

H₂Ph₄TCHP⁺ - atomic coordinates

Model chemistry: B3LYP/6-31G

Stoichiometry C60H54N4 (1+,2)
Framework group C1[X(C60H54N4)]
Deg. of freedom 348
Full point group C1 NOP 1
Largest Abelian subgroup C1 NOP 1
Largest concise Abelian subgroup C1 NOP 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.408251	4.010706	-1.074366
2	6	0	0.900232	2.878980	-0.329991
3	6	0	-0.982286	3.902178	-1.152122
4	6	0	1.192286	5.077572	-1.797633
5	7	0	-0.189957	2.091566	-0.035888
6	6	0	-1.367022	2.694590	-0.454804
7	6	0	2.225589	2.606122	0.131000
8	1	0	2.143060	4.673423	-2.159747
9	6	0	0.371667	5.654279	-2.969703
10	1	0	1.455185	5.893404	-1.111060
11	6	0	-1.833745	4.834065	-1.981104
12	1	0	-0.141158	1.150160	0.329514
13	6	0	2.683578	1.323428	0.493028
14	1	0	0.294011	4.907364	-3.772301
15	6	0	-2.648783	2.197256	-0.114306
16	6	0	-1.034498	6.052276	-2.494589
17	6	0	3.164164	3.758260	0.214417
18	1	0	-2.704910	5.184600	-1.424707
19	1	0	-2.233688	4.270007	-2.837623
20	1	0	0.895096	6.520903	-3.389100
21	6	0	3.914418	0.979252	1.217856
22	7	0	2.037974	0.165668	0.070340
23	6	0	4.379337	3.741746	-0.499456
24	6	0	2.850328	4.885324	1.000563
25	6	0	-2.892690	0.871475	0.345538
26	1	0	-1.595707	6.532675	-3.303958
27	6	0	-3.810705	3.124908	-0.234719
28	1	0	-0.943156	6.795951	-1.689832
29	6	0	-4.831239	2.864578	-1.168378
30	6	0	2.891669	-0.872441	0.364082
31	6	0	-4.077397	0.379212	1.072516
32	6	0	5.252556	4.831053	-0.436681
33	1	0	4.624027	2.881186	-1.113301
34	6	0	4.055117	-0.386250	1.125943
35	6	0	4.798241	1.849681	2.077483
36	6	0	-3.907101	4.263216	0.588075
37	7	0	-2.029494	-0.165660	0.071715
38	6	0	3.737445	5.961874	1.081657
39	1	0	1.919622	4.904631	1.558539
40	6	0	2.653279	-2.195085	-0.108220
41	1	0	4.211155	2.647902	2.545835
42	6	0	-3.934273	-0.985108	1.168549
43	1	0	3.494284	6.815482	1.705533
44	6	0	-2.682806	-1.326409	0.476299
45	6	0	5.113768	-1.168679	1.865194
46	6	0	-5.170893	1.154224	1.767847
47	6	0	-5.919566	3.734836	-1.285596
48	1	0	5.557367	2.357179	1.467443
49	6	0	-5.007173	5.119391	0.483654
50	6	0	5.505933	1.000238	3.154883
51	1	0	-3.125740	4.466955	1.313346
52	6	0	4.937071	5.940350	0.358226
53	1	0	-4.763332	1.986975	-1.802946
54	1	0	6.176721	4.814741	-1.004702
55	6	0	-2.220600	-2.610541	0.125310
56	6	0	1.371268	-2.687095	-0.452416
57	1	0	-5.080075	5.985836	1.132505
58	6	0	-4.842653	-1.859264	1.998335
59	6	0	6.159926	-0.238382	2.520590

60	1	0	-5.662691	1.853818	1.087497
61	1	0	4.776812	0.683981	3.914363
62	6	0	-6.234169	0.218275	2.386289
63	1	0	-4.721331	1.774717	2.558808
64	6	0	3.813399	-3.117774	-0.242902
65	6	0	-6.012581	4.860343	-0.457128
66	1	0	5.620149	6.781267	0.413629
67	1	0	5.624767	-1.876792	1.208100
68	1	0	4.627031	-1.780379	2.641175
69	1	0	-6.694228	3.533399	-2.017914
70	1	0	6.258051	1.610445	3.668201
71	7	0	0.190467	-2.095861	-0.031245
72	6	0	-0.894219	-2.890482	-0.330242
73	6	0	0.996944	-3.888467	-1.159410
74	6	0	-3.161260	-3.762980	0.220066
75	1	0	6.727330	-0.802844	3.269515
76	6	0	-5.595350	-1.013594	3.047204
77	1	0	-4.267404	-2.651531	2.490107
78	6	0	4.884107	-2.787963	-1.098436
79	1	0	-6.862163	5.529419	-0.542662
80	6	0	3.867833	-4.319620	0.488680
81	1	0	-5.575025	-2.374189	1.362256
82	1	0	-6.832523	0.780982	3.112112
83	1	0	-6.925637	-0.116947	1.599820
84	1	0	6.882049	0.090274	1.759286
85	6	0	-0.391247	-4.021049	-1.074536
86	1	0	4.849062	-1.862140	-1.663236
87	6	0	-2.883368	-4.842631	1.082203
88	1	0	-4.897072	-0.690157	3.832248
89	6	0	1.859800	-4.806998	-1.988217
90	1	0	-6.360934	-1.628870	3.533834
91	1	0	3.052930	-4.574246	1.158760
92	1	0	0.130432	-1.157046	0.338772
93	6	0	4.972888	-5.167881	0.374920
94	6	0	-4.334085	-3.793399	-0.557672
95	6	0	5.975855	-3.650551	-1.229133
96	6	0	-5.203606	-4.885888	-0.483908
97	1	0	6.787440	-3.394959	-1.902094
98	6	0	-1.163708	-5.093191	-1.807379
99	1	0	2.676584	-4.245747	-2.453668
100	6	0	1.015343	-5.523729	-3.062095
101	6	0	-3.766583	-5.921884	1.171783
102	1	0	-1.981225	-4.826362	1.685431
103	1	0	-4.550822	-2.968033	-1.227908
104	1	0	2.340714	-5.561649	-1.351673
105	1	0	5.013790	-6.081809	0.958102
106	6	0	6.025570	-4.839125	-0.488752
107	1	0	-3.551332	-6.740493	1.850396
108	1	0	0.711874	-4.805606	-3.836745
109	6	0	-0.231746	-6.158202	-2.426973
110	6	0	-4.925312	-5.948960	0.384051
111	1	0	1.626774	-6.287496	-3.555670
112	1	0	6.878792	-5.502413	-0.582750
113	1	0	-1.754847	-4.616499	-2.604089
114	1	0	-1.886680	-5.584808	-1.153468
115	1	0	-6.095885	-4.907223	-1.100691
116	1	0	-5.605038	-6.792087	0.446558
117	1	0	-0.793040	-6.737221	-3.168906
118	1	0	0.084409	-6.866493	-1.647638
