085
32	6	0	-0.843336	3.439272	0.011657
33	6	0	-1.784003	2.931546	-0.874419
34	6	0	-2.847166	2.069470	-0.389656
35	6	0	-3.240993	0.397478	1.370838
36	6	0	-2.453939	0.090174	2.551637
37	6	0	-1.649904	1.256633	2.870820
38	6	0	-0.355760	1.098125	3.347042
39	6	0	0.707342	1.960557	2.863109
40	6	0	0.430403	2.943371	1.922389
41	6	0	0.559372	3.477466	-0.361486
42	6	0	0.960482	3.007300	-1.604719
43	6	0	-0.023023	2.476013	-2.530920
44	6	0	-1.364527	2.439438	-2.174215
45	6	0	-2.169033	1.273394	-2.493286
46	6	0	-3.085783	1.044804	-1.390663
47	6	0	-3.388865	-0.251836	-0.997712
48	6	0	-3.468725	-0.582443	0.414106
49	6	0	-1.928900	-1.183239	2.723840
50	6	0	-2.166995	-2.208174	1.723380
51	6	0	-2.919432	-1.914396	0.594194
52	6	0	-2.499844	-2.406197	-0.705618
53	6	0	-2.789966	-1.379088	-1.689995
54	6	0	-1.913369	-1.160775	-2.744288
55	6	0	-1.595928	0.195325	-3.154160
56	6	0	-0.193481	0.233922	-3.526741
57	6	0	0.575292	1.348866	-3.222907
58	6	0	1.346698	3.170434	0.819053
59	6	0	2.166996	2.208173	-1.723380
60	6	0	-2.922829	1.753121	0.959790

72	6	0	4.620942	-1.229582	0.699655
73	6	0	3.976749	0.000024	1.292597
74	1	0	3.996015	0.000041	2.387284
75	6	0	4.620889	1.229631	0.699646
76	6	0	5.131145	2.313597	1.402697
77	1	0	5.117029	2.316585	2.490142
78	6	0	5.657710	3.397948	0.697026
79	1	0	6.065094	4.247200	1.237763
80	6	0	5.657739	3.397922	-0.697054
81	1	0	6.065147	4.247155	-1.237806
82	6	0	5.131291	2.313508	-1.402721
83	1	0	5.117242	2.316469	-2.490167
84	6	0	4.620959	1.229582	-0.699669

$AC_{60}MA$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.467649	-0.000003	-0.800841
2	6	0	2.467647	0.000009	0.800840
3	6	0	1.709899	1.170131	1.427746
4	6	0	1.284379	2.277091	0.740834
5	6	0	1.284379	2.277079	-0.740875
6	6	0	1.709906	1.170111	-1.427771
7	6	0	0.966108	0.725386	-2.573810
8	6	0	0.966107	-0.725412	-2.573794
9	6	0	1.709898	-1.170124	-1.427753
10	6	0	1.284383	-2.277085	-0.740838
11	6	0	1.284381	-2.277070	0.740876
12	6	0	1.709901	-1.170101	1.427775
13	6	0	0.966106	-0.725369	2.573807
14	6	0	0.966108	0.725428	2.573796
15	6	0	-0.150359	1.422936	3.026837
16	6	0	-0.591442	2.590399	2.307782
17	6	0	0.110575	2.996514	1.175453
18	6	0	-0.614117	3.442077	-0.000030
19	6	0	0.110575	2.996493	-1.175504
20	6	0	-0.591442	2.590362	-2.307827
21	6	0	-0.150359	1.422886	-3.026862
22	6	0	-1.323346	0.693571	-3.480309
23	6	0	-1.323347	-0.693617	-3.480296
24	6	0	-0.150359	-1.422925	-3.026836
25	6	0	-0.591440	-2.590386	-2.307783
26	6	0	0.110576	-2.996502	-1.175452
27	6	0	-0.614117	-3.442067	0.000030
28	6	0	0.110576	-2.996480	1.175502
29	6	0	-0.591441	-2.590348	2.307828
30	6	0	-0.150360	-1.422874	3.026861
31	6	0	-1.323348	-0.693558	3.480309
32	6	0	-1.323347	0.693630	3.480297
33	6	0	-2.495540	1.421129	3.031411
34	6	0	-2.042018	2.594032	2.303320
35	6	0	-2.732817	3.018828	1.175820
36	6	0	-2.001908	3.459333	-0.000030
37	6	0	-2.732817	3.018808	-1.175870
38	6	0	-2.042018	2.593995	-2.303364
39	6	0	-2.495539	1.421079	-3.031435
40	6	0	-3.617801	0.726215	-2.598740
41	6	0	-3.617801	-0.726248	-2.598727
42	6	0	-2.495540	-1.421117	-3.031412
43	6	0	-2.042016	-2.594019	-2.303319
44	6	0	-2.732815	-3.018815	-1.175820
45	6	0	-2.001907	-3.459319	0.000030
46	6	0	-2.732816	-3.018795	1.175871
47	6	0	-2.042018	-2.593981	2.303364
48	6	0	-2.495541	-1.421066	3.031436
49	6	0	-3.617802	-0.726203	2.598739
50	6	0	-3.617802	0.726260	2.598727
51	6	0	-4.339512	1.173923	1.422042
52	6	0	-3.905450	2.295505	0.727063
53	6	0	-3.905450	2.295492	-0.727102
54	6	0	-4.339511	1.173898	-1.422063
55	6	0	-4.786460	0.000001	-0.694365
56	6	0	-4.339513	-1.173910	-1.422042
57	6	0	-3.905448	-2.295491	-0.727063
58	6	0	-3.905448	-2.295478	0.727101
59	6	0	-4.339513	-1.173886	1.422062
60	6	0	-4.786460	0.000013	0.694364
61	6	0	3.976746	-0.000012	-1.292606
62	1	0	3.995995	-0.000028	-2.387293
63	6	0	4.620878	-1.229634	-0.699657
64	6	0	5.131062	-2.313644	-1.402693
65	1	0	5.116971	-2.316652	-2.490138
66	6	0	5.657456	-3.398071	-0.697009
67	1	0	6.064735	-4.247372	-1.237750
68	6	0	5.657534	-3.398015	0.697070
69	1	0	6.064839	-4.247292	1.237829
70	6	0	5.131162	-2.313556	1.402721
71	1	0	5.117093	-2.316499	2.490167

C_{70}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.201751	3.091604	1.547133
2	6	0	0.000205	3.441961	0.884986
3	6	0	-1.201494	3.091714	1.546979
4	6	0	-1.201400	2.204703	2.663771
5	6	0	-0.000035	1.637623	3.152965
6	6	0	1.201688	2.204341	2.663699
7	6	0	2.440369	1.447541	2.635216
8	6	0	3.219795	1.882746	1.497261
9	6	0	2.440501	2.892961	0.816459
10	6	0	2.440786	2.953077	-0.562238
11	6	0	1.201992	3.215218	-1.273475
12	6	0	0.000184	3.505970	-0.583464
13	6	0	-1.201551	3.215279	-1.273427
14	6	0	-2.440079	2.953488	-0.562471
15	6	0	-2.440026	2.893103	0.816207
16	6	0	-3.219629	1.883112	1.497279
17	6	0	-2.440171	1.447798	2.635114
18	6	0	-2.440212	0.117982	3.004049
19	6	0	-1.201739	-0.516110	3.418378
20	6	0	-0.000063	0.221385	3.545606
21	6	0	1.201629	-0.516185	3.418378
22	6	0	2.440141	0.117545	3.003885
23	6	0	3.219454	-0.842420	2.253553
24	6	0	3.966919	-0.432413	1.155980
25	6	0	3.966908	0.965438	0.767930
26	6	0	3.967283	1.028417	-0.680749
27	6	0	3.220345	2.005798	-1.327847
28	6	0	2.440418	1.670740	-2.499156
29	6	0	1.201736	2.427147	-2.462032
30	6	0	0.000159	1.905105	-2.998832
31	6	0	-1.201410	2.427208	-2.462036
32	6	0	-2.440134	1.670910	-2.499127
33	6	0	-3.220001	2.006204	-1.328174
34	6	0	-3.966873	1.028804	-0.680689
35	6	0	-3.966553	0.965832	0.767877
36	6	0	-3.967178	-0.431941	1.155913
37	6	0	-3.219625	-0.842144	2.253421
38	6	0	-2.440478	-2.059070	2.190516
39	6	0	-1.202059	-1.852208	2.919544
40	6	0	-0.000123	-2.492578	2.531963
41	6	0	1.201540	-1.852357	2.919454
42	6	0	2.440244	-2.059392	2.190703
43	6	0	2.440197	-2.821589	1.039991
44	6	0	3.219380	-2.404014	-0.104560
45	6	0	3.966334	-1.232904	-0.053369
46	6	0	3.966915	-0.330556	-1.188261
47	6	0	3.220022	-0.643527	-2.317803
48	6	0	2.440307	0.377869	-2.981647
49	6	0	1.201502	-0.217464	-3.450294
50	6	0	0.000071	0.528911	-3.512929
51	6	0	-1.201547	-0.217248	-3.450313
52	6	0	-2.440233	0.378040	-2.981761
53	6	0	-3.219986	-0.643144	-2.317843
54	6	0	-3.966875	-0.329952	-1.188269
55	6	0	-3.966687	-1.232597	-0.053528
56	6	0	-3.219789	-2.403562	-0.104581
57	6	0	-2.440727	-2.821462	1.040039
58	6	0	-1.201749	-3.411100	0.565324
59	6	0	-0.000226	-3.304117	1.306725
60	6	0	1.201179	-3.411245	0.565287
61	6	0	1.201133	-3.348915	-0.859650
62	6	0	2.439833	-2.719709	-1.281142
63	6	0	2.440506	-1.861000	-2.361570
64	6	0	1.201564	-1.591707	-3.069492
65	6	0	-0.000041	-2.263768	-2.739327
66	6	0	-1.201630	-1.591443	-3.069724
67	6	0	-2.440493	-1.860634	-2.361623
68	6	0	-2.440271	-2.719547	-1.281323
69	6	0	-1.201672	-3.348769	-0.859629
70	6	0	-0.000233	-3.178785	-1.589228

$AC_{70}MA$ isomer *a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.338292	2.559794	1.660906
2	6	0	2.018900	3.070936	1.687297
3	6	0	1.171860	2.559010	2.700050
4	6	0	1.537865	1.410561	3.462159
5	6	0	2.762557	0.734992	3.231494
6	6	0	3.705115	1.410515	2.421362
7	6	0	4.722504	0.689810	1.674819
8	6	0	5.001278	1.412649	0.454390
9	6	0	4.129827	2.565257	0.442690
10	6	0	3.565420	2.994505	-0.741258
11	6	0	2.182324	3.434704	-0.763041
12	6	0	1.415253	3.517859	0.423730
13	6	0	0.010494	3.406534	0.271315
14	6	0	-0.839369	2.964298	1.357854
15	6	0	-0.273356	2.561145	2.556362
16	6	0	-0.804086	1.416910	3.233025
17	6	0	0.320664	0.689604	3.783756
18	6	0	0.320650	-0.689961	3.783667
19	6	0	1.537898	-1.410858	3.462082
20	6	0	2.762547	-0.735233	3.231410
21	6	0	3.705134	-1.410678	2.421258
22	6	0	4.722502	-0.689896	1.674762
23	6	0	5.001265	-1.412613	0.454280
24	6	0	5.269675	-0.724174	-0.724996
25	6	0	5.269620	0.724262	-0.724929
26	6	0	4.674077	1.173209	-1.968252
27	6	0	3.843588	2.287877	-1.972527
28	6	0	2.616706	2.278407	-2.737897
29	6	0	1.601474	2.995565	-1.989468
30	6	0	0.235711	2.631741	-2.068054
31	6	0	-0.571324	2.970622	-0.954512
32	6	0	-1.794813	2.258546	-0.651901
33	6	0	-1.970925	2.263611	0.809251
34	6	0	-2.489810	1.166867	1.452389
35	6	0	-1.878928	0.722773	2.671139
36	6	0	-1.878891	-0.723092	2.671107
37	6	0	-0.804091	-1.417286	3.232982
38	6	0	-0.273316	-2.561451	2.556199
39	6	0	1.171903	-2.559241	2.699854
40	6	0	2.018953	-3.071096	1.687088
41	6	0	3.338323	-2.559898	1.660695
42	6	0	4.129878	-2.565271	0.442498
43	6	0	3.565464	-2.994421	-0.741476
44	6	0	3.843643	-2.287714	-1.972697
45	6	0	4.674117	-1.173054	-1.968343
46	6	0	4.308574	0.000121	-2.740328
47	6	0	3.131353	0.000114	-3.478046
48	6	0	2.269300	1.162749	-3.474969
49	6	0	0.890886	0.713599	-3.490757
50	6	0	-0.129215	1.449017	-2.841256
51	6	0	-1.272254	0.712775	-2.433616
52	6	0	-2.140465	1.159051	-1.377729
53	6	0	-2.971107	-0.000074	-0.845568
54	6	0	-3.175762	-0.000056	0.742804
55	6	0	-2.489899	-1.167145	1.452395
56	6	0	-1.970840	-2.263688	0.809096
57	6	0	-0.839279	-2.964437	1.357612
58	6	0	0.010550	-3.406620	0.271069
59	6	0	1.415315	-3.517907	0.423461
60	6	0	2.182385	-3.434662	-0.763290
61	6	0	1.601529	-2.995426	-1.989680
62	6	0	2.616745	-2.278266	-2.738106
63	6	0	2.269348	-1.162523	-3.475045
64	6	0	0.890899	-0.713433	-3.490859
65	6	0	-0.129145	-1.448871	-2.841315
66	6	0	-1.272202	-0.712629	-2.433672
67	6	0	-2.140266	-1.158985	-1.377767
68	6	0	-1.794868	-2.258654	-0.652064
69	6	0	-0.571320	-2.970641	-0.954731
70	6	0	0.235720	-2.631696	-2.068232
71	6	0	-4.405873	-0.000053	-1.526994
72	1	0	-4.285902	0.000122	-2.615160
73	6	0	-5.119912	1.229589	-1.020746
74	6	0	-5.537652	2.312808	-1.783449
75	1	0	-5.386956	2.315165	-2.860502
76	6	0	-6.148527	3.398033	-1.150315
77	1	0	-6.482609	4.247433	-1.738766
78	6	0	-6.324042	3.398934	0.232767
79	1	0	-6.795807	4.248307	0.717831
80	6	0	-5.890698	2.314893	0.999987
81	1	0	-6.014214	2.318423	2.080487
82	6	0	-5.296590	1.230084	0.367473
83	6	0	-4.732500	0.000030	1.036884
84	1	0	-4.891450	-0.000064	2.119957
85	6	0	-5.296922	-1.229819	0.367374
86	6	0	-5.891558	-2.314377	0.999860
87	1	0	-6.015239	-2.317804	2.080344
88	6	0	-6.324865	-3.398464	0.232723
89	1	0	-6.796903	-4.247666	0.717821
90	6	0	-6.149090	-3.397801	-1.150339
91	1	0	-6.483291	-4.247222	-1.738692
92	6	0	-5.537828	-2.312825	-1.783470
93	1	0	-5.386931	-2.315268	-2.860493
94	6	0	-5.119945	-1.229610	-1.020822

$AC_{70}MA$ isomer *b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.302069	0.486928	3.439516
2	6	0	0.942505	0.107683	3.529681
3	6	0	0.671887	-1.279216	3.436912
4	6	0	1.666218	-2.199079	3.003312
5	6	0	2.965520	-1.760595	2.640889
6	6	0	3.300763	-0.434662	3.001802
7	6	0	4.311148	0.316229	2.278551
8	6	0	3.944538	1.715702	2.288432
9	6	0	2.688166	1.814717	2.996917
10	6	0	1.722720	2.704404	2.570355
11	6	0	0.326456	2.304733	2.567301
12	6	0	-0.078610	1.054638	3.065289
13	6	0	-1.289059	0.538794	2.523648
14	6	0	-1.575224	-0.885048	2.537213
15	6	0	-0.622641	-1.776908	2.996390
16	6	0	-0.428015	-3.012746	2.297533
17	6	0	0.995334	-3.267646	2.283067
18	6	0	1.587042	-3.812432	1.161466
19	6	0	2.876318	-3.317889	0.712636
20	6	0	3.595671	-2.344972	1.449967
21	6	0	4.512973	-1.557232	0.713363
22	6	0	4.907220	-0.233907	1.161905
23	6	0	5.163500	0.588959	0.000009
24	6	0	4.810398	1.933044	0.000019
25	6	0	4.184898	2.511662	1.174004
26	6	0	3.169908	3.444599	0.725462
27	6	0	1.964661	3.535875	1.413415
28	6	0	0.714999	3.620756	0.689533
29	6	0	-0.294683	2.865999	1.408653
30	6	0	-1.354489	2.210349	0.740826
31	6	0	-1.924187	1.107332	1.406150
32	6	0	-2.899565	0.107909	0.791314
33	6	0	-2.407264	-1.191204	1.415967
34	6	0	-2.223495	-2.370920	0.740560
35	6	0	-1.206006	-3.297835	1.174520
36	6	0	-0.580317	-3.869761	-0.000021
37	6	0	0.786765	-4.130199	-0.000016
38	6	0	1.587051	-3.812431	-1.161505
39	6	0	2.876321	-3.317877	-0.712655
40	6	0	3.595681	-2.344973	-1.449980
41	6	0	4.512978	-1.557223	-0.713372
42	6	0	4.907216	-0.233898	-1.161892
43	6	0	4.311160	0.316244	-2.278541
44	6	0	3.944538	1.715722	-2.288394
45	6	0	4.184901	2.511680	-1.173975
46	6	0	3.169911	3.444614	-0.725416
47	6	0	1.964667	3.535876	-1.413371
48	6	0	0.714982	3.620768	-0.689496
49	6	0	-0.294678	2.866011	-1.408619
50	6	0	-1.354501	2.210363	-0.740810
51	6	0	-1.924203	1.107363	-1.406157
52	6	0	-2.899561	0.107910	-0.791342
53	6	0	-2.407237	-1.191187	-1.415981
54	6	0	-2.223489	-2.370919	-0.740605
55	6	0	-1.205999	-3.297825	-1.174560
56	6	0	-0.428004	-3.012734	-2.297572
57	6	0	0.995346	-3.267630	-2.283092
58	6	0	1.666235	-2.199057	-3.003338
59	6	0	2.965525	-1.760577	-2.640899
60	6	0	3.300776	-0.434637	-3.001788
61	6	0	2.302079	0.486955	-3.439498
62	6	0	2.688178	1.814743	-2.996893

63	6	0	1.722727	2.704422	-2.570315
64	6	0	0.326462	2.304753	-2.567284
65	6	0	-0.078602	1.054662	-3.065267
66	6	0	-1.289057	0.538816	-2.523652
67	6	0	-1.575208	-0.885021	-2.537229
68	6	0	-0.622623	-1.776883	-2.996399
69	6	0	0.671896	-1.279189	-3.436919
70	6	0	0.942521	0.107710	-3.529678
71	6	0	-4.374638	0.426879	-1.290899
72	1	0	-4.387619	0.429866	-2.385410
73	6	0	-4.748865	1.764144	-0.699815
74	6	0	-5.019554	2.931108	-1.403155
75	1	0	-5.004892	2.930721	-2.490610
76	6	0	-5.306526	4.102007	-0.697197
77	1	0	-5.526740	5.017560	-1.238070
78	6	0	-5.306611	4.102017	0.697083
79	1	0	-5.526838	5.017589	1.237918
80	6	0	-5.019603	2.931155	1.403083
81	1	0	-5.004959	2.930802	2.490538
82	6	0	-4.748862	1.764175	0.699782
83	6	0	-4.374632	0.426938	1.290903
84	1	0	-4.387580	0.429952	2.385412
85	6	0	-5.263685	-0.639866	0.699552
86	6	0	-5.990300	-1.592336	1.402937
87	1	0	-5.976642	-1.598684	2.490353
88	6	0	-6.733693	-2.541295	0.697180
89	1	0	-7.309075	-3.286760	1.238140
90	6	0	-6.733642	-2.541363	-0.697090
91	1	0	-7.308988	-3.286873	-1.238026
92	6	0	-5.990208	-1.592463	-1.402877
93	1	0	-5.976495	-1.598897	-2.490292
94	6	0	-5.263655	-0.639922	-0.699521

$AC_{70}MA$ isomer *c*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.302069	0.486928	3.439516
2	6	0	0.942505	0.107683	3.529681
3	6	0	0.671887	-1.279216	3.436912
4	6	0	1.666218	-2.199079	3.003312
5	6	0	2.965520	-1.760595	2.640889
6	6	0	3.300763	-0.434662	3.001802
7	6	0	4.311148	0.316229	2.278551
8	6	0	3.944538	1.715702	2.288432
9	6	0	2.688166	1.814717	2.996917
10	6	0	1.722720	2.704404	2.570355
11	6	0	0.326456	2.304733	2.567301
12	6	0	-0.078610	1.054638	3.065289
13	6	0	-1.289059	0.538794	2.523648
14	6	0	-1.575224	-0.885048	2.537213
15	6	0	-0.622641	-1.776908	2.996390
16	6	0	-0.428015	-3.012746	2.297533
17	6	0	0.995334	-3.267646	2.283067
18	6	0	1.587042	-3.812432	1.161466
19	6	0	2.876318	-3.317889	0.712636
20	6	0	3.595671	-2.344972	1.449967
21	6	0	4.512973	-1.557232	0.713363
22	6	0	4.907220	-0.233907	1.161905
23	6	0	5.163500	0.588959	0.000009
24	6	0	4.810398	1.933044	0.000019
25	6	0	4.184898	2.511662	1.174004
26	6	0	3.169908	3.444599	0.725462
27	6	0	1.964661	3.535875	1.413415
28	6	0	0.714999	3.620756	0.689533
29	6	0	-0.294683	2.865999	1.408653
30	6	0	-1.354489	2.210349	0.740826
31	6	0	-1.924187	1.107332	1.406150
32	6	0	-2.899565	0.107909	0.791314
33	6	0	-2.407264	-1.191204	1.415967
34	6	0	-2.223495	-2.370920	0.740560
35	6	0	-1.206006	-3.297835	1.174520
36	6	0	-0.580317	-3.869761	-0.000021
37	6	0	0.786765	-4.130199	-0.000016
38	6	0	1.587051	-3.812431	-1.161505
39	6	0	2.876321	-3.317877	-0.712655
40	6	0	3.595681	-2.344973	-1.449980
41	6	0	4.512978	-1.557223	-0.713372
42	6	0	4.907216	-0.233898	-1.161892
43	6	0	4.311160	0.316244	-2.278541
44	6	0	3.944538	1.715722	-2.288394
45	6	0	4.184901	2.511680	-1.173975
46	6	0	3.169911	3.444614	-0.725416
47	6	0	1.964667	3.535876	-1.413371
48	6	0	0.714982	3.620768	-0.689496
49	6	0	-0.294678	2.866011	-1.408619
50	6	0	-1.354501	2.210363	-0.740810
51	6	0	-1.924203	1.107363	-1.406157
52	6	0	-2.899561	0.107910	-0.791342
53	6	0	-2.407237	-1.191187	-1.415981
54	6	0	-2.223489	-2.370919	-0.740605
55	6	0	-1.205999	-3.297825	-1.174560
56	6	0	-0.428004	-3.012734	-2.297572
57	6	0	0.995346	-3.267630	-2.283092
58	6	0	1.666235	-2.199057	-3.003338
59	6	0	2.965525	-1.760577	-2.640899
60	6	0	3.300776	-0.434637	-3.001788
61	6	0	2.302079	0.486955	-3.439498
62	6	0	2.688178	1.814743	-2.996893
63	6	0	1.722727	2.704422	-2.570315
64	6	0	0.326462	2.304753	-2.567284
65	6	0	-0.078602	1.054662	-3.065267
66	6	0	-1.289057	0.538816	-2.523652
67	6	0	-1.575208	-0.885021	-2.537229
68	6	0	-0.622623	-1.776883	-2.996399
69	6	0	0.671896	-1.279189	-3.436919
70	6	0	0.942521	0.107710	-3.529678
71	6	0	-4.374638	0.426879	-1.290899
72	1	0	-4.387619	0.429866	-2.385410
73	6	0	-4.748865	1.764144	-0.699815
74	6	0	-5.019554	2.931108	-1.403155
75	1	0	-5.004892	2.930721	-2.490610
76	6	0	-5.306526	4.102007	-0.697197
77	1	0	-5.526740	5.017560	-1.238070
78	6	0	-5.306611	4.102017	0.697083
79	1	0	-5.526838	5.017589	1.237918
80	6	0	-5.019603	2.931155	1.403083
81	1	0	-5.004959	2.930802	2.490538
82	6	0	-4.748862	1.764175	0.699782
83	6	0	-4.374632	0.426938	1.290903
84	1	0	-4.387580	0.429952	2.385412
85	6	0	-5.263685	-0.639866	0.699552
86	6	0	-5.990300	-1.592336	1.402937
87	1	0	-5.976642	-1.598684	2.490353
88	6	0	-6.733693	-2.541295	0.697180
89	1	0	-7.309075	-3.286760	1.238140
90	6	0	-6.733642	-2.541363	-0.697090
91	1	0	-7.308988	-3.286873	-1.238026
92	6	0	-5.990208	-1.592463	-1.402877
93	1	0	-5.976495	-1.598897	-2.490292
94	6	0	-5.263655	-0.639922	-0.699521

$AC_{70}MA$ isomer *d*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.338292	2.559794	1.660906
2	6	0	2.018900	3.070936	1.687297
3	6	0	1.171860	2.559010	2.700050
4	6	0	1.537865	1.410561	3.462159
5	6	0	2.762557	0.734992	3.231494
6	6	0	3.705115	1.410515	2.421362
7	6	0	4.722504	0.689810	1.674819
8	6	0	5.001278	1.412649	0.454390
9	6	0	4.129827	2.565257	0.442690
10	6	0	3.565420	2.994505	-0.741258
11	6	0	2.182324	3.434704	-0.763041
12	6	0	1.415253	3.517859	0.423730
13	6	0	0.010494	3.406534	0.271315
14	6	0	-0.839369	2.964298	1.357854
15	6	0	-0.273356	2.561145	2.556362
16	6	0	-0.804086	1.416910	3.233025
17	6	0	0.320664	0.689604	3.783756
18	6	0	0.320650	-0.689961	3.783667
19	6	0	1.537898	-1.410858	3.462082
20	6	0	2.762547	-0.735233	3.231410
21	6	0	3.705134	-1.410678	2.421258
22	6	0	4.722502	-0.689896	1.674762
23	6	0	5.001265	-1.412613	0.454280
24	6	0	5.269675	-0.724174	-0.724996
25	6	0	5.269620	0.724262	-0.724929
26	6	0	4.674077	1.173209	-1.968252
27	6	0	3.843588	2.287877	-1.972527
28	6	0	2.616706	2.278407	-2.737897
29	6	0	1.601474	2.995565	-1.989468
30	6	0	0.235711	2.631741	-2.068054
31	6	0	-0.571324	2.970622	-0.954512
32	6	0	-1.794813	2.258546	-0.651901
33	6	0	-1.970925	2.263611	0.809251
34	6	0	-2.489810	1.166867	1.452389
35	6	0	-1.878928	0.722773	2.671139
36	6	0	-1.878891	-0.723092	2.671107
37	6	0	-0.804091	-1.417286	3.232982
38	6	0	-0.273316	-2.561451	2.556199
39	6	0	1.171903	-2.559241	2.699854
40	6	0	2.018953	-3.071096	1.687088
41	6	0	3.338323	-2.559898	1.660695
42	6	0	4.129878	-2.565271	0.442498
43	6	0	3.565464	-2.994421	-0.741476
44	6	0	3.843643	-2.287714	-1.972697

45	6	0	4.674117	-1.173054	-1.968343
46	6	0	4.308574	0.000121	-2.740328
47	6	0	3.131353	0.000114	-3.478046
48	6	0	2.269300	1.162749	-3.474969
49	6	0	0.890886	0.713599	-3.490757
50	6	0	-0.129215	1.449017	-2.841256
51	6	0	-1.272254	0.712775	-2.433616
52	6	0	-2.140465	1.159051	-1.377729
53	6	0	-2.971107	-0.000074	-0.845568
54	6	0	-3.175762	-0.000056	0.742804
55	6	0	-2.489899	-1.167145	1.452395
56	6	0	-1.970840	-2.263688	0.809096
57	6	0	-0.839279	-2.964437	1.357612
58	6	0	0.010550	-3.406620	0.271069
59	6	0	1.415315	-3.517907	0.423461
60	6	0	2.182385	-3.434662	-0.763290
61	6	0	1.601529	-2.995426	-1.989680
62	6	0	2.616745	-2.278266	-2.738106
63	6	0	2.269348	-1.162523	-3.475045
64	6	0	0.890899	-0.713433	-3.490859
65	6	0	-0.129145	-1.448871	-2.841315
66	6	0	-1.272202	-0.712629	-2.433672
67	6	0	-2.140266	-1.158985	-1.377767
68	6	0	-1.794868	-2.258654	-0.652064
69	6	0	-0.571320	-2.970641	-0.954731
70	6	0	0.235720	-2.631696	-2.068232
71	6	0	-4.405873	-0.000053	-1.526994
72	1	0	-4.285902	0.000122	-2.615160
73	6	0	-5.119912	1.229589	-1.020746
74	6	0	-5.537652	2.312808	-1.783449
75	1	0	-5.386956	2.315165	-2.860502
76	6	0	-6.148527	3.398033	-1.150315
77	1	0	-6.482609	4.247433	-1.738766
78	6	0	-6.324042	3.398934	0.232767
79	1	0	-6.795807	4.248307	0.717831
80	6	0	-5.890698	2.314893	0.999987
81	1	0	-6.014214	2.318423	2.080487
82	6	0	-5.296590	1.230084	0.367473
83	6	0	-4.732500	0.000030	1.036884
84	1	0	-4.891450	-0.000064	2.119957
85	6	0	-5.296922	-1.229819	0.367374
86	6	0	-5.891558	-2.314377	0.999860
87	1	0	-6.015239	-2.317804	2.080344
88	6	0	-6.324865	-3.398464	0.232723
89	1	0	-6.796903	-4.247666	0.717821
90	6	0	-6.149090	-3.397801	-1.150339
91	1	0	-6.483291	-4.247222	-1.738692
92	6	0	-5.537828	-2.312825	-1.783470
93	1	0	-5.386931	-2.315268	-2.860493
94	6	0	-5.119945	-1.229610	-1.020822

ICMA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.194329	-1.418024	1.131578
2	1	0	4.303092	-1.763086	2.162095
3	6	0	5.102585	-0.290164	0.700824
4	6	0	5.798218	0.673012	1.414833
5	1	0	5.786340	0.685682	2.501864
6	6	0	6.525270	1.630075	0.697353
7	1	0	7.093735	2.384852	1.232949
8	6	0	6.525434	1.629740	-0.697852
9	1	0	7.094019	2.384271	-1.233663
10	6	0	5.798495	0.672350	-1.415015
11	1	0	5.786779	0.684481	-2.502056
12	6	0	5.102657	-0.290414	-0.700661
13	6	0	4.194320	-1.418350	-1.131124
14	1	0	4.303166	-1.763779	-2.161502
15	6	0	4.440727	-2.436254	0.000393
16	1	0	5.464576	-2.819420	0.000381
17	1	0	3.731930	-3.271332	0.000516
18	6	0	-0.351861	-3.233664	1.176208
19	6	0	0.971423	-2.853007	0.741621
20	6	0	1.681636	-1.903050	1.431801
21	6	0	1.081937	-1.275503	2.577748
22	6	0	-0.181954	-1.647842	3.027543
23	6	0	-0.919261	-2.654689	2.308508
24	6	0	-1.168546	-3.470324	0.000349
25	6	0	-0.351840	-3.233936	-1.175544
26	6	0	0.971440	-2.853170	-0.741002
27	6	0	1.681662	-1.903383	-1.431389
28	6	0	2.715506	-0.971787	0.803275
29	6	0	1.470139	0.122323	2.578937
30	6	0	0.578304	1.092248	3.029096
31	6	0	-0.747455	0.703576	3.480654
32	6	0	-1.118370	-0.632605	3.480753
33	6	0	-2.442516	-1.020038	3.031474
34	6	0	-2.318327	-2.271502	2.304452
35	6	0	-3.096862	-2.497527	1.176683
36	6	0	-2.510041	-3.116291	0.000297
37	6	0	-0.919194	-2.655174	-2.307978
38	6	0	-2.318258	-2.271979	-2.304032
39	6	0	-3.096822	-2.497776	-1.176236
40	6	0	-4.034559	-1.488835	-0.727037
41	6	0	-4.034584	-1.488687	0.727248
42	6	0	-4.152737	-0.291034	1.420985
43	6	0	-3.338936	-0.051159	2.598239
44	6	0	-2.950161	1.348326	2.597861
45	6	0	-1.682687	1.717473	3.031088
46	6	0	2.308319	0.352138	1.435303
47	6	0	-0.660977	3.548335	-0.000363
48	6	0	0.670522	3.158682	-0.000301
49	6	0	1.250119	2.536374	-1.176109
50	6	0	0.465598	2.333348	-2.309085
51	6	0	-0.931362	2.725039	-2.304326
52	6	0	-2.805935	2.936698	-0.727456
53	6	0	-2.805955	2.936848	0.726792
54	6	0	-1.483071	3.319441	1.175848
55	6	0	-0.931423	2.725522	2.303763
56	6	0	0.465534	2.333836	2.308643
57	6	0	1.250087	2.536629	1.175651
58	6	0	2.190466	1.530332	-0.741481
59	6	0	2.308370	0.351832	-1.435293
60	6	0	1.470223	0.121783	-2.578900
61	6	0	0.578381	1.091620	-3.029262
62	6	0	-0.747362	0.702858	-3.480802
63	6	0	-1.682605	1.716842	-3.031467
64	6	0	-2.950097	1.347792	-2.598201
65	6	0	-3.524966	1.972131	-1.422000
66	6	0	-3.525003	1.972423	1.421518
67	6	0	-4.269710	0.960093	0.693982
68	6	0	-4.269691	0.959950	-0.694274
69	6	0	-4.152697	-0.291328	-1.421020
70	6	0	-3.338861	-0.051690	-2.598302
71	6	0	-2.442434	-1.020657	-3.031313
72	6	0	-1.118270	-0.633326	-3.480634
73	6	0	-0.181868	-1.648485	-3.027222
74	6	0	1.082000	-1.276037	-2.577452
75	6	0	2.190454	1.530485	0.741246
76	6	0	2.715536	-0.971935	-0.802955
77	6	0	-1.483041	3.319199	-1.176558

AICBA *trans*-1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.680698	0.887427	1.131000
2	1	0	-5.840507	1.211652	2.161654
3	6	0	-6.405875	-0.366476	0.700881
4	6	0	-6.937223	-1.429328	1.414911
5	1	0	-6.921806	-1.440718	2.501945
6	6	0	-7.499669	-2.491472	0.697766
7	1	0	-7.940204	-3.327753	1.233038
8	6	0	-7.499659	-2.491557	-0.697456
9	1	0	-7.940196	-3.327894	-1.232634
10	6	0	-6.937160	-1.429503	-1.414695
11	1	0	-6.921705	-1.440986	-2.501731
12	6	0	-6.405802	-0.366606	-0.700742
13	6	0	-5.680645	0.887252	-1.131077
14	1	0	-5.840633	1.211288	-2.161761
15	6	0	-6.078811	1.855493	-0.000108
16	1	0	-7.148776	2.079987	-0.000193
17	1	0	-5.502991	2.787198	-0.000132
18	6	0	-1.454740	3.363047	1.177086
19	6	0	-2.705986	2.791218	0.741272
20	6	0	-3.269991	1.747378	1.432654
21	6	0	-2.587188	1.217872	2.580551
22	6	0	-1.393587	1.775967	3.034075
23	6	0	-0.811059	2.879183	2.312987
24	6	0	-0.680042	3.710985	-0.000247
25	6	0	-1.454726	3.362908	-1.177547
26	6	0	-2.705958	2.791095	-0.741666
27	6	0	-3.270047	1.747275	-1.432968
28	6	0	-4.150961	0.670264	0.803198
29	6	0	-2.758599	-0.223008	2.581553
30	6	0	-1.731054	-1.047767	3.035703
31	6	0	-0.480455	-0.463168	3.486716
32	6	0	-0.316339	0.913287	3.486604
33	6	0	0.933688	1.497985	3.032879
34	6	0	0.629006	2.707324	2.312812
35	6	0	1.368963	3.025620	1.176537
36	6	0	0.698054	3.547240	-0.000229
37	6	0	-0.811049	2.878871	-2.313380
38	6	0	0.629017	2.707016	-2.313162
39	6	0	1.368964	3.025466	-1.176924
40	6	0	2.450151	2.176666	-0.741278
41	6	0	2.450124	2.176736	0.741005
42	6	0	2.745711	1.026895	1.428767
43	6	0	1.959649	0.672796	2.575699
44	6	0	1.788276	-0.768164	2.575898
45	6	0	0.596030	-1.326723	3.033429

46	6	0	-3.549275	-0.576490	1.437622
47	6	0	-0.119299	-3.261049	0.000218
48	6	0	-1.496940	-3.094430	0.000206
49	6	0	-2.167828	-2.572127	-1.176301
50	6	0	-1.427366	-2.256384	-2.313131
51	6	0	0.012779	-2.429881	-2.313262
52	6	0	1.907886	-2.345363	-0.740872
53	6	0	1.907897	-2.345308	0.741183
54	6	0	0.656324	-2.914371	1.177576
55	6	0	0.012778	-2.429584	2.313585
56	6	0	-1.427368	-2.256103	2.313426
57	6	0	-2.167836	-2.571985	1.176639
58	6	0	-3.249696	-1.722897	-0.741619
59	6	0	-3.549235	-0.576668	-1.437555
60	6	0	-2.758593	-0.223312	-2.581533
61	6	0	-1.731028	-1.048140	-3.035545
62	6	0	-0.480419	-0.463625	-3.486658
63	6	0	0.596057	-1.327138	-3.033271
64	6	0	1.788314	-0.768554	-2.575810
65	6	0	2.468102	-1.298697	-1.428333
66	6	0	2.467994	-1.298453	1.428462
67	6	0	3.358513	-0.225147	0.800511
68	6	0	3.358532	-0.225196	-0.800474
69	6	0	2.745614	1.026683	-1.428868
70	6	0	1.959627	0.672418	-2.575779
71	6	0	0.933679	1.497576	-3.033052
72	6	0	-0.316349	0.912834	-3.486732
73	6	0	-1.393599	1.775587	-3.034362
74	6	0	-2.587199	1.217572	-2.580743
75	6	0	-3.249701	-1.722788	0.741839
76	6	0	-4.150979	0.670106	-0.803275
77	6	0	0.656326	-2.914506	-1.177184
78	6	0	4.857025	-0.402304	1.292031
79	1	0	4.875729	-0.404216	2.386668
80	6	0	5.642010	0.742979	0.699750
81	6	0	6.274232	1.760679	1.402949
82	1	0	6.259387	1.765644	2.490370
83	6	0	6.922828	2.777109	0.697181
84	1	0	7.425056	3.574010	1.237674
85	6	0	6.922831	2.777157	-0.696925
86	1	0	7.425067	3.574096	-1.237356
87	6	0	6.274214	1.760789	-1.402764
88	1	0	6.259361	1.765820	-2.490183
89	6	0	5.641991	0.743041	-0.699631
90	6	0	4.857030	-0.402210	-1.291959
91	1	0	4.875704	-0.404178	-2.386600
92	6	0	5.354425	-1.698225	-0.699679
93	6	0	5.737672	-2.833496	-1.402627
94	1	0	5.723475	-2.834770	-2.490095
95	6	0	6.136578	-3.971409	-0.697081
96	1	0	6.442586	-4.861611	-1.238713
97	6	0	6.136532	-3.971469	0.696975
98	1	0	6.442491	-4.861722	1.238552
99	6	0	5.737620	-2.833597	1.402583
100	1	0	5.723352	-2.834933	2.490050
101	6	0	5.354422	-1.698271	0.699695

AICBA *trans*-2 *a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.747329	0.037750	-0.575875
2	1	0	-6.185779	-0.701316	-1.249888
3	6	0	-5.954768	1.489207	-0.943666
4	6	0	-6.253710	2.115370	-2.143796
5	1	0	-6.437790	1.540907	-3.048316
6	6	0	-6.317206	3.513586	-2.161697
7	1	0	-6.566757	4.028198	-3.085100
8	6	0	-6.058486	4.256023	-1.008993
9	1	0	-6.109252	5.340383	-1.047538
10	6	0	-5.730637	3.620960	0.194313
11	1	0	-5.510277	4.201596	1.086652
12	6	0	-5.697106	2.235313	0.214631
13	6	0	-5.333340	1.242743	1.293317
14	1	0	-5.394861	1.600501	2.323423
15	6	0	-6.213708	0.042439	0.892736
16	1	0	-7.281198	0.257575	0.990750
17	1	0	-5.969287	-0.878503	1.432890
18	6	0	-2.586233	-3.403149	0.899620
19	6	0	-3.497239	-2.282399	0.897761
20	6	0	-3.816933	-1.648405	-0.277313
21	6	0	-3.214842	-2.097862	-1.503068
22	6	0	-2.349900	-3.190195	-1.525226
23	6	0	-2.027558	-3.863160	-0.290799
24	6	0	-1.771168	-3.328459	2.096420
25	6	0	-2.171642	-2.152676	2.846517
26	6	0	-3.233538	-1.494228	2.124848
27	6	0	-3.300495	-0.122470	2.090200
28	6	0	-4.192654	-0.172620	-0.387777
29	6	0	-2.931970	-0.934535	-2.320667
30	6	0	-1.796788	-0.909057	-3.129506
31	6	0	-0.886071	-2.042941	-3.135852
32	6	0	-1.158509	-3.154681	-2.350593
33	6	0	-0.090209	-3.803108	-1.611084
34	6	0	-0.632002	-4.246281	-0.337089
35	6	0	0.148637	-4.175255	0.810368
36	6	0	-0.437130	-3.711811	2.057327
37	6	0	-1.211641	-1.408411	3.530703
38	6	0	0.182606	-1.798457	3.475611
39	6	0	0.562193	-2.923227	2.755818
40	6	0	1.753835	-2.893801	1.930417
41	6	0	1.501251	-3.664534	0.738060
42	6	0	2.016619	-3.223136	-0.479057
43	6	0	1.201280	-3.296648	-1.675689
44	6	0	1.489685	-2.132877	-2.493995
45	6	0	0.464330	-1.524965	-3.217803
46	6	0	-3.358793	0.230182	-1.596684
47	6	0	0.928636	1.834633	-1.810378
48	6	0	-0.413322	2.202153	-1.767142
49	6	0	-0.982490	2.664080	-0.529001
50	6	0	-0.169670	2.737940	0.603739
51	6	0	1.225529	2.368763	0.534492
52	6	0	2.939007	0.961605	-0.758163
53	6	0	2.413412	0.034358	-1.855591
54	6	0	1.336370	0.663302	-2.564100
55	6	0	0.385960	-0.086885	-3.252669
56	6	0	-1.015203	0.295761	-3.203868
57	6	0	-1.408526	1.409741	-2.467677
58	6	0	-2.335980	2.167213	-0.434610
59	6	0	-2.835943	1.759641	0.775776
60	6	0	-1.993799	1.806689	1.938342
61	6	0	-0.693095	2.298279	1.869912
62	6	0	0.371235	1.645232	2.610543
63	6	0	1.566110	1.679243	1.802292
64	6	0	2.424344	0.609497	1.795060
65	6	0	3.307099	0.216338	0.610430
66	6	0	2.481366	-1.336154	-1.815405
67	6	0	2.815596	-2.022451	-0.546398
68	6	0	3.061926	-1.291797	0.587145
69	6	0	2.505256	-1.723643	1.838325
70	6	0	2.112537	-0.547039	2.588303
71	6	0	0.979590	-0.583848	3.400030
72	6	0	0.085466	0.542342	3.409830
73	6	0	-1.272234	0.030690	3.484488
74	6	0	-2.288773	0.646127	2.758612
75	6	0	-2.604749	1.376232	-1.660764
76	6	0	-3.899500	0.683295	0.939733
77	6	0	1.765815	1.934436	-0.646725
78	6	0	4.829490	0.516765	0.940155
79	1	0	5.098550	0.010497	1.872866
80	6	0	4.961167	2.017322	1.034097
81	6	0	5.305800	2.746709	2.165114
82	1	0	5.540884	2.235031	3.095553
83	6	0	5.342077	4.141377	2.092762
84	1	0	5.616353	4.719830	2.969986
85	6	0	5.021826	4.793491	0.902952
86	1	0	5.047901	5.878223	0.856638
87	6	0	4.660527	4.059150	-0.229387
88	1	0	4.396292	4.565706	-1.154771
89	6	0	4.638401	2.672060	-0.159973
90	6	0	4.234985	1.725694	-1.264835
91	1	0	4.001132	2.245329	-2.199706
92	6	0	5.311871	0.681935	-1.433747
93	6	0	5.928010	0.317454	-2.624155
94	1	0	5.666053	0.820332	-3.552200
95	6	0	6.882161	-0.702815	-2.614187
96	1	0	7.373753	-0.990960	-3.538764
97	6	0	7.200980	-1.357052	-1.425079
98	1	0	7.939440	-2.153556	-1.427044
99	6	0	6.570415	-0.998738	-0.231108
100	1	0	6.807369	-1.516521	0.695445
101	6	0	5.632737	0.026109	-0.239759

AICBA *trans*-2 *b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.283707	-0.474739	-1.758655
2	1	0	-5.300297	0.018620	-2.750694
3	6	0	-6.547567	-0.491625	-0.810619
4	6	0	-7.701566	0.218196	-0.549483
5	1	0	-7.927244	0.969356	-1.049972
6	6	0	-8.517549	-0.223028	0.482953
7	1	0	-9.310746	0.225558	0.663891
8	6	0	-8.270478	-1.424946	1.190924
9	1	0	-8.914206	-1.703474	1.800158
10	6	0	-7.193584	-2.252965	0.906117
11	1	0	-7.095987	-3.074425	1.331955
12	6	0	-6.274333	-1.820815	-0.027680

13	6	0	-4.917101	-2.258152	-0.708162
14	1	0	-4.613744	-3.321229	-0.783406
15	6	0	-5.010112	-1.878655	-2.134493
16	1	0	-5.734390	-2.250962	-2.513795
17	1	0	-4.183705	-1.931653	-2.512872
18	6	0	-0.718417	-0.717745	-3.218004
19	6	0	-2.042527	-0.962715	-2.643814
20	6	0	-2.861926	0.103508	-2.313520
21	6	0	-2.404089	1.475651	-2.538498
22	6	0	-1.151639	1.707332	-3.081637
23	6	0	-0.285360	0.580121	-3.430847
24	6	0	0.202717	-1.716671	-2.673336
25	6	0	-0.552074	-2.578976	-1.762490
26	6	0	-1.939749	-2.113003	-1.744227
27	6	0	-2.661899	-2.134840	-0.562996
28	6	0	-3.787984	-0.015290	-1.094034
29	6	0	-2.884605	2.300563	-1.428721
30	6	0	-2.086676	3.312538	-0.922186
31	6	0	-0.762580	3.557484	-1.496427
32	6	0	-0.308073	2.777196	-2.546133
33	6	0	1.079560	2.311202	-2.564406
34	6	0	1.093594	0.953344	-3.111194
35	6	0	1.964884	0.008489	-2.596006
36	6	0	1.507049	-1.363658	-2.370984
37	6	0	0.038301	-3.041594	-0.598557
38	6	0	1.417225	-2.668388	-0.278888
39	6	0	2.131181	-1.852737	-1.140456
40	6	0	2.974757	-0.782871	-0.604946
41	6	0	2.871969	0.367424	-1.504536
42	6	0	2.858692	1.651805	-0.987322
43	6	0	1.937569	2.650723	-1.532003
44	6	0	1.457043	3.475673	-0.422236
45	6	0	0.144514	3.916451	-0.404938
46	6	0	-3.639403	1.438284	-0.517870
47	6	0	-0.783449	2.568384	2.918666
48	6	0	-2.087778	2.215382	2.616327
49	6	0	-2.545603	0.843247	2.841314
50	6	0	-1.674310	-0.101603	3.356523
51	6	0	-0.295382	0.271615	3.676196
52	6	0	1.461786	1.814429	2.889116
53	6	0	1.358999	2.964730	1.989534
54	6	0	-0.028621	3.430720	2.007800
55	6	0	-0.618982	3.893334	0.843860
56	6	0	-1.997948	3.520095	0.524166
57	6	0	-2.711916	2.704463	1.385744
58	6	0	-3.452662	0.484304	1.749829
59	6	0	-3.439399	-0.800051	1.232607
60	6	0	-2.518252	-1.798990	1.777265
61	6	0	-1.660261	-1.459466	2.809694
62	6	0	-0.272661	-1.925455	2.791444
63	6	0	0.570899	-0.855599	3.326945
64	6	0	1.823335	-0.623903	2.783776
65	6	0	2.281172	0.748233	2.558782
66	6	0	2.081178	2.986580	0.808298
67	6	0	2.947439	1.859370	0.459064
68	6	0	3.044664	0.771330	1.309961
69	6	0	3.058702	-0.586539	0.763158
70	6	0	2.303879	-1.448841	1.674037
71	6	0	1.505974	-2.460814	1.167519
72	6	0	0.181869	-2.705758	1.741741
73	6	0	-0.725201	-3.064686	0.650287
74	6	0	-2.037733	-2.623911	0.667561
75	6	0	-3.555450	1.634629	0.850243
76	6	0	-3.613231	-1.138612	-0.311723
77	6	0	0.137665	1.569494	3.463344
78	6	0	4.412186	-0.981198	-1.391183
79	1	0	4.345751	-1.133377	-2.484752
80	6	0	5.072722	-2.139566	-0.679843
81	6	0	5.497204	-3.342048	-1.262692
82	1	0	5.406629	-3.490885	-2.349299
83	6	0	6.047479	-4.346268	-0.446409
84	1	0	6.402912	-5.284500	-0.897540
85	6	0	6.160139	-4.148851	0.940742
86	1	0	6.602470	-4.934579	1.571019
87	6	0	5.718169	-2.948246	1.528843
88	1	0	5.798462	-2.795020	2.615785
89	6	0	5.179080	-1.944459	0.714613
90	6	0	4.604620	-0.623821	1.173948
91	1	0	4.702070	-0.472278	2.265153
92	6	0	5.204383	0.508160	0.371584
93	6	0	5.755612	1.690167	0.881073
94	1	0	5.831421	1.840990	1.968622
95	6	0	6.214679	2.676875	-0.012375
96	1	0	6.666364	3.600216	0.379548
97	6	0	6.107913	2.485432	-1.400618
98	1	0	6.478440	3.257488	-2.091012
99	6	0	5.542936	1.303209	-1.911683
100	1	0	5.455281	1.148611	-2.997768
101	6	0	5.099855	0.313851	-1.022936

AICBA *trans*-3 *a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.446324	-1.112061	-0.654702
2	1	0	-6.226730	-0.367516	-0.483394
3	6	0	-5.535377	-2.379240	0.162945
4	6	0	-6.168924	-2.674639	1.359820
5	1	0	-6.778488	-1.933797	1.871186
6	6	0	-6.007104	-3.958619	1.893345
7	1	0	-6.509173	-4.221979	2.819772
8	6	0	-5.205484	-4.903027	1.251557
9	1	0	-5.090521	-5.891784	1.686141
10	6	0	-4.544598	-4.591217	0.057663
11	1	0	-3.906027	-5.323543	-0.430118
12	6	0	-4.731500	-3.328425	-0.483359
13	6	0	-4.151057	-2.644207	-1.699934
14	1	0	-3.753243	-3.297107	-2.479888
15	6	0	-5.305448	-1.694193	-2.075067
16	1	0	-6.201345	-2.232651	-2.395495
17	1	0	-5.030476	-0.948121	-2.828317
18	6	0	-2.608538	2.511182	-2.318105
19	6	0	-3.236952	1.218936	-2.158875
20	6	0	-3.870096	0.896085	-0.984626
21	6	0	-3.874876	1.846279	0.093743
22	6	0	-3.299075	3.106688	-0.050123
23	6	0	-2.651044	3.450211	-1.288880
24	6	0	-1.394379	2.336988	-3.086313
25	6	0	-1.257355	0.926312	-3.403078
26	6	0	-2.389061	0.220422	-2.847078
27	6	0	-2.232064	-1.037186	-2.320012
28	6	0	-3.998256	-0.521974	-0.435387
29	6	0	-3.723692	1.115808	1.337338
30	6	0	-2.995229	1.671718	2.387301
31	6	0	-2.377873	2.980526	2.228748
32	6	0	-2.529978	3.682609	1.041180
33	6	0	-1.399957	4.384307	0.464319
34	6	0	-1.475118	4.239077	-0.979207
35	6	0	-0.311007	4.070325	-1.719548
36	6	0	-0.270777	3.101911	-2.803479
37	6	0	0.005422	0.340974	-3.412991
38	6	0	1.179537	1.131456	-3.102436
39	6	0	1.044685	2.488996	-2.813127
40	6	0	1.804742	3.056911	-1.734733
41	6	0	0.974056	4.040048	-1.053860
42	6	0	1.047051	4.177256	0.324958
43	6	0	-0.164648	4.353460	1.101840
44	6	0	-0.006827	3.618075	2.344707
45	6	0	-1.092538	2.946314	2.894050
46	6	0	-3.633615	-0.281950	1.024566
47	6	0	0.458903	-0.394534	3.098431
48	6	0	-0.679946	-1.139226	2.802313
49	6	0	-0.642373	-2.087406	1.720370
50	6	0	0.539423	-2.242869	0.993734
51	6	0	1.717390	-1.489130	1.316736
52	6	0	2.306224	0.747210	2.185208
53	6	0	1.467055	1.713156	2.856780
54	6	0	0.333300	1.014926	3.426152
55	6	0	-0.917857	1.615408	3.453280
56	6	0	-2.103714	0.837505	3.144318
57	6	0	-1.986168	-0.512380	2.813921
58	6	0	-1.923764	-2.075460	1.048527
59	6	0	-1.989225	-2.218689	-0.312827
60	6	0	-0.773251	-2.352932	-1.068883
61	6	0	0.472015	-2.377540	-0.438484
62	6	0	1.610921	-1.714411	-1.012903
63	6	0	2.615255	-1.362680	0.085078
64	6	0	3.295309	0.075341	-0.087430
65	6	0	2.933279	1.075497	1.010734
66	6	0	1.302152	2.995220	2.333336
67	6	0	1.949253	3.335274	1.093864
68	6	0	2.729825	2.380353	0.446001
69	6	0	2.659014	2.239731	-0.996216
70	6	0	2.822392	0.850648	-1.317480
71	6	0	2.092800	0.308034	-2.345174
72	6	0	1.465093	-1.022676	-2.185277
73	6	0	0.180160	-0.971732	-2.847525
74	6	0	-0.924050	-1.631551	-2.305733
75	6	0	-2.770491	-1.076641	1.739937
76	6	0	-3.078707	-1.606913	-1.182415
77	6	0	1.674629	-0.580682	2.342554
78	6	0	3.769666	-2.450750	0.140928
79	1	0	3.320243	-3.441745	0.261270
80	6	0	4.661303	-2.072262	1.299547
81	6	0	4.875563	-2.812881	2.455028
82	1	0	4.401897	-3.783974	2.579135
83	6	0	5.702493	-2.294831	3.454848
84	1	0	5.881329	-2.869250	4.359072
85	6	0	6.294375	-1.041767	3.300738
86	1	0	6.932163	-0.644348	4.084789
87	6	0	6.066945	-0.292024	2.144622
88	1	0	6.515764	0.691540	2.026807
89	6	0	5.256511	-0.814628	1.145054
90	6	0	4.867759	-0.128797	-0.141693

91	1	0	5.349830	0.846698	-0.262166
92	6	0	5.143475	-1.059211	-1.297628
93	6	0	5.854612	-0.752924	-2.450748
94	1	0	6.301816	0.230823	-2.573190
95	6	0	5.985263	-1.720606	-3.449856
96	1	0	6.545666	-1.492021	-4.351535
97	6	0	5.395165	-2.974546	-3.297024
98	1	0	5.498821	-3.720280	-4.079647
99	6	0	4.667194	-3.276025	-2.143277
100	1	0	4.194548	-4.248567	-2.026654
101	6	0	4.550428	-2.317800	-1.144253

AICBA *trans*-3 *b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.179444	-0.773473	-1.906577
2	1	0	-5.770374	0.068267	-2.274453
3	6	0	-5.848714	-1.673386	-0.892723
4	6	0	-6.908736	-1.476057	-0.021055
5	1	0	-7.465386	-0.542242	-0.014099
6	6	0	-7.248654	-2.515625	0.852388
7	1	0	-8.085979	-2.392746	1.533312
8	6	0	-6.522593	-3.707255	0.863713
9	1	0	-6.803014	-4.499180	1.552279
10	6	0	-5.435385	-3.891632	0.002308
11	1	0	-4.857653	-4.812308	0.025996
12	6	0	-5.119163	-2.870266	-0.879550
13	6	0	-4.000143	-2.703836	-1.880414
14	1	0	-3.515733	-3.620423	-2.224209
15	6	0	-4.683654	-1.810366	-2.933498
16	1	0	-5.505909	-2.320210	-3.442712
17	1	0	-3.989396	-1.395566	-3.672088
18	6	0	-1.133851	1.711062	-3.131874
19	6	0	-2.076456	0.636557	-2.919593
20	6	0	-3.149321	0.810456	-2.080047
21	6	0	-3.309817	2.066109	-1.400352
22	6	0	-2.426077	3.122233	-1.613329
23	6	0	-1.310226	2.941155	-2.500099
24	6	0	0.193197	1.139379	-3.237342
25	6	0	0.085589	-0.287534	-3.086229
26	6	0	-1.307512	-0.629203	-2.893398
27	6	0	-1.660846	-1.634216	-2.031910
28	6	0	-3.807167	-0.310338	-1.277436
29	6	0	-3.804172	1.794586	-0.064255
30	6	0	-3.405077	2.591927	1.005901
31	6	0	-2.473711	3.685972	0.785253
32	6	0	-1.993781	3.943655	-0.491455
33	6	0	-0.596404	4.264567	-0.691303
34	6	0	-0.169665	3.635954	-1.931299
35	6	0	1.098270	3.077228	-2.020810
36	6	0	1.289103	1.803452	-2.692059
37	6	0	1.085999	-0.976052	-2.397747
38	6	0	2.226644	-0.291252	-1.858070
39	6	0	2.319408	1.069841	-1.996023
40	6	0	2.764404	1.904179	-0.858711
41	6	0	2.002243	3.131645	-0.891346
42	6	0	1.597470	3.746951	0.292722
43	6	0	0.268584	4.316175	0.395630
44	6	0	-0.233172	4.046781	1.732514
45	6	0	-1.575872	3.738529	1.922110
46	6	0	-3.945711	0.372850	0.075750
47	6	0	-1.076330	0.525201	3.661309
48	6	0	-2.152459	-0.146420	3.096873
49	6	0	-1.948913	-1.415029	2.419162
50	6	0	-0.666934	-1.951976	2.331339
51	6	0	0.461249	-1.245523	2.904811
52	6	0	1.178835	1.047149	3.349143
53	6	0	0.425324	2.293184	3.324240
54	6	0	-0.971608	1.968817	3.521896
55	6	0	-1.953877	2.675372	2.837663
56	6	0	-3.085554	1.972457	2.265021
57	6	0	-3.177631	0.585805	2.384216
58	6	0	-2.854215	-1.484741	1.295608
59	6	0	-2.455973	-2.081364	0.124874
60	6	0	-1.125465	-2.609282	0.022130
61	6	0	-0.239856	-2.563703	1.100070
62	6	0	1.157203	-2.255812	0.890307
63	6	0	1.596928	-1.421918	2.030795
64	6	0	2.476293	-0.389289	1.824489
65	6	0	2.251142	0.867985	2.477701
66	6	0	0.787348	3.308164	2.449695
67	6	0	1.916465	3.126674	1.551429
68	6	0	2.624386	1.926932	1.559901
69	6	0	3.077954	1.318937	0.340711
70	6	0	3.286436	-0.181927	0.544464
71	6	0	2.811587	-1.084658	-0.688120
72	6	0	1.627888	-1.999970	-0.369936
73	6	0	0.715709	-2.023757	-1.481002
74	6	0	-0.634250	-2.331930	-1.302815
75	6	0	-3.623745	-0.220725	1.270783
76	6	0	-2.971877	-1.682397	-1.251837
77	6	0	0.258972	-0.034873	3.566551
78	6	0	4.819215	-0.487294	0.815589
79	1	0	5.160860	0.121855	1.658712
80	6	0	5.553189	-0.171042	-0.464722
81	6	0	6.508682	0.821442	-0.642805
82	1	0	6.814976	1.442167	0.195984
83	6	0	7.066095	1.012762	-1.909448
84	1	0	7.818956	1.781305	-2.057070
85	6	0	6.656382	0.225597	-2.984743
86	1	0	7.091839	0.382707	-3.967172
87	6	0	5.682881	-0.760939	-2.807485
88	1	0	5.351492	-1.366098	-3.648173
89	6	0	5.139394	-0.959335	-1.544447
90	6	0	4.054123	-1.943248	-1.177404
91	1	0	3.746985	-2.566443	-2.023461
92	6	0	4.510576	-2.756596	0.009353
93	6	0	4.498390	-4.141703	0.114619
94	1	0	4.167858	-4.751370	-0.723164
95	6	0	4.911685	-4.739460	1.307660
96	1	0	4.911100	-5.821773	1.397473
97	6	0	5.318015	-3.953556	2.385125
98	1	0	5.632230	-4.425806	3.311343
99	6	0	5.318294	-2.560464	2.281980
100	1	0	5.621390	-1.944454	3.125369
101	6	0	4.921753	-1.967916	1.089830

AICBA *trans*-4 *a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.008165	2.510058	-1.926050
2	1	0	-3.879308	2.655190	-3.000911
3	6	0	-3.903697	3.747418	-1.064093
4	6	0	-3.302186	4.979862	-1.267925
5	1	0	-2.820823	5.220798	-2.212540
6	6	0	-3.332431	5.910851	-0.223290
7	1	0	-2.884485	6.890425	-0.363645
8	6	0	-3.928451	5.595824	0.998171
9	1	0	-3.938800	6.333432	1.795625
10	6	0	-4.509188	4.340052	1.210033
11	1	0	-4.955683	4.090359	2.169437
12	6	0	-4.499752	3.430147	0.164329
13	6	0	-4.964071	1.996465	0.058765
14	1	0	-5.704027	1.669100	0.792388
15	6	0	-5.345626	1.924235	-1.432461
16	1	0	-6.198112	2.563616	-1.676984
17	1	0	-5.532430	0.904847	-1.786929
18	6	0	-2.690777	-2.170351	-2.541314
19	6	0	-3.359477	-0.981752	-2.066244
20	6	0	-2.801301	0.256014	-2.268584
21	6	0	-1.531326	0.348443	-2.935889
22	6	0	-0.886068	-0.780810	-3.425985
23	6	0	-1.479253	-2.076017	-3.224677
24	6	0	-2.886455	-3.224897	-1.566667
25	6	0	-3.682203	-2.697219	-0.475485
26	6	0	-3.984682	-1.313014	-0.762872
27	6	0	-4.006196	-0.386220	0.247153
28	6	0	-2.992628	1.454048	-1.339181
29	6	0	-0.767914	1.401818	-2.288491
30	6	0	0.616130	1.268615	-2.141189
31	6	0	1.286776	0.079295	-2.638721
32	6	0	0.557722	-0.918319	-3.275783
33	6	0	0.846350	-2.296515	-2.983110
34	6	0	-0.411846	-3.018803	-2.945459
35	6	0	-0.604928	-4.026532	-2.007204
36	6	0	-1.871164	-4.138215	-1.310534
37	6	0	-3.433135	-3.112493	0.829547
38	6	0	-2.367207	-4.058122	1.101331
39	6	0	-1.601184	-4.558026	0.055331
40	6	0	-0.168361	-4.693697	0.204802
41	6	0	0.448874	-4.358441	-1.068698
42	6	0	1.647166	-3.655682	-1.094602
43	6	0	1.854187	-2.601653	-2.068602
44	6	0	2.620547	-1.550494	-1.443061
45	6	0	2.349589	-0.236504	-1.726388
46	6	0	-1.557865	1.955986	-1.244769
47	6	0	1.778996	0.877339	1.744960
48	6	0	0.760344	1.753958	1.475519
49	6	0	-0.508020	1.634470	2.155617
50	6	0	-0.700467	0.639205	3.115205
51	6	0	0.361108	-0.294953	3.388653
52	6	0	2.236829	-1.366575	2.208714
53	6	0	2.873892	-1.038252	0.961869
54	6	0	2.867743	0.475785	0.749227
55	6	0	2.574531	0.926027	-0.757867
56	6	0	1.258314	1.682402	-0.942363

57	6	0	0.484389	2.172611	0.085022
58	6	0	-1.566581	1.973674	1.233123
59	6	0	-2.766131	1.308276	1.279003
60	6	0	-2.942951	0.244460	2.230884
61	6	0	-1.948916	-0.078013	3.150569
62	6	0	-1.665655	-1.471666	3.451566
63	6	0	-0.229673	-1.606760	3.600285
64	6	0	0.413105	-2.743041	3.128537
65	6	0	1.678869	-2.624354	2.426415
66	6	0	2.891621	-1.965544	-0.046244
67	6	0	2.285637	-3.262615	0.146967
68	6	0	1.702127	-3.599004	1.365672
69	6	0	0.446316	-4.324721	1.395223
70	6	0	-0.351025	-3.797424	2.488381
71	6	0	-1.727725	-3.667310	2.344831
72	6	0	-2.398178	-2.477845	2.836527
73	6	0	-3.448615	-2.139373	1.892472
74	6	0	-3.709909	-0.804864	1.592313
75	6	0	-0.939097	2.307848	-0.064456
76	6	0	-3.668450	1.091952	0.071483
77	6	0	1.562800	-0.180415	2.695163
78	6	0	3.788548	1.819101	-1.248941
79	1	0	3.603738	2.135770	-2.280545
80	6	0	5.031044	0.973348	-1.114187
81	6	0	5.852753	0.544169	-2.148639
82	1	0	5.641605	0.839067	-3.173977
83	6	0	6.948604	-0.271648	-1.856717
84	1	0	7.600211	-0.606907	-2.658273
85	6	0	7.205892	-0.661695	-0.543310
86	1	0	8.057454	-1.299234	-0.324462
87	6	0	6.370031	-0.241573	0.494165
88	1	0	6.560168	-0.555480	1.518015
89	6	0	5.288598	0.580948	0.204090
90	6	0	4.262601	1.094562	1.185286
91	1	0	4.479426	0.797252	2.216450
92	6	0	4.137453	2.590537	1.026784
93	6	0	4.205033	3.536909	2.041364
94	1	0	4.393984	3.227837	3.066882
95	6	0	4.025145	4.886510	1.728898
96	1	0	4.084137	5.634234	2.514426
97	6	0	3.765825	5.277226	0.415986
98	1	0	3.621669	6.328176	0.183017
99	6	0	3.684880	4.322985	-0.601081
100	1	0	3.468521	4.621972	-1.624108
101	6	0	3.879016	2.982909	-0.291412

AICBA *trans*-4 *b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.644677	-3.380478	-0.776271
2	1	0	-3.233520	-4.045944	-1.538401
3	6	0	-5.047584	-2.872740	-1.013733
4	6	0	-5.812722	-2.746933	-2.162682
5	1	0	-5.441596	-3.089294	-3.125456
6	6	0	-7.083431	-2.170646	-2.050805
7	1	0	-7.710958	-2.079344	-2.932690
8	6	0	-7.553355	-1.710170	-0.820365
9	1	0	-8.541761	-1.264278	-0.756462
10	6	0	-6.765917	-1.812786	0.332230
11	1	0	-7.127529	-1.436226	1.285830
12	6	0	-5.519845	-2.410348	0.222585
13	6	0	-4.405787	-2.634134	1.218911
14	1	0	-4.687175	-2.618285	2.274154
15	6	0	-3.772268	-3.923688	0.660590
16	1	0	-4.446679	-4.781854	0.724733
17	1	0	-2.809569	-4.171481	1.120800
18	6	0	0.954307	-2.286655	0.522491
19	6	0	-0.454736	-2.567239	0.584262
20	6	0	-1.244631	-2.471460	-0.540447
21	6	0	-0.644089	-2.034723	-1.754705
22	6	0	0.724938	-1.759089	-1.813494
23	6	0	1.545914	-1.911014	-0.661595
24	6	0	1.342791	-1.621027	1.783791
25	6	0	0.156509	-1.501020	2.598672
26	6	0	-0.959607	-2.079789	1.886385
27	6	0	-2.209987	-1.523784	1.981423
28	6	0	-2.730367	-2.118091	-0.529100
29	6	0	-1.585506	-1.175434	-2.453020
30	6	0	-1.125965	-0.091273	-3.191974
31	6	0	0.301649	0.194829	-3.254405
32	6	0	1.202712	-0.616638	-2.574142
33	6	0	2.323462	-0.060692	-1.869136
34	6	0	2.784752	-1.021316	-0.771476
35	6	0	3.199785	-0.301401	0.596937
36	6	0	2.285056	-0.625996	1.778364
37	6	0	-0.031258	-0.380865	3.407997
38	6	0	0.947274	0.675420	3.392690
39	6	0	2.066114	0.552714	2.573588
40	6	0	2.547316	1.695657	1.825536
41	6	0	3.065946	1.220757	0.571030
42	6	0	2.867754	1.964164	-0.561820
43	6	0	2.482276	1.300845	-1.829690
44	6	0	1.540398	2.162679	-2.502883
45	6	0	0.472314	1.622408	-3.218692
46	6	0	-2.771944	-1.085930	-1.649201
47	6	0	-2.216267	3.470423	-1.505970
48	6	0	-3.150618	2.442613	-1.482590
49	6	0	-3.751405	2.034879	-0.227333
50	6	0	-3.400540	2.683944	0.953934
51	6	0	-2.417355	3.750709	0.933198
52	6	0	-0.418577	4.418410	-0.333006
53	6	0	0.079326	3.931674	-1.609764
54	6	0	-1.034435	3.355865	-2.337943
55	6	0	-0.843794	2.227595	-3.126247
56	6	0	-1.828451	1.161153	-3.114599
57	6	0	-2.955847	1.260516	-2.299619
58	6	0	-3.934844	0.601528	-0.255648
59	6	0	-3.742984	-0.139525	0.882253
60	6	0	-3.336928	0.521761	2.093242
61	6	0	-3.187516	1.905423	2.147526
62	6	0	-2.076268	2.486466	2.880213
63	6	0	-1.598984	3.630880	2.126458
64	6	0	-0.236979	3.902878	2.065079
65	6	0	0.366845	4.307453	0.808261
66	6	0	1.335278	3.342028	-1.684233
67	6	0	2.152350	3.217804	-0.492474
68	6	0	1.681276	3.699841	0.725979
69	6	0	1.886615	2.918492	1.918777
70	6	0	0.705095	3.040853	2.754761
71	6	0	0.246700	1.946817	3.475737
72	6	0	-1.173508	1.663677	3.540100
73	6	0	-1.338097	0.219544	3.496184
74	6	0	-2.391813	-0.336941	2.776986
75	6	0	-3.434143	0.114310	-1.563545
76	6	0	-3.271586	-1.586824	0.886456
77	6	0	-1.835845	4.134172	-0.269164
78	6	0	4.027105	-1.868369	-1.276985
79	1	0	3.760671	-2.366991	-2.214540
80	6	0	4.361349	-2.844241	-0.174661
81	6	0	4.296406	-4.229705	-0.250656
82	1	0	4.006861	-4.714345	-1.180287
83	6	0	4.605131	-4.990670	0.879710
84	1	0	4.563715	-6.074720	0.827893
85	6	0	4.959944	-4.365516	2.074191
86	1	0	5.194614	-4.963731	2.949688
87	6	0	5.012807	-2.971770	2.152554
88	1	0	5.277755	-2.480260	3.085888
89	6	0	4.721018	-2.216874	1.023470
90	6	0	4.694797	-0.710350	0.934057
91	1	0	4.994503	-0.227499	1.869900
92	6	0	5.535388	-0.272645	-0.241058
93	6	0	6.538923	0.687611	-0.226190
94	1	0	6.807978	1.184456	0.703098
95	6	0	7.193537	1.009388	-1.417684
96	1	0	7.984250	1.754061	-1.414606
97	6	0	6.833155	0.384336	-2.610537
98	1	0	7.343758	0.644166	-3.533144
99	6	0	5.813568	-0.570347	-2.626576
100	1	0	5.519349	-1.049227	-3.557714
101	6	0	5.173468	-0.899911	-1.438604

AICBA *e*-face *a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.865136	4.704651	-1.130755
2	1	0	-1.143346	4.933967	-2.161724
3	6	0	0.521179	5.124429	-0.700863
4	6	0	1.676081	5.403448	-1.414941
5	1	0	1.682578	5.387011	-2.501968
6	6	0	2.837879	5.712990	-0.697706
7	1	0	3.750566	5.957056	-1.233782
8	6	0	2.837821	5.713185	0.697686
9	1	0	3.750469	5.957388	1.233766
10	6	0	1.675974	5.403797	1.414908
11	1	0	1.682390	5.387590	2.501941
12	6	0	0.521146	5.124532	0.700809
13	6	0	-0.865157	4.704670	1.130695
14	1	0	-1.143415	4.934025	2.161642
15	6	0	-1.716719	5.314187	-0.000048
16	1	0	-1.691361	6.407278	-0.000037
17	1	0	-2.755387	4.966821	-0.000050
18	6	0	1.448065	-2.333277	-1.170817
19	6	0	0.591160	-3.393039	-0.726116
20	6	0	-0.567848	-3.728748	-1.423901
21	6	0	-0.930164	-2.972653	-2.592750
22	6	0	-0.111703	-1.921790	-3.003460
23	6	0	1.099307	-1.608363	-2.282325
24	6	0	2.262215	-1.782922	-0.000009

25	6	0	1.448062	-2.333251	1.170810
26	6	0	0.591158	-3.393021	0.726125
27	6	0	-0.567847	-3.728709	1.423926
28	6	0	-1.782418	-4.052465	-0.693585
29	6	0	-2.372289	-2.814204	-2.596769
30	6	0	-2.937374	-1.618710	-3.025807
31	6	0	-2.084982	-0.529829	-3.468396
32	6	0	-0.707180	-0.677786	-3.450666
33	6	0	0.141232	0.412834	-3.001323
34	6	0	1.251838	-0.137317	-2.284846
35	6	0	1.731138	0.510910	-1.169615
36	6	0	2.419045	-0.189893	-0.000017
37	6	0	1.099316	-1.608336	2.282322
38	6	0	1.251848	-0.137289	2.284828
39	6	0	1.731130	0.510916	1.169574
40	6	0	1.124708	1.731120	0.738197
41	6	0	1.124711	1.731119	-0.738252
42	6	0	0.078292	2.296970	-1.435888
43	6	0	-0.437498	1.608789	-2.570286
44	6	0	-1.880868	1.760149	-2.577037
45	6	0	-2.687946	0.717947	-3.022879
46	6	0	-2.900895	-3.482766	-1.421282
47	6	0	-4.747260	0.470775	0.000000
48	6	0	-4.914409	-0.908375	0.000006
49	6	0	-4.556477	-1.682022	1.175560
50	6	0	-4.052415	-1.041227	2.302001
51	6	0	-3.893668	0.401804	2.305630
52	6	0	-3.391400	2.238287	0.741727
53	6	0	-3.391410	2.238286	-0.741758
54	6	0	-4.227981	1.143495	-1.174625
55	6	0	-3.893679	0.401772	-2.305632
56	6	0	-4.052426	-1.041259	-2.301986
57	6	0	-4.556482	-1.682043	-1.175536
58	6	0	-3.969606	-2.927297	0.727133
59	6	0	-2.900896	-3.482756	1.421330
60	6	0	-2.372284	-2.814173	2.596808
61	6	0	-2.937357	-1.618670	3.025828
62	6	0	-2.084966	-0.529783	3.468398
63	6	0	-2.687938	0.717990	3.022877
64	6	0	-1.880864	1.760183	2.577007
65	6	0	-2.247628	2.550767	1.432748
66	6	0	-2.247625	2.550736	-1.432778
67	6	0	-1.000175	3.166323	-0.802548
68	6	0	-1.000150	3.166332	0.802497
69	6	0	0.078280	2.296972	1.435826
70	6	0	-0.437493	1.608819	2.570244
71	6	0	0.141246	0.412871	3.001294
72	6	0	-0.707165	-0.677745	3.450669
73	6	0	-0.111690	-1.921755	3.003469
74	6	0	-0.930159	-2.972620	2.592776
75	6	0	-3.969615	-2.927317	-0.727092
76	6	0	-1.782421	-4.052440	0.693624
77	6	0	-4.227979	1.143512	1.174614
78	6	0	3.969218	0.151352	-0.000001
79	1	0	4.094243	1.239155	-0.000015
80	6	0	4.552674	-0.501344	-1.229382
81	6	0	5.128314	0.148151	-2.314138
82	1	0	5.217960	1.232068	-2.317593
83	6	0	5.584912	-0.605870	-3.397754
84	1	0	6.042803	-0.107563	-4.247180
85	6	0	5.450220	-1.993576	-3.396810
86	1	0	5.801872	-2.572069	-4.246059
87	6	0	4.857290	-2.644117	-2.312035
88	1	0	4.737072	-3.725005	-2.314824
89	6	0	4.416519	-1.894192	-1.228992
90	6	0	3.715868	-2.420374	0.000019
91	1	0	3.627956	-3.511705	0.000015
92	6	0	4.416498	-1.894171	1.229033
93	6	0	4.857223	-2.644075	2.312111
94	1	0	4.737003	-3.724963	2.314913
95	6	0	5.450103	-1.993513	3.396900
96	1	0	5.801714	-2.571988	4.246178
97	6	0	5.584797	-0.605807	3.397821
98	1	0	6.042655	-0.107483	4.247255
99	6	0	5.128251	0.148192	2.314167
100	1	0	5.217901	1.232108	2.317603
101	6	0	4.552652	-0.501324	1.229401

AICBA *e*-face *b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.917031	-3.663538	-1.130800
2	1	0	-2.734488	-3.974945	-2.161705
3	6	0	-4.363231	-3.575728	-0.700819
4	6	0	-5.542732	-3.432951	-1.414822
5	1	0	-5.543292	-3.412314	-2.501821
6	6	0	-6.739084	-3.317174	-0.697553
7	1	0	-7.679504	-3.221802	-1.232724
8	6	0	-6.739031	-3.317177	0.697797
9	1	0	-7.679411	-3.221831	1.233035
10	6	0	-5.542613	-3.432951	1.414954
11	1	0	-5.543055	-3.412350	2.501957
12	6	0	-4.363185	-3.575702	0.700831
13	6	0	-2.916947	-3.663510	1.130739
14	1	0	-2.734372	-3.975076	2.161581
15	6	0	-2.331837	-4.531901	-0.000074
16	1	0	-2.737911	-5.547106	0.000021
17	1	0	-1.236966	-4.569366	-0.000123
18	6	0	1.494796	-1.526027	-1.169138
19	6	0	0.321076	-2.219831	-0.738028
20	6	0	-0.866925	-2.127854	-1.431311
21	6	0	-0.924973	-1.270384	-2.568218
22	6	0	0.210162	-0.580321	-2.998230
23	6	0	1.442976	-0.721023	-2.283322
24	6	0	2.452107	-1.310804	-0.000001
25	6	0	1.494777	-1.525980	1.169111
26	6	0	0.321056	-2.219770	0.737999
27	6	0	-0.866875	-2.127945	1.431364
28	6	0	-2.251248	-2.270087	-0.802341
29	6	0	-2.219849	-0.614818	-2.578087
30	6	0	-2.331761	0.698705	-3.024595
31	6	0	-1.147230	1.418576	-3.467208
32	6	0	0.090328	0.795796	-3.449370
33	6	0	1.266432	1.517175	-3.003536
34	6	0	2.114724	0.596666	-2.282623
35	6	0	2.801779	1.016159	-1.171786
36	6	0	3.187811	0.111990	-0.000006
37	6	0	1.442968	-0.721021	2.283327
38	6	0	2.114721	0.596665	2.282642
39	6	0	2.801775	1.016146	1.171795
40	6	0	2.656387	2.371330	0.726070
41	6	0	2.656389	2.371340	-0.726054
42	6	0	1.864182	3.281858	-1.423209
43	6	0	1.149679	2.844186	-2.593122
44	6	0	-0.148523	3.492313	-2.596586
45	6	0	-1.272426	2.795621	-3.025262
46	6	0	-2.958262	-1.079493	-1.436362
47	6	0	-3.317304	3.272253	-0.000014
48	6	0	-3.924554	2.023363	-0.000023
49	6	0	-3.855657	1.175614	1.174766
50	6	0	-3.173105	1.617702	2.306496
51	6	0	-2.522791	2.916307	2.302213
52	6	0	-1.427340	4.454608	0.727337
53	6	0	-1.427334	4.454609	-0.727340
54	6	0	-2.596557	3.727769	-1.175342
55	6	0	-2.522782	2.916322	-2.302241
56	6	0	-3.173105	1.617724	-2.306536
57	6	0	-3.855660	1.175624	-1.174812
58	6	0	-3.748681	-0.198085	0.741560
59	6	0	-2.958235	-1.079484	1.436310
60	6	0	-2.219838	-0.614853	2.578055
61	6	0	-2.331757	0.698689	3.024536
62	6	0	-1.147243	1.418570	3.467197
63	6	0	-1.272447	2.795615	3.025255
64	6	0	-0.148543	3.492308	2.596584
65	6	0	-0.228709	4.340687	1.422119
66	6	0	-0.228699	4.340687	-1.422115
67	6	0	1.019315	4.212399	-0.693568
68	6	0	1.019309	4.212397	0.693578
69	6	0	1.864166	3.281844	1.423219
70	6	0	1.149659	2.844180	2.593133
71	6	0	1.266416	1.517168	3.003540
72	6	0	0.090309	0.795774	3.449362
73	6	0	0.210149	-0.580346	2.998258
74	6	0	-0.924969	-1.270427	2.568226
75	6	0	-3.748667	-0.198087	-0.741603
76	6	0	-2.251310	-2.270073	0.802270
77	6	0	-2.596571	3.727769	1.175329
78	6	0	4.754335	-0.144323	-0.000027
79	1	0	5.273553	0.819619	-0.000073
80	6	0	5.056465	-0.967865	-1.229704
81	6	0	5.834135	-0.581011	-2.314217
82	1	0	6.321115	0.391471	-2.320022
83	6	0	5.979425	-1.453245	-3.395952
84	1	0	6.589943	-1.161944	-4.245529
85	6	0	5.339896	-2.691928	-3.393301
86	1	0	5.453921	-3.362293	-4.240161
87	6	0	4.546558	-3.073399	-2.308749
88	1	0	4.033855	-4.032623	-2.309099
89	6	0	4.414391	-2.210908	-1.227998
90	6	0	3.568344	-2.439257	0.000043
91	1	0	3.081621	-3.420057	0.000065
92	6	0	4.414415	-2.210846	1.228045
93	6	0	4.546607	-3.073280	2.308840
94	1	0	4.033896	-4.032498	2.309277
95	6	0	5.339980	-2.691751	3.393345
96	1	0	5.454016	-3.362066	4.240245
97	6	0	5.979528	-1.453077	3.395913
98	1	0	6.590067	-1.161755	4.245468
99	6	0	5.834220	-0.580901	2.314135
100	1	0	6.321205	0.391578	2.319845
101	6	0	5.056507	-0.967813	1.229670

AICBA *e*-edge

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.162296	2.699186	1.254098
2	1	0	-5.116274	2.299363	1.604683
3	6	0	-4.222608	3.651862	0.083697
4	6	0	-5.171595	3.850387	-0.906672
5	1	0	-6.108063	3.298170	-0.906270
6	6	0	-4.892880	4.784852	-1.910513
7	1	0	-5.627376	4.972031	-2.688483
8	6	0	-3.680187	5.474626	-1.926833
9	1	0	-3.483931	6.193239	-2.717345
10	6	0	-2.712388	5.249413	-0.940542
11	1	0	-1.760445	5.773940	-0.968031
12	6	0	-3.003370	4.343179	0.068064
13	6	0	-2.194959	3.815437	1.231538
14	1	0	-1.356380	4.433036	1.560273
15	6	0	-3.313332	3.515136	2.248485
16	1	0	-3.824956	4.420326	2.586645
17	1	0	-2.974704	2.934789	3.113312
18	6	0	-1.320544	-2.418985	-3.258359
19	6	0	-0.277142	-3.326277	-2.822681
20	6	0	-0.538907	-4.255968	-1.821888
21	6	0	-1.854143	-4.321512	-1.220336
22	6	0	-2.855762	-3.453780	-1.640256
23	6	0	-2.583416	-2.479574	-2.681208
24	6	0	-0.706120	-1.130474	-3.523295
25	6	0	0.720135	-1.254456	-3.260154
26	6	0	0.981040	-2.601624	-2.829654
27	6	0	1.919410	-2.824058	-1.823457
28	6	0	0.442485	-4.494588	-0.779203
29	6	0	-1.687756	-4.608241	0.195865
30	6	0	-2.529766	-4.012930	1.128577
31	6	0	-3.567654	-3.100858	0.687116
32	6	0	-3.727597	-2.828622	-0.663788
33	6	0	-3.988349	-1.469684	-1.108326
34	6	0	-3.289150	-1.256397	-2.347945
35	6	0	-2.691157	-0.019789	-2.587227
36	6	0	-1.373395	0.037456	-3.189392
37	6	0	1.411219	-0.201864	-2.667252
38	6	0	0.713894	1.024692	-2.327117
39	6	0	-0.653597	1.146352	-2.585911
40	6	0	-1.506019	1.777645	-1.624036
41	6	0	-2.793567	1.048090	-1.618999
42	6	0	-3.473076	0.847316	-0.441557
43	6	0	-4.053193	-0.436431	-0.175803
44	6	0	-3.885280	-0.721782	1.238239
45	6	0	-3.659351	-2.028776	1.663733
46	6	0	-0.269611	-4.717970	0.466301
47	6	0	-0.581541	-1.319879	3.524012
48	6	0	0.090402	-2.495451	3.227429
49	6	0	1.413930	-2.443851	2.623567
50	6	0	2.002227	-1.214355	2.341739
51	6	0	1.301103	0.015371	2.661878
52	6	0	-0.982319	0.879217	2.815388
53	6	0	-2.269033	0.148469	2.820146
54	6	0	-2.001621	-1.202793	3.257495
55	6	0	-2.692265	-2.277304	2.700682
56	6	0	-1.987239	-3.502291	2.374018
57	6	0	-0.625563	-3.609826	2.632791
58	6	0	1.510663	-3.509053	1.662263
59	6	0	2.188712	-3.286316	0.465373
60	6	0	2.816121	-2.013156	0.203356
61	6	0	2.733095	-1.000247	1.123182
62	6	0	2.751942	0.489293	0.777284
63	6	0	1.598246	0.976613	1.654187
64	6	0	0.599233	1.826782	1.236093
65	6	0	-0.703819	1.796213	1.825874
66	6	0	-3.198802	0.386489	1.838157
67	6	0	-3.141687	1.558673	0.863202
68	6	0	-1.743364	2.348510	0.854572
69	6	0	-0.967348	2.257803	-0.450337
70	6	0	0.432422	2.118383	-0.200268
71	6	0	1.274066	1.538456	-1.123923
72	6	0	2.570878	0.803826	-0.780891
73	6	0	2.406766	-0.438347	-1.658080
74	6	0	2.646856	-1.721495	-1.240369
75	6	0	0.251363	-4.231071	1.659945
76	6	0	1.639855	-3.790337	-0.778601
77	6	0	0.034426	-0.033184	3.246603
78	6	0	4.113639	1.145496	1.256354
79	1	0	4.252275	0.941094	2.322956
80	6	0	4.006901	2.621073	0.957818
81	6	0	4.000039	3.652701	1.887979
82	1	0	4.106988	3.434566	2.948126
83	6	0	3.852050	4.969646	1.445800
84	1	0	3.853466	5.783788	2.164795
85	6	0	3.699398	5.243110	0.087110
86	1	0	3.583357	6.269535	-0.248620
87	6	0	3.691517	4.203134	-0.845758
88	1	0	3.558568	4.411742	-1.904823
89	6	0	3.852094	2.895121	-0.405927
90	6	0	3.823906	1.650168	-1.260282
91	1	0	3.715643	1.873566	-2.326569
92	6	0	5.048473	0.819386	-0.960185
93	6	0	5.938586	0.293274	-1.888370
94	1	0	5.805793	0.494192	-2.948921
95	6	0	6.999348	-0.499465	-1.443561
96	1	0	7.703357	-0.910289	-2.161167
97	6	0	7.155013	-0.770704	-0.084935
98	1	0	7.979816	-1.392073	0.251274
99	6	0	6.251403	-0.252237	0.845984
100	1	0	6.361389	-0.473277	1.905176
101	6	0	5.205159	0.546878	0.403397

AICBA *cis*-2 *a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.348223	-4.038419	-1.698251
2	1	0	0.707548	-4.885643	-1.952258
3	6	0	2.463975	-4.312430	-0.728715
4	6	0	2.654270	-5.323068	0.199604
5	1	0	1.934085	-6.130774	0.303367
6	6	0	3.803600	-5.280920	0.996214
7	1	0	3.985675	-6.067387	1.722820
8	6	0	4.718471	-4.238095	0.861170
9	1	0	5.609862	-4.220633	1.481654
10	6	0	4.504463	-3.209581	-0.063929
11	1	0	5.223133	-2.406249	-0.152597
12	6	0	3.369736	-3.251367	-0.858295
13	6	0	2.803957	-2.322928	-1.920931
14	1	0	3.513273	-1.639595	-2.391098
15	6	0	2.113114	-3.346914	-2.842379
16	1	0	2.826687	-4.017075	-3.329292
17	1	0	1.460561	-2.889973	-3.593746
18	6	0	-3.774103	2.740571	1.209121
19	6	0	-3.408521	3.187096	-0.123901
20	6	0	-3.893362	2.511534	-1.237883
21	6	0	-4.770392	1.368412	-1.070259
22	6	0	-5.125390	0.944968	0.205750
23	6	0	-4.611751	1.643561	1.368541
24	6	0	-2.613800	2.897635	2.065787
25	6	0	-1.538092	3.443627	1.255763
26	6	0	-2.027798	3.624673	-0.087705
27	6	0	-1.183425	3.353384	-1.162254
28	6	0	-3.016735	2.240647	-2.361090
29	6	0	-4.445114	0.393732	-2.095130
30	6	0	-4.492021	-0.964604	-1.804084
31	6	0	-4.856871	-1.406048	-0.468502
32	6	0	-5.164499	-0.472259	0.513457
33	6	0	-4.669103	-0.650261	1.866485
34	6	0	-4.328231	0.655458	2.394112
35	6	0	-3.213186	0.803890	3.211482
36	6	0	-2.335948	1.949903	3.041309
37	6	0	-0.232162	3.001588	1.451070
38	6	0	0.060369	2.012589	2.471389
39	6	0	-0.972466	1.502512	3.256679
40	6	0	-1.001134	0.094869	3.547953
41	6	0	-2.387265	-0.343654	3.528649
42	6	0	-2.713225	-1.594428	3.022321
43	6	0	-3.880177	-1.752859	2.178181
44	6	0	-3.557963	-2.726546	1.149656
45	6	0	-4.039542	-2.558705	-0.141942
46	6	0	-3.358579	0.928474	-2.891737
47	6	0	-0.789490	-2.713066	-1.873103
48	6	0	-1.051926	-1.783237	-2.840285
49	6	0	-0.151068	-0.618798	-2.991209
50	6	0	0.961291	-0.470867	-2.176411
51	6	0	1.545139	-1.581991	-1.302603
52	6	0	0.019659	-3.012775	0.291742
53	6	0	-1.357255	-3.408567	0.279588
54	6	0	-1.861249	-3.230659	-1.069080
55	6	0	-3.175165	-2.823908	-1.279178
56	6	0	-3.455442	-1.846056	-2.301627
57	6	0	-2.405870	-1.330012	-3.058623
58	6	0	-0.967893	0.508379	-3.314812
59	6	0	-0.642681	1.766770	-2.806936
60	6	0	0.502051	1.912430	-1.968207
61	6	0	1.279337	0.812687	-1.654752
62	6	0	2.140370	0.709630	-0.398793
63	6	0	1.837451	-0.759391	-0.042981
64	6	0	1.416267	-1.150145	1.174496
65	6	0	0.507428	-2.306924	1.362063
66	6	0	-2.193175	-3.167149	1.368292
67	6	0	-1.669872	-2.467933	2.510386
68	6	0	-0.347075	-2.030765	2.489498
69	6	0	-0.005730	-0.725066	3.021419
70	6	0	1.066440	-0.174208	2.232303
71	6	0	1.114327	1.171594	1.984581
72	6	0	1.741668	1.776467	0.736762

73	6	0	0.638300	2.752930	0.338621
74	6	0	0.173985	2.918969	-0.936309
75	6	0	-2.358365	0.086605	-3.356572
76	6	0	-1.691913	2.647367	-2.321646
77	6	0	0.528005	-2.823373	-1.122406
78	6	0	3.664866	0.981599	-0.773888
79	1	0	3.975234	0.306842	-1.576368
80	6	0	4.505528	0.820147	0.470380
81	6	0	5.614075	-0.000539	0.620143
82	1	0	5.975870	-0.581742	-0.223297
83	6	0	6.284821	-0.038476	1.844813
84	1	0	7.151829	-0.681767	1.966285
85	6	0	5.851576	0.753837	2.906060
86	1	0	6.371193	0.714379	3.858875
87	6	0	4.772651	1.625718	2.737960
88	1	0	4.458477	2.278440	3.549043
89	6	0	4.119337	1.668885	1.513104
90	6	0	3.022961	2.621351	1.113774
91	1	0	2.763859	3.323504	1.912799
92	6	0	3.438935	3.321772	-0.160507
93	6	0	3.450873	4.692080	-0.383656
94	1	0	3.185994	5.379580	0.416385
95	6	0	3.797980	5.174509	-1.648201
96	1	0	3.816426	6.244891	-1.830823
97	6	0	4.112642	4.289158	-2.677742
98	1	0	4.375390	4.672018	-3.659535
99	6	0	4.087336	2.910002	-2.454799
100	1	0	4.320423	2.216600	-3.259834
101	6	0	3.756962	2.432414	-1.193100

AICBA *cis*-2 *b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.226033	4.048653	1.656274
2	1	0	0.685065	4.597261	2.430257
3	6	0	1.617530	4.829554	0.424676
4	6	0	1.125449	5.998655	-0.133308
5	1	0	0.343074	6.570625	0.359365
6	6	0	1.662205	6.424733	-1.353651
7	1	0	1.306351	7.346852	-1.804119
8	6	0	2.643970	5.675308	-2.002693
9	1	0	3.041730	6.022351	-2.951958
10	6	0	3.118844	4.481023	-1.447852
11	1	0	3.870641	3.890669	-1.966586
12	6	0	2.606434	4.077712	-0.223743
13	6	0	2.834779	2.847175	0.623500
14	1	0	3.784968	2.338290	0.469939
15	6	0	2.570542	3.403821	2.034718
16	1	0	3.317607	4.142257	2.339103
17	1	0	2.482913	2.623186	2.798334
18	6	0	-3.415312	-2.776585	1.773392
19	6	0	-2.779146	-2.038152	2.845562
20	6	0	-3.179091	-0.738239	3.125753
21	6	0	-4.232191	-0.119825	2.346922
22	6	0	-4.839262	-0.825038	1.313014
23	6	0	-4.421644	-2.181757	1.020192
24	6	0	-2.395308	-3.578098	1.118477
25	6	0	-1.134812	-3.330242	1.792130
26	6	0	-1.366533	-2.381652	2.847957
27	6	0	-0.413195	-1.395867	3.092409
28	6	0	-2.185848	0.281794	3.420555
29	6	0	-3.890496	1.280669	2.165945
30	6	0	-4.171281	1.915599	0.963793
31	6	0	-4.798903	1.178939	-0.116348
32	6	0	-5.124967	-0.161460	0.053542
33	6	0	-4.880480	-1.109858	-1.016160
34	6	0	-4.448104	-2.359739	-0.420333
35	6	0	-3.473242	-3.128684	-1.045039
36	6	0	-2.426147	-3.751740	-0.258375
37	6	0	0.045313	-3.252669	1.052855
38	6	0	0.014375	-3.437806	-0.386222
39	6	0	-1.195641	-3.689365	-1.028953
40	6	0	-1.478947	-3.035290	-2.281507
41	6	0	-2.884999	-2.681271	-2.295649
42	6	0	-3.292765	-1.478374	-2.860067
43	6	0	-4.311972	-0.677138	-2.209086
44	6	0	-3.969519	0.721836	-2.386003
45	6	0	-4.211761	1.633239	-1.364919
46	6	0	-2.627693	1.520315	2.837332
47	6	0	-0.781691	2.959544	-1.090458
48	6	0	-0.759051	3.138343	0.268400
49	6	0	0.426808	2.782816	1.153129
50	6	0	1.575763	1.905225	0.436735
51	6	0	1.252696	1.528688	-0.998938
52	6	0	-0.372964	1.409289	-2.807218
53	6	0	-1.783607	1.752246	-2.832178
54	6	0	-2.031916	2.706014	-1.768154
55	6	0	-3.227166	2.651475	-1.054409
56	6	0	-3.200841	2.823469	0.376389
57	6	0	-1.982574	3.044228	1.013764
58	6	0	-0.288711	2.070660	2.288188
59	6	0	0.126104	0.872379	2.808162
60	6	0	1.174885	0.073512	2.132968
61	6	0	1.780167	0.499339	1.010005
62	6	0	2.304372	-0.454100	-0.075388
63	6	0	1.650497	0.196018	-1.286311
64	6	0	1.062609	-0.506373	-2.319025
65	6	0	0.028055	0.101601	-3.091806
66	6	0	-2.731443	0.787150	-3.138555
67	6	0	-2.312600	-0.576001	-3.432172
68	6	0	-0.966694	-0.908361	-3.407432
69	6	0	-0.536178	-2.162597	-2.819371
70	6	0	0.721878	-1.935390	-2.148180
71	6	0	1.000531	-2.567274	-0.965239
72	6	0	1.907640	-1.997105	0.126973
73	6	0	1.043256	-2.269343	1.348716
74	6	0	0.808828	-1.346984	2.332334
75	6	0	-1.688436	2.380109	2.269926
76	6	0	-0.831211	-0.037861	3.384115
77	6	0	0.255172	2.130043	-1.745078
78	6	0	3.887452	-0.391267	-0.201925
79	1	0	4.203509	0.633454	-0.404427
80	6	0	4.290167	-1.313981	-1.326003
81	6	0	4.896172	-0.940607	-2.519395
82	1	0	5.138678	0.102904	-2.708185
83	6	0	5.187189	-1.919126	-3.472689
84	1	0	5.666203	-1.637679	-4.405869
85	6	0	4.861466	-3.253773	-3.234040
86	1	0	5.086847	-4.008029	-3.982269
87	6	0	4.236911	-3.625182	-2.041140
88	1	0	3.965850	-4.662468	-1.858395
89	6	0	3.960344	-2.651774	-1.089992
90	6	0	3.241521	-2.851996	0.219822
91	1	0	2.981013	-3.899492	0.402467
92	6	0	4.066126	-2.256585	1.335545
93	6	0	4.422664	-2.882337	2.523536
94	1	0	4.129315	-3.913005	2.709311
95	6	0	5.156840	-2.172022	3.476567
96	1	0	5.443469	-2.655053	4.406120
97	6	0	5.517858	-0.846052	3.243064
98	1	0	6.085508	-0.300224	3.991002
99	6	0	5.148183	-0.213988	2.053098
100	1	0	5.420441	0.824162	1.873690
101	6	0	4.427848	-0.924923	1.101608

AICBA *cis*-3 *a*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.950938	3.760230	1.228133
2	1	0	-2.245362	3.717996	2.279023
3	6	0	-3.074528	3.744204	0.220285
4	6	0	-4.401160	3.360516	0.310555
5	1	0	-4.814371	2.987557	1.244067
6	6	0	-5.198562	3.469364	-0.835766
7	1	0	-6.251467	3.202532	-0.785142
8	6	0	-4.661191	3.917563	-2.041935
9	1	0	-5.298405	3.990707	-2.918729
10	6	0	-3.311707	4.282644	-2.134045
11	1	0	-2.894375	4.629113	-3.076198
12	6	0	-2.535828	4.209223	-0.988504
13	6	0	-1.084244	4.526035	-0.716865
14	1	0	-0.590508	5.181677	-1.437559
15	6	0	-1.165967	4.998697	0.749313
16	1	0	-1.741117	5.922156	0.857513
17	1	0	-0.187999	5.113402	1.228026
18	6	0	3.775375	-2.390903	1.741172
19	6	0	3.502481	-3.101628	0.504218
20	6	0	4.028479	-2.636846	-0.694216
21	6	0	4.853702	-1.446324	-0.713450
22	6	0	5.112529	-0.761595	0.468176
23	6	0	4.560932	-1.242881	1.723174
24	6	0	2.578172	-2.434495	2.555473
25	6	0	1.565448	-3.170258	1.814124
26	6	0	2.134415	-3.583289	0.558551
27	6	0	1.342083	-3.558116	-0.586956
28	6	0	3.209927	-2.630254	-1.895557
29	6	0	4.554387	-0.710437	-1.930455
30	6	0	4.528452	0.680215	-1.911866
31	6	0	4.792059	1.392567	-0.673960
32	6	0	5.076364	0.686735	0.487722
33	6	0	4.492098	1.099851	1.752985
34	6	0	4.182978	-0.093515	2.519323
35	6	0	3.033964	-0.136804	3.303259
36	6	0	2.214783	-1.334156	3.319522
37	6	0	0.236448	-2.757355	1.857795
38	6	0	-0.143051	-1.606072	2.655075
39	6	0	0.823688	-0.917179	3.381083
40	6	0	0.790155	0.521260	3.394423

41	6	0	2.146059	1.008319	3.352948
42	6	0	2.434441	2.144793	2.602923
43	6	0	3.634768	2.191268	1.793494
44	6	0	3.335322	2.930668	0.580227
45	6	0	3.912637	2.546310	-0.626738
46	6	0	3.542796	-1.444104	-2.662667
47	6	0	0.760857	2.196686	-2.481028
48	6	0	1.127773	1.106883	-3.263950
49	6	0	0.310071	-0.077412	-3.237240
50	6	0	-0.825481	-0.106687	-2.422255
51	6	0	-1.205741	1.049681	-1.649367
52	6	0	-0.320128	3.159744	-0.533428
53	6	0	1.191596	3.366530	-0.507143
54	6	0	1.773637	2.932136	-1.746343
55	6	0	3.108592	2.544673	-1.820901
56	6	0	3.487664	1.393450	-2.624765
57	6	0	2.518668	0.691449	-3.328239
58	6	0	1.174599	-1.228366	-3.297447
59	6	0	0.854214	-2.355837	-2.546170
60	6	0	-0.346308	-2.386759	-1.744171
61	6	0	-1.165766	-1.290492	-1.681734
62	6	0	-2.064501	-0.941871	-0.498562
63	6	0	-1.806715	0.564576	-0.390587
64	6	0	-1.564909	1.219902	0.760061
65	6	0	-0.938767	2.607729	0.842945
66	6	0	1.955858	3.350442	0.631893
67	6	0	1.384265	2.848968	1.902995
68	6	0	0.093657	2.386584	1.941728
69	6	0	-0.207721	1.189528	2.680405
70	6	0	-1.222970	0.451272	1.972509
71	6	0	-1.205030	-0.920872	1.972955
72	6	0	-1.737686	-1.776536	0.828513
73	6	0	-0.584940	-2.768559	0.681986
74	6	0	-0.039741	-3.152747	-0.514718
75	6	0	2.545581	-0.758986	-3.349833
76	6	0	1.895407	-3.073484	-1.838843
77	6	0	-0.442103	2.191242	-1.695967
78	6	0	-3.580650	-1.218999	-0.886957
79	1	0	-3.827297	-0.656669	-1.793468
80	6	0	-4.433329	-0.817864	0.291077
81	6	0	-5.429564	0.147739	0.294486
82	1	0	-5.657480	0.696848	-0.615271
83	6	0	-6.127780	0.404957	1.477408
84	1	0	-6.917670	1.152125	1.487045
85	6	0	-5.815393	-0.288795	2.645378
86	1	0	-6.358153	-0.078146	3.562294
87	6	0	-4.812044	-1.262010	2.639982
88	1	0	-4.568041	-1.809318	3.547460
89	6	0	-4.136059	-1.532479	1.457350
90	6	0	-3.047355	-2.556857	1.258886
91	1	0	-2.837587	-3.130685	2.167367
92	6	0	-3.419353	-3.437225	0.088085
93	6	0	-3.436759	-4.825977	0.072905
94	1	0	-3.197488	-5.386244	0.973768
95	6	0	-3.758451	-5.491871	-1.112414
96	1	0	-3.780237	-6.577503	-1.132299
97	6	0	-4.044803	-4.770229	-2.270368
98	1	0	-4.288725	-5.296017	-3.188767
99	6	0	-4.012096	-3.373606	-2.257602
100	1	0	-4.220361	-2.807941	-3.162829
101	6	0	-3.705285	-2.712500	-1.075205

AICBA *cis*-3 *b*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.766194	3.789650	-1.963270
2	1	0	1.993240	3.773925	-3.031496
3	6	0	2.783293	4.462797	-1.070592
4	6	0	4.131700	4.739920	-1.233870
5	1	0	4.645706	4.506225	-2.162922
6	6	0	4.818124	5.335676	-0.169021
7	1	0	5.870746	5.580171	-0.278694
8	6	0	4.168046	5.616100	1.033205
9	1	0	4.720806	6.076693	1.846959
10	6	0	2.813421	5.308330	1.204245
11	1	0	2.313718	5.509686	2.148579
12	6	0	2.130483	4.744637	0.137887
13	6	0	0.714466	4.240816	-0.011538
14	1	0	-0.020585	4.630575	0.696480
15	6	0	0.472521	4.495462	-1.511313
16	1	0	0.470136	5.560631	-1.758233
17	1	0	-0.440174	4.022908	-1.890332
18	6	0	1.005831	-3.816664	2.431957
19	6	0	0.250611	-4.426092	1.351497
20	6	0	0.875410	-4.716739	0.145774
21	6	0	2.280684	-4.414944	-0.036645
22	6	0	3.004274	-3.825291	0.993458
23	6	0	2.353083	-3.518555	2.255713
24	6	0	0.138519	-2.870639	3.104071
25	6	0	-1.152614	-2.897400	2.433335
26	6	0	-1.083752	-3.854173	1.360487
27	6	0	-1.729507	-3.575137	0.158590
28	6	0	0.195376	-4.445463	-1.110201
29	6	0	2.471933	-3.968661	-1.406073
30	6	0	3.380637	-2.952553	-1.684687
31	6	0	4.129215	-2.333380	-0.605219
32	6	0	3.943567	-2.761335	0.702442
33	6	0	3.864344	-1.790129	1.781235
34	6	0	2.888580	-2.265258	2.744835
35	6	0	2.057309	-1.359176	3.394858
36	6	0	0.651299	-1.670790	3.575948
37	6	0	-1.864190	-1.714633	2.247561
38	6	0	-1.325116	-0.459876	2.739151
39	6	0	-0.100627	-0.440313	3.400389
40	6	0	0.834255	0.614291	3.109161
41	6	0	2.163407	0.058274	3.107024
42	6	0	3.085637	0.510389	2.166806
43	6	0	3.957622	-0.433767	1.498993
44	6	0	4.150750	0.017589	0.131925
45	6	0	4.248076	-0.915852	-0.897093
46	6	0	1.185127	-3.991900	-2.070993
47	6	0	1.559105	0.491937	-2.958969
48	6	0	1.054294	-0.708174	-3.449361
49	6	0	-0.341479	-1.010378	-3.262690
50	6	0	-1.153474	-0.097355	-2.587062
51	6	0	-0.612735	1.154103	-2.119866
52	6	0	1.525358	2.341741	-1.381912
53	6	0	2.787660	1.500709	-1.249072
54	6	0	2.849936	0.519004	-2.295985
55	6	0	3.576445	-0.659437	-2.143274
56	6	0	3.038352	-1.916706	-2.639159
57	6	0	1.806281	-1.939175	-3.277350
58	6	0	-0.470294	-2.418197	-2.984745
59	6	0	-1.412300	-2.840787	-2.050753
60	6	0	-2.277229	-1.887902	-1.393996
61	6	0	-2.149526	-0.549196	-1.653738
62	6	0	-2.501675	0.563077	-0.672274
63	6	0	-1.297221	1.483840	-0.856187
64	6	0	-0.607861	2.053916	0.146173
65	6	0	0.782936	2.661949	0.006685
66	6	0	3.412465	1.244177	-0.053389
67	6	0	2.732676	1.550779	1.227667
68	6	0	1.468201	2.082490	1.232332
69	6	0	0.494505	1.590064	2.169485
70	6	0	-0.794598	1.567912	1.526187
71	6	0	-1.695073	0.575240	1.815899
72	6	0	-2.737797	0.059982	0.829341
73	6	0	-2.562185	-1.447260	1.021437
74	6	0	-2.483389	-2.355023	-0.003417
75	6	0	0.858053	-2.999126	-2.988558
76	6	0	-1.072833	-3.880109	-1.100751
77	6	0	0.710647	1.460164	-2.319628
78	6	0	-3.816448	1.312943	-1.152915
79	1	0	-3.673944	1.660799	-2.181518
80	6	0	-4.039074	2.446752	-0.182883
81	6	0	-3.997841	3.803893	-0.476680
82	1	0	-3.831971	4.137708	-1.498766
83	6	0	-4.169610	4.731613	0.553647
84	1	0	-4.148400	5.794798	0.332219
85	6	0	-4.365297	4.298938	1.864701
86	1	0	-4.494507	5.026595	2.660490
87	6	0	-4.393600	2.933792	2.160431
88	1	0	-4.532972	2.593058	3.183790
89	6	0	-4.238167	2.012247	1.132291
90	6	0	-4.192500	0.509269	1.273767
91	1	0	-4.369990	0.177681	2.301987
92	6	0	-5.154220	-0.109554	0.288569
93	6	0	-6.125191	-1.062413	0.570117
94	1	0	-6.271336	-1.410412	1.590094
95	6	0	-6.905365	-1.570635	-0.471193
96	1	0	-7.670845	-2.311734	-0.260573
97	6	0	-6.701658	-1.137075	-1.780448
98	1	0	-7.309012	-1.541455	-2.584896
99	6	0	-5.714875	-0.190047	-2.064358
100	1	0	-5.543154	0.139735	-3.086479
101	6	0	-4.949295	0.324873	-1.025932

Anthracene (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.653260	-0.714753	0.000004
2	6	0	2.476222	-1.406638	-0.000001
3	6	0	1.219718	-0.718773	-0.000005
4	6	0	1.219719	0.718773	-0.000002
5	6	0	2.476222	1.406638	0.000006
6	6	0	3.653260	0.714752	0.000008
7	6	0	0.000000	-1.402089	-0.000004
8	6	0	0.000000	1.402089	-0.000005
9	6	0	-1.219719	0.718773	-0.000005

10	6	0	-1.219719	-0.718773	-0.000001
11	6	0	-2.476221	-1.406638	0.000007
12	1	0	-2.471225	-2.494356	0.000012
13	6	0	-3.653260	-0.714752	0.000003
14	6	0	-3.653260	0.714752	0.000000
15	6	0	-2.476221	1.406638	-0.000004
16	1	0	-0.000001	-2.491033	-0.000007
17	1	0	4.599942	-1.247591	0.000003
18	1	0	2.471225	-2.494356	-0.000013
19	1	0	2.471224	2.494356	0.000004
20	1	0	4.599942	1.247592	0.000016
21	1	0	-0.000001	2.491033	-0.000009
22	1	0	-4.599942	-1.247592	0.000008
23	1	0	-4.599942	1.247592	-0.000002
24	1	0	-2.471225	2.494356	-0.000012

Indene (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.230355	-0.686724	0.000009
2	6	0	-1.664280	-1.155881	0.000041
3	6	0	-0.211419	0.720689	0.000004
4	6	0	-2.435728	0.140809	-0.000093
5	6	0	-1.601809	1.196096	0.000053
6	6	0	0.955500	-1.409010	-0.000004
7	6	0	0.997877	1.414837	-0.000005
8	6	0	2.168633	-0.712779	-0.000013
9	6	0	2.187819	0.684762	-0.000010
10	1	0	-1.898224	-1.767870	-0.881361
11	1	0	-1.898239	-1.767715	0.881555
12	1	0	-3.519514	0.186087	-0.000153
13	1	0	-1.890301	2.242520	0.000090
14	1	0	0.946621	-2.496755	0.000001
15	1	0	1.016644	2.501907	0.000010
16	1	0	3.105429	-1.263108	-0.000017
17	1	0	3.140152	1.208141	-0.000006

C_{60} (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.520419	0.354175	0.162846
2	6	0	-3.293342	-0.775521	1.046430
3	6	0	-2.656531	-0.585561	2.265217
4	6	0	-2.219501	0.742569	2.656807
5	6	0	-2.436332	1.822391	1.811958
6	6	0	-3.102942	1.624442	0.537308
7	6	0	-3.329471	-0.099603	-1.202755
8	6	0	-2.987083	-1.510276	-1.163080
9	6	0	-2.962857	-1.927511	0.227355
10	6	0	-2.010402	-2.839255	0.662950
11	6	0	-1.661562	-1.539377	2.721203
12	6	0	-0.952411	0.609264	3.352031
13	6	0	0.041775	1.561677	3.176936
14	6	0	-0.184983	2.689877	2.292592
15	6	0	-1.396365	2.818696	1.626777
16	6	0	-1.418878	3.235728	0.236716
17	6	0	-2.472860	2.497585	-0.436385
18	6	0	-2.289311	2.063023	-1.742046
19	6	0	-2.726829	0.735422	-2.133551
20	6	0	-2.054506	-2.021380	-2.055651
21	6	0	-1.425701	-1.148064	-3.030248
22	6	0	-1.754326	0.199916	-3.068042
23	6	0	-0.714379	1.195625	-3.253161
24	6	0	-1.045901	2.348176	-2.434880
25	6	0	-0.039142	3.054585	-1.791209
26	6	0	-0.229882	3.508900	-0.425600
27	6	0	1.036456	3.374061	0.271655
28	6	0	1.059069	2.975615	1.601065
29	6	0	-0.608414	-0.800446	3.393060
30	6	0	3.329471	0.099603	1.202755
31	6	0	2.726829	-0.735422	2.133552
32	6	0	2.289311	-2.063023	1.742046
33	6	0	2.472860	-2.497585	0.436385
34	6	0	3.102942	-1.624442	-0.537308
35	6	0	3.293341	0.775521	-1.046430
36	6	0	2.962857	1.927511	-0.227355
37	6	0	2.987083	1.510277	1.163080
38	6	0	2.054506	2.021380	2.055651
39	6	0	1.425701	1.148064	3.030248
40	6	0	1.754326	-0.199916	3.068042
41	6	0	1.045901	-2.348176	2.434880
42	6	0	0.039142	-3.054585	1.791209
43	6	0	0.229883	-3.508900	0.425600
44	6	0	1.418878	-3.235728	-0.236716
45	6	0	1.396364	-2.818696	-1.626777
46	6	0	2.436332	-1.822391	-1.811958
47	6	0	2.219500	-0.742570	-2.656807
48	6	0	2.656531	0.585561	-2.265217
49	6	0	2.010403	2.839255	-0.662950
50	6	0	1.345043	2.640861	-1.937633
51	6	0	1.661562	1.539377	-2.721203
52	6	0	0.608414	0.800446	-3.393060
53	6	0	0.952410	-0.609265	-3.352031
54	6	0	-0.041775	-1.561677	-3.176936
55	6	0	0.184983	-2.689876	-2.292591
56	6	0	-1.059069	-2.975615	-1.601065
57	6	0	-1.036456	-3.374061	-0.271655
58	6	0	0.714379	-1.195625	3.253161
59	6	0	-1.345042	-2.640861	1.937633
60	6	0	3.520419	-0.354175	-0.162846

$AC_{60}MA$ (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.467113	0.000008	-0.801214
2	6	0	-2.467112	-0.000008	0.801216
3	6	0	-1.707917	-1.169662	1.427841
4	6	0	-1.281465	-2.276628	0.740740
5	6	0	-1.281465	-2.276612	-0.740789
6	6	0	-1.707916	-1.169631	-1.427865
7	6	0	-0.962939	-0.725196	-2.573455
8	6	0	-0.962939	0.725252	-2.573439
9	6	0	-1.707918	1.169662	-1.427840
10	6	0	-1.281466	2.276627	-0.740739
11	6	0	-1.281465	2.276611	0.740790
12	6	0	-1.707916	1.169631	1.427866
13	6	0	-0.962937	0.725195	2.573456
14	6	0	-0.962937	-0.725252	2.573440
15	6	0	0.153475	-1.423148	3.026686
16	6	0	0.594711	-2.590590	2.307822
17	6	0	-0.107650	-2.995979	1.175300
18	6	0	0.617534	-3.439984	-0.000038
19	6	0	-0.107650	-2.995953	-1.175366
20	6	0	0.594710	-2.590539	-2.307879
21	6	0	0.153473	-1.423081	-3.026717
22	6	0	1.326407	-0.693383	-3.478695
23	6	0	1.326407	0.693460	-3.478680
24	6	0	0.153472	1.423148	-3.026685
25	6	0	0.594710	2.590590	-2.307822
26	6	0	-0.107651	2.995978	-1.175300
27	6	0	0.617534	3.439984	0.000038
28	6	0	-0.107650	2.995953	1.175366
29	6	0	0.594712	2.590539	2.307879
30	6	0	0.153475	1.423081	3.026717
31	6	0	1.326409	0.693383	3.478694
32	6	0	1.326409	-0.693460	3.478679
33	6	0	2.498648	-1.421419	3.031347
34	6	0	2.045190	-2.594240	2.303269
35	6	0	2.736426	-3.019038	1.175767
36	6	0	2.004977	-3.457848	-0.000039
37	6	0	2.736425	-3.019012	-1.175835
38	6	0	2.045188	-2.594189	-2.303328
39	6	0	2.498646	-1.421352	-3.031381
40	6	0	3.621019	-0.726165	-2.598888
41	6	0	3.621019	0.726222	-2.598872
42	6	0	2.498646	1.421419	-3.031349
43	6	0	2.045188	2.594240	-2.303270
44	6	0	2.736425	3.019038	-1.175769
45	6	0	2.004977	3.457848	0.000037
46	6	0	2.736426	3.019012	1.175833
47	6	0	2.045190	2.594189	2.303326
48	6	0	2.498648	1.421352	3.031379
49	6	0	3.621021	0.726165	2.598886
50	6	0	3.621021	-0.726222	2.598870
51	6	0	4.342802	-1.173909	1.422362
52	6	0	3.908856	-2.295544	0.727024
53	6	0	3.908855	-2.295528	-0.727078
54	6	0	4.342802	-1.173878	-1.422390
55	6	0	4.788189	0.000008	-0.694169
56	6	0	4.342801	1.173909	-1.422365
57	6	0	3.908855	2.295544	-0.727027
58	6	0	3.908855	2.295528	0.727075
59	6	0	4.342803	1.173878	1.422387
60	6	0	4.788189	-0.000008	0.694166
61	6	0	-3.977301	0.000008	-1.293814
62	1	0	-3.997669	0.000014	-2.387831
63	6	0	-4.623695	1.228639	-0.699845
64	6	0	-5.143673	2.308481	-1.403391
65	1	0	-5.131534	2.310845	-2.490994
66	6	0	-5.679111	3.388510	-0.697189
67	1	0	-6.095034	4.234081	-1.237724
68	6	0	-5.679108	3.388503	0.697231
69	1	0	-6.095028	4.234070	1.237776
70	6	0	-5.143664	2.308469	1.403421
71	1	0	-5.131521	2.310823	2.491024
72	6	0	-4.623691	1.228633	0.699863

73	6	0	-3.977301	-0.000008	1.293817
74	1	0	-3.997669	-0.000014	2.387834
75	6	0	-4.623696	-1.228639	0.699848
76	6	0	-5.143673	-2.308480	1.403395
77	1	0	-5.131534	-2.310844	2.490997
78	6	0	-5.679113	-3.388509	0.697193
79	1	0	-6.095036	-4.234080	1.237728
80	6	0	-5.679109	-3.388503	-0.697227
81	1	0	-6.095029	-4.234069	-1.237772
82	6	0	-5.143665	-2.308469	-1.403417
83	1	0	-5.131522	-2.310824	-2.491020
84	6	0	-4.623692	-1.228633	-0.699860

C_{70} (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.201756	-3.376529	0.747402
2	6	0	-0.000033	-3.228699	1.481138
3	6	0	-1.201815	-3.376523	0.747381
4	6	0	-1.201746	-3.390242	-0.678597
5	6	0	0.000000	-3.260537	-1.416252
6	6	0	1.201700	-3.390302	-0.678573
7	6	0	2.440207	-2.784689	-1.133232
8	6	0	3.219978	-2.406180	0.024366
9	6	0	2.440350	-2.761426	1.189668
10	6	0	2.439909	-1.938117	2.297407
11	6	0	1.201734	-1.693229	3.014304
12	6	0	-0.000023	-2.353792	2.661713
13	6	0	-1.201804	-1.693213	3.014299
14	6	0	-2.440032	-1.938093	2.297335
15	6	0	-2.440439	-2.761426	1.189617
16	6	0	-3.220021	-2.406134	0.024327
17	6	0	-2.440247	-2.784649	-1.133269
18	6	0	-2.440458	-1.984655	-2.258000
19	6	0	-1.201603	-1.753616	-2.978557
20	6	0	0.000014	-2.407055	-2.612671
21	6	0	1.201621	-1.753649	-2.978544
22	6	0	2.440452	-1.984729	-2.257967
23	6	0	3.220161	-0.766826	-2.280388
24	6	0	3.967085	-0.393293	-1.169253
25	6	0	3.966497	-1.233644	0.012270
26	6	0	3.966294	-0.369355	1.176532
27	6	0	3.219074	-0.720073	2.294563
28	6	0	2.439879	0.278270	2.992394
29	6	0	1.201740	-0.332413	3.440862
30	6	0	-0.000026	0.411178	3.527180
31	6	0	-1.201785	-0.332389	3.440856
32	6	0	-2.439925	0.278291	2.992372
33	6	0	-3.219140	-0.720043	2.294482
34	6	0	-3.966357	-0.369286	1.176507
35	6	0	-3.966553	-1.233593	0.012223
36	6	0	-3.967049	-0.393242	-1.169315
37	6	0	-3.220141	-0.766801	-2.280430
38	6	0	-2.440340	0.217300	-2.997905
39	6	0	-1.201394	-0.401811	-3.432051
40	6	0	0.000022	0.339943	-3.535326
41	6	0	1.201477	-0.401842	-3.432055
42	6	0	2.440382	0.217278	-2.997855
43	6	0	2.440120	1.534102	-2.584512
44	6	0	3.220184	1.932079	-1.433706
45	6	0	3.966499	0.990344	-0.734968
46	6	0	3.966657	1.005260	0.714818
47	6	0	3.219528	1.960503	1.394008
48	6	0	2.440266	1.586629	2.553382
49	6	0	1.201917	2.343974	2.541739
50	6	0	-0.000002	1.803536	3.059661
51	6	0	-1.201904	2.344001	2.541710
52	6	0	-2.440283	1.586653	2.553350
53	6	0	-3.219534	1.960557	1.393968
54	6	0	-3.966661	1.005336	0.714772
55	6	0	-3.966446	0.990377	-0.735020
56	6	0	-3.220113	1.932137	-1.433753
57	6	0	-2.440034	1.534139	-2.584519
58	6	0	-1.201699	2.291612	-2.587964
59	6	0	0.000038	1.742557	-3.097206
60	6	0	1.201796	2.291587	-2.587962
61	6	0	1.202021	3.142531	-1.443500
62	6	0	2.440713	2.919493	-0.719762
63	6	0	2.440209	2.932798	0.660292
64	6	0	1.201891	3.170863	1.379643
65	6	0	0.000010	3.484799	0.699717
66	6	0	-1.201868	3.170872	1.379583
67	6	0	-2.440197	2.932845	0.660236
68	6	0	-2.440630	2.919502	-0.719800
69	6	0	-1.201920	3.142544	-1.443513
70	6	0	0.000044	3.468207	-0.769651

$AC_{70}MA$ isomer *a* (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.338955	2.559345	1.661315
2	6	0	2.019759	3.070494	1.687388
3	6	0	1.172147	2.558793	2.699898
4	6	0	1.537831	1.410859	3.463104
5	6	0	2.762260	0.734947	3.231678
6	6	0	3.705314	1.410177	2.421919
7	6	0	4.722802	0.689757	1.675729
8	6	0	5.003085	1.412975	0.456087
9	6	0	4.131201	2.565053	0.443830
10	6	0	3.568506	2.995606	-0.740511
11	6	0	2.185392	3.436051	-0.762970
12	6	0	1.417349	3.517424	0.423452
13	6	0	0.012635	3.405627	0.270539
14	6	0	-0.837742	2.963769	1.356435
15	6	0	-0.272685	2.561082	2.555695
16	6	0	-0.803725	1.416714	3.231768
17	6	0	0.320433	0.689802	3.783883
18	6	0	0.320424	-0.690035	3.783831
19	6	0	1.537819	-1.411080	3.463013
20	6	0	2.762251	-0.735162	3.231626
21	6	0	3.705302	-1.410348	2.421827
22	6	0	4.722795	-0.689888	1.675684
23	6	0	5.003070	-1.413028	0.455996
24	6	0	5.272110	-0.724066	-0.723041
25	6	0	5.272112	0.724084	-0.722993
26	6	0	4.678400	1.173398	-1.966732
27	6	0	3.846813	2.287477	-1.970964
28	6	0	2.620829	2.278666	-2.737461
29	6	0	1.605150	2.995421	-1.989317
30	6	0	0.239567	2.630929	-2.068497
31	6	0	-0.568121	2.968757	-0.955293
32	6	0	-1.792155	2.257629	-0.653756
33	6	0	-1.968427	2.262646	0.807056
34	6	0	-2.488661	1.166320	1.449856
35	6	0	-1.878331	0.722615	2.669023
36	6	0	-1.878335	-0.722762	2.668977
37	6	0	-0.803741	-1.416909	3.231682
38	6	0	-0.272705	-2.561236	2.555531
39	6	0	1.172126	-2.558963	2.699732
40	6	0	2.019734	-3.070607	1.687190
41	6	0	3.338932	-2.559463	1.661148
42	6	0	4.131184	-2.565103	0.443665
43	6	0	3.568480	-2.995567	-0.740703
44	6	0	3.846797	-2.287365	-1.971112
45	6	0	4.678390	-1.173295	-1.966807
46	6	0	4.313729	0.000080	-2.739495
47	6	0	3.135845	0.000106	-3.476468
48	6	0	2.273762	1.162743	-3.474572
49	6	0	0.895417	0.713584	-3.491039
50	6	0	-0.125075	1.448330	-2.841449
51	6	0	-1.269274	0.712634	-2.435033
52	6	0	-2.139430	1.158737	-1.380360
53	6	0	-2.972957	0.000037	-0.849104
54	6	0	-3.176148	-0.000003	0.740447
55	6	0	-2.488680	-1.166390	1.449787
56	6	0	-1.968438	-2.262660	0.806907
57	6	0	-0.837759	-2.963836	1.356241
58	6	0	0.012607	-3.405639	0.270320
59	6	0	1.417321	-3.517448	0.423224
60	6	0	2.185366	-3.436008	-0.763192
61	6	0	1.605128	-2.995290	-1.989508
62	6	0	2.620810	-2.278500	-2.737611
63	6	0	2.273756	-1.162525	-3.474646
64	6	0	0.895412	-0.713358	-3.491092
65	6	0	-0.125080	-1.448133	-2.841537
66	6	0	-1.269275	-0.712449	-2.435080
67	6	0	-2.139411	-1.158611	-1.380427
68	6	0	-1.792183	-2.257576	-0.653904
69	6	0	-0.568148	-2.968685	-0.955487
70	6	0	0.239542	-2.630791	-2.068666
71	6	0	-4.410626	0.000020	-1.529073
72	1	0	-4.295164	0.000044	-2.616874
73	6	0	-5.126001	1.228688	-1.020480
74	6	0	-5.551500	2.309271	-1.783523
75	1	0	-5.404540	2.311398	-2.861194
76	6	0	-6.164953	3.392795	-1.149086
77	1	0	-6.504399	4.240325	-1.737743
78	6	0	-6.336183	3.394659	0.234924
79	1	0	-6.810102	4.242896	0.720522
80	6	0	-5.897061	2.312741	1.002511
81	1	0	-6.019133	2.316031	2.083299
82	6	0	-5.299958	1.229536	0.368626
83	6	0	-4.733154	-0.000004	1.037918
84	1	0	-4.891516	-0.000022	2.120561
85	6	0	-5.299961	-1.229523	0.368588
86	6	0	-5.897072	-2.312736	1.002456
87	1	0	-6.019150	-2.316037	2.083243

88	6	0	-6.336171	-3.394653	0.234858
89	1	0	-6.810089	-4.242898	0.720441
90	6	0	-6.164927	-3.392776	-1.149154
91	1	0	-6.504362	-4.240304	-1.737819
92	6	0	-5.551464	-2.309249	-1.783569
93	1	0	-5.404487	-2.311359	-2.861239
94	6	0	-5.125974	-1.228669	-1.020513

ICMA (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.197722	-1.411232	-1.132343
2	1	0	-4.305547	-1.755271	-2.162745
3	6	0	-5.110551	-0.286871	-0.701110
4	6	0	-5.818278	0.668012	-1.415451
5	1	0	-5.808696	0.679565	-2.502761
6	6	0	-6.555635	1.617601	-0.697610
7	1	0	-7.133087	2.365725	-1.233465
8	6	0	-6.555647	1.617444	0.697852
9	1	0	-7.133109	2.365446	1.233865
10	6	0	-5.818303	0.667695	1.415492
11	1	0	-5.808739	0.679006	2.502805
12	6	0	-5.110564	-0.287029	0.700950
13	6	0	-4.197739	-1.411485	1.131947
14	1	0	-4.305582	-1.755753	2.162271
15	6	0	-4.439955	-2.429355	-0.000311
16	1	0	-5.461556	-2.818635	-0.000361
17	1	0	-3.729867	-3.263151	-0.000398
18	6	0	0.345250	-3.231353	-1.176320
19	6	0	-0.976672	-2.846894	-0.741427
20	6	0	-1.684876	-1.895023	-1.431205
21	6	0	-1.082622	-1.269368	-2.576683
22	6	0	0.179957	-1.645532	-3.027416
23	6	0	0.914511	-2.655025	-2.309399
24	6	0	1.160884	-3.470606	-0.000384
25	6	0	0.345227	-3.231621	1.175591
26	6	0	-0.976686	-2.847065	0.740759
27	6	0	-1.684901	-1.895349	1.430739
28	6	0	-2.718060	-0.962302	-0.803429
29	6	0	-1.467213	0.129025	-2.578233
30	6	0	-0.572720	1.096602	-3.028945
31	6	0	0.751763	0.704383	-3.481139
32	6	0	1.118860	-0.633027	-3.481227
33	6	0	2.441892	-1.024014	-3.031575
34	6	0	2.314373	-2.275017	-2.304658
35	6	0	3.092399	-2.503378	-1.176802
36	6	0	2.503150	-3.119011	-0.000331
37	6	0	0.914466	-2.655547	2.308811
38	6	0	2.314327	-2.275538	2.304180
39	6	0	3.092373	-2.503640	1.176288
40	6	0	4.032888	-1.497546	0.726948
41	6	0	4.032905	-1.497383	-0.727219
42	6	0	4.153754	-0.299914	-1.420713
43	6	0	3.340975	-0.057525	-2.598074
44	6	0	2.956081	1.342832	-2.597645
45	6	0	1.689641	1.715581	-3.031080
46	6	0	-2.305717	0.360699	-1.434813
47	6	0	0.674032	3.549344	0.000409
48	6	0	-0.657975	3.161332	0.000353
49	6	0	-1.240222	2.542347	1.176241
50	6	0	-0.456568	2.337507	2.309593
51	6	0	0.941285	2.725781	2.305159
52	6	0	2.816297	2.931399	0.727439
53	6	0	2.816312	2.931566	-0.726720
54	6	0	1.494892	3.318042	-1.176011
55	6	0	0.941331	2.726301	-2.304521
56	6	0	-0.456521	2.338030	-2.309067
57	6	0	-1.240196	2.542608	-1.175682
58	6	0	-2.183299	1.539102	0.741453
59	6	0	-2.305745	0.360375	1.434853
60	6	0	-1.467265	0.128437	2.578236
61	6	0	-0.572776	1.095912	3.029179
62	6	0	0.751697	0.703592	3.481314
63	6	0	1.689581	1.714893	3.031498
64	6	0	2.956027	1.342240	2.598004
65	6	0	3.532564	1.964932	1.422135
66	6	0	3.532591	1.965257	-1.421620
67	6	0	4.273589	0.950638	-0.693902
68	6	0	4.273574	0.950479	0.694201
69	6	0	4.153723	-0.300237	1.420720
70	6	0	3.340920	-0.058117	2.598122
71	6	0	2.441836	-1.024705	3.031393
72	6	0	1.118794	-0.633818	3.481104
73	6	0	0.179898	-1.646220	3.027047
74	6	0	-1.082674	-1.269955	2.576374
75	6	0	-2.183283	1.539268	-0.741140
76	6	0	-2.718073	-0.962484	0.803158
77	6	0	1.494868	3.317774	1.176793

AICBA *e*-face *a* (in *m*-xylene, SMD)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.874722	4.706165	-1.131565
2	1	0	-1.153732	4.933726	-2.162399
3	6	0	0.509931	5.133263	-0.701268
4	6	0	1.662897	5.422891	-1.415478
5	1	0	1.669952	5.408329	-2.502767
6	6	0	2.822863	5.740429	-0.697837
7	1	0	3.734045	5.990148	-1.234442
8	6	0	2.822855	5.740440	0.697773
9	1	0	3.734032	5.990165	1.234384
10	6	0	1.662882	5.422911	1.415406
11	1	0	1.669924	5.408365	2.502695
12	6	0	0.509924	5.133274	0.701186
13	6	0	-0.874734	4.706183	1.131475
14	1	0	-1.153755	4.933762	2.162302
15	6	0	-1.727184	5.312239	-0.000055
16	1	0	-1.705246	6.405448	-0.000064
17	1	0	-2.766123	4.966862	-0.000057
18	6	0	1.450000	-2.335140	-1.170487
19	6	0	0.593281	-3.395488	-0.726027
20	6	0	-0.566135	-3.731694	-1.423652
21	6	0	-0.929338	-2.975501	-2.591980
22	6	0	-0.111961	-1.923684	-3.001920
23	6	0	1.098939	-1.609682	-2.281355
24	6	0	2.265676	-1.784589	0.000029
25	6	0	1.449989	-2.335119	1.170547
26	6	0	0.593273	-3.395474	0.726098
27	6	0	-0.566150	-3.731668	1.423717
28	6	0	-1.780501	-4.056343	-0.693596
29	6	0	-2.371324	-2.818279	-2.596366
30	6	0	-2.937403	-1.623382	-3.026108
31	6	0	-2.085844	-0.533730	-3.468166
32	6	0	-0.707822	-0.680398	-3.449976
33	6	0	0.139959	0.410873	-3.001446
34	6	0	1.250635	-0.138738	-2.284617
35	6	0	1.729462	0.509450	-1.169083
36	6	0	2.419279	-0.190321	0.000016
37	6	0	1.098916	-1.609641	2.281398
38	6	0	1.250612	-0.138697	2.284637
39	6	0	1.729451	0.509471	1.169096
40	6	0	1.122158	1.729719	0.738208
41	6	0	1.122165	1.729705	-0.738224
42	6	0	0.075362	2.295828	-1.435708
43	6	0	-0.439603	1.606617	-2.570346
44	6	0	-1.882793	1.755893	-2.576187
45	6	0	-2.689386	0.713274	-3.022231
46	6	0	-2.899244	-3.486677	-1.420690
47	6	0	-4.750299	0.465496	-0.000028
48	6	0	-4.915496	-0.914235	-0.000016
49	6	0	-4.557038	-1.687760	1.175516
50	6	0	-4.052543	-1.046845	2.301933
51	6	0	-3.895130	0.396171	2.305638
52	6	0	-3.393592	2.232578	0.741478
53	6	0	-3.393584	2.232565	-0.741552
54	6	0	-4.229186	1.137351	-1.174272
55	6	0	-3.895106	0.396129	-2.305684
56	6	0	-4.052519	-1.046887	-2.301954
57	6	0	-4.557026	-1.687781	-1.175531
58	6	0	-3.968887	-2.932272	0.726946
59	6	0	-2.899259	-3.486652	1.420726
60	6	0	-2.371351	-2.818232	2.596395
61	6	0	-2.937435	-1.623327	3.026110
62	6	0	-2.085881	-0.533667	3.468157
63	6	0	-2.689418	0.713328	3.022192
64	6	0	-1.882820	1.755939	2.576138
65	6	0	-2.249649	2.546688	1.431966
66	6	0	-2.249634	2.546663	-1.432032
67	6	0	-1.003471	3.166078	-0.802842
68	6	0	-1.003479	3.166093	0.802778
69	6	0	0.075346	2.295853	1.435670
70	6	0	-0.439630	1.606664	2.570315
71	6	0	0.139927	0.410927	3.001443
72	6	0	-0.707859	-0.680335	3.449984
73	6	0	-0.111993	-1.923629	3.001957
74	6	0	-0.929365	-2.975454	2.592028
75	6	0	-3.968880	-2.932285	-0.726932
76	6	0	-1.780508	-4.056330	0.693654
77	6	0	-4.229199	1.137373	1.174210
78	6	0	3.969533	0.155378	0.000019
79	1	0	4.093221	1.242707	0.000012
80	6	0	4.555999	-0.496681	-1.228994
81	6	0	5.134851	0.154178	-2.312081
82	1	0	5.222411	1.238361	-2.315757
83	6	0	5.598289	-0.600230	-3.393027
84	1	0	6.058771	-0.101592	-4.241179
85	6	0	5.468535	-1.988804	-3.390928
86	1	0	5.826539	-2.567401	-4.237836
87	6	0	4.872876	-2.640615	-2.307969
88	1	0	4.757246	-3.722103	-2.309979

89	6	0	4.423590	-1.890342	-1.228018
90	6	0	3.722235	-2.419169	0.000036
91	1	0	3.639127	-3.510179	0.000044
92	6	0	4.423587	-1.890325	1.228085
93	6	0	4.872876	-2.640584	2.308044
94	1	0	4.757247	-3.722072	2.310067
95	6	0	5.468535	-1.988759	3.390994
96	1	0	5.826542	-2.567345	4.237908
97	6	0	5.598287	-0.600185	3.393076
98	1	0	6.058771	-0.101536	4.241220
99	6	0	5.134848	0.154209	2.312121
100	1	0	5.222407	1.238392	2.315783
101	6	0	4.555994	-0.496664	1.229042