Electronic Supplementary Information

for

How great is the stabilization of crowded polyphenylbiphenyls by London dispersion?

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1. DSC results

The melting temperatures, T_m, and the standard molar enthalpies of melting, $\Delta_{melt}H_m^0(T_m)$, at T_m, were determined using equations S1 and S2:

$$T_m = 0.99701 \cdot T_m(\text{onset}) + 1.5089 \quad \text{(S1)}$$

$$\Delta_{melt}H_m^0(T_m) = \varphi \cdot M_M / S \quad \text{(S2)}$$

where T_m(onset) is the onset temperature of the melting peak, φ is the measured heat flow area of the peak, M_M is the molar mass of the compound, and S is the DSC sensitivity, which was determined by previous calibration of the DSC and is a function of temperature. The standard molar entropies of melting, $\Delta_{melt}S_m^0(T_m)$, at T_m, were determined using equations S3:

$$\Delta_{melt}S_m^0(T_{fus}) = \Delta_{melt}H_m^0(T_m) / T_m \quad \text{(S3)}$$

The heat capacity corrections for the calculation of the standard molar enthalpies and entropies of melting at another temperature, T, were made according to equations S4 and S5:

$$\Delta_{melt}H_m^0(T) = \Delta_{melt}H_m^0(T_{melt}) + \Delta_{melt}C_{p,m}^0 \cdot (T - T_m) \quad \text{(S4)}$$

$$\Delta_{melt}S_m^0(T) = \Delta_{melt}S_m^0(T_m) + \Delta_{melt}C_{p,m}^0 \cdot \ln(T / T_m) \quad \text{(S5)}$$

where $\Delta_{melt}C_{p,m}^0$ is the change in the standard molar heat capacity upon melting, given by $\Delta_{melt}C_{p,m}^0 = C_{p,m}^0(\text{l}) - C_{p,m}^0(\text{cr})$, and its value was taken as +54.4 $J \cdot K^{-1} \cdot mol^{-1}$, according to the equation proposed by Sidgewick[S1] and recommended by Chickos;[S2] the associated uncertainty was taken as ± 20 $J \cdot K^{-1} \cdot mol^{-1}$. The DSC results are presented in tables S1–S3 and the uncertainties quoted are expanded uncertainties calculated as $u = 2 \cdot \sigma_m$, where σ_m is the standard deviation of the mean. The uncertainties of the calculated enthalpies and entropies of melting are the combined uncertainties considering equations S2 – S5.

Table S1. DSC results for the C_1 polymorph of decaphenylbiphenyl (**1**); S = (2.48 ± 0.10) μV·s·J^{-1}.

Exp.	m / mg	T_m / K	φ / μV·s·mg^{-1}
1	2.9171	603.75	156.3
2	2.9171	604.09	150.8
3	2.8571	604.13	153.5
4	6.3911	603.88	159.5
5	6.3911	604.08	161.7
6	6.3911	604.03	160.5
7	6.4054	603.93	155.1
8	6.4054	603.99	158.9
9	5.9950	603.93	169.0
10	5.9910	603.71	158.7
11	3.0917	603.76	166.1
12	3.0846	603.69	154.4
13	3.0775	603.69	155.2
14	4.8285	603.64	166.6
15	4.8205	603.77	153.5
16	4.8124	603.77	152.8
17	4.8044	603.81	153.3
18	4.6609	603.57	166.6
19	4.6527	603.53	167.2
20	4.6444	603.59	167.3
21	5.9025	603.92	163.2
22	5.8943	603.67	162.5
23	5.8860	603.69	163.1
24	4.8449	603.77	166.6
25	4.8374	603.74	159.5
26	4.8300	603.71	159.5
27	4.8225	603.87	160.4
average		**603.8 ± 0.1**	**160.1 ± 2.1**

Table S2. DSC results for the D_2 polymorph of decaphenylbiphenyl (**1**); S = (3.33 ± 0.10) μV·s·J^{-1}.

Exp.	m / mg	T_m / K	φ / μV·s·mg^{-1}
1	8.0914	563.40	199.1
2	5.1852	563.14	203.5
3	4.9961	563.25	205.7
4	3.3699	563.22	197.5
average		**563.3 ± 0.1**	**201.5 ± 3.8**

Table S3. DSC results for hexaphenylbiphenyl (**2**); S = (2.82 ± 0.10) μV·s·J^{-1}.

Exp.	m / mg	T_m / K	φ / μV·s·mg^{-1}
1	3.6270	634.50	332.3
2	3.1489	634.34	328.9
3	2.6707	634.32	335.6
4	2.2377	634.29	327.6
average		**634.4 ± 0.1**	**331.1 ± 3.6**

2. High-precision heat capacity drop calorimetry

Tables S4 presents the experimental results obtained for the compounds studied. In these tables N_{drop} is the total number of drops for each compound (each experiment has several drops), $A_{ampoule+sample}$ is the average normalized integrated area of the calorimetric peak, $T_{furnace}$ is the average temperature of the furnace, T_{cal} is the average temperature of the calorimeter, and <*T*> is the mean temperature of the experiments. The value of C_p, at <*T*> ≅ 298.15 K, is calculated according to equation (S6):

$$C_{p,m}^{0} = \frac{\varepsilon \cdot (A_{ampoule+sample} - A_{ampoule}) \cdot M_M}{m_{sample}} \quad \text{(S6)}$$

where ε is the calibration constant (determined by calibration with α-Al_2O_3 pellets, NIST-RM 720), m_{sample} is the weighed mass of sample, $A_{ampoule+sample}$ and $A_{ampoule}$ are the normalized integrated areas of the filled and empty (blank) ampoules, respectively (both are the average of the corresponding N_{drop} measurements), and M_M is the molar mass of the compound. In all experiments <*T*> is around 298.2 K, which is ≈ 298.15 K. Since the samples were measured in different periods of time, the values of $A_{ampoule}$ and ε are not necessarily the same for all the measurements. In the main manuscript, the results of $C_{p,m}^{0}$(cr) are shown as the mean and the standard deviation of the mean. The errors in the heat capacity values were calculated by applying propagation of uncertainty to equation S6.

Table S4. Experimental results obtained by Drop calorimetry for the compounds studied.

Compound	N_{drop}	m / g	$T_{furnace}$ / K	T_{cal} / K	<*T*> / K	$A_{ampoule+sample}$ / V·s·K^{-1}
decaphenylbiphenyl (**1**), C_1 [a]	37	0.26038	303.24	293.17	298.20	0.25784 ± 0.00017
decaphenylbiphenyl (**1**), D_2 [b]	39	0.21842	303.17	293.18	298.18	0.25139 ± 0.00007
hexaphenylbiphenyl (**2**) [b]	31	0.19150	303.12	293.18	298.15	0.24500 ± 0.00011

[a] ε = (6.676 ± 0.024) W·V^{-1}, $A_{ampoule}$ = (0.21360 ± 0.00017) V·s·K^{-1}.
[b] ε = (6.647 ± 0.019) W·V^{-1}, $A_{ampoule}$ = (0.21248 ± 0.00013) V·s·K^{-1}.

3. Vapor pressure measurements by Knudsen/Quartz crystal effusion

During the effusion experiment, the rate of mass loss from the Knudsen effusion cell, $(dm(\text{cell})/dt)$, is proportional to the rate of change of the mass deposited on the quartz crystal, (dm/dt), as shown by equation (S7):

$$\left(\frac{dm(\text{cell})}{dt}\right) = g \cdot \left(\frac{dm}{dt}\right) = g \cdot \frac{A_\text{q}}{S_\text{q}} \cdot \left(\frac{df}{dt}\right) \tag{S7}$$

where g is a geometric factor of the mass detection, A_q is the area of the quartz crystal, S_q is the mass sensitivity of the crystal, and (df/dt) is the rate of change of the resonance frequency of the quartz crystal. Taking $W = -S_\text{q} / (A_\text{q} \cdot g)$, where W is defined as the effective mass sensitivity coefficient, equation (S7) becomes:

$$\left(\frac{df}{dt}\right) = -W \cdot \left(\frac{dm(\text{cell})}{dt}\right) \tag{S8}$$

To derive the vapor pressure, p, the value of W must be known for each compound. This value can be determined by weighing the total mass loss of the Knudsen cell, $\Delta m(\text{cell})$, during the experiment, and using equation (S9):

$$W = -\frac{\Delta f}{\Delta m(\text{cell})} \tag{S9}$$

where Δf is the total change in the crystal's resonance frequency in the whole experiment. The vapor pressures at each temperature are subsequently obtained from equation (S10):

$$p = -\left(\frac{df}{dt}\right) \cdot \frac{1}{w_\text{o} \cdot A_\text{o} \cdot W} \cdot \left(\frac{2 \cdot \pi \cdot R \cdot T}{M_\text{M}}\right)^{1/2} \tag{S10}$$

where M is the molar mass of the effusing vapor, R is the gas constant, 8.314 462 618 J mol^{-1} K^{-1},[S3] A_o is the area of the effusion orifice and w_o is the transmission probability factor, which is usually calculated by means of equation (S10), where l is the length of the effusion orifice and r its radius:

$$w_o = \{1 + (3l / 8r)\}^{-1} \tag{S11}$$

In this technique only one effusion cell is used, with l = 0.0125 mm and r = 0.500 mm, giving A_o = 0.7854 mm^2 and w_o = 0.9907.

The $\ln p = f(1 / T)$ results were fitted using the integrated linear form of the Clausius-Clapeyron equation:

$$\ln(p / p^*) = a - b / T \tag{S12}$$

where $b = \Delta_{cr}^{g} H_m^0(\langle T \rangle) / R$, and p^* = 1 Pa. The mean temperature, <T>, was taken as the average temperature concerning all the experimental data points, and <p> (denoted $p(\langle T \rangle)$ in the tables that follow) is the pressure at that temperature, given by the ln $p = f(1/T)$ linear regression. $\Delta_{cr}^{g} S_m^0(\langle T \rangle)$ was then calculated according to the following equation:

$$\Delta_{cr}^{g} S_m^0(\langle T \rangle) = \Delta_{cr}^{g} S_m(\langle T \rangle, \langle p \rangle) + R \cdot \ln\left(\frac{\langle p \rangle}{10^5}\right) \tag{S13}$$

Table S5. Experimental results obtained for the sublimation of decaphenylbiphenyl (**1**), C_1 polymorph, in the Knudsen/Quartz crystal effusion apparatus.

Exp.	T / K	T^{-1} / K^{-1}	$(df/dt)_{corr}$ / Hz·s^{-1}	p / Pa	ln (p / p*)
1	547.09	0.0018279	-0.7131	0.2524	-1.3769
	549.04	0.0018214	-0.8356	0.2962	-1.2166
	551.00	0.0018149	-0.9795	0.3479	-1.0559
	552.91	0.0018086	-1.1493	0.4089	-0.8943
	554.85	0.0018023	-1.3418	0.4782	-0.7377
	556.78	0.0017960	-1.5677	0.5597	-0.5803
	558.74	0.0017898	-1.8226	0.6519	-0.4279
	Δm / mg	38.95	W / Hz·mg^{-1}	641.7	
2	542.77	0.0018424	-0.5013	0.1774	-1.7294
	544.69	0.0018359	-0.5866	0.2079	-1.5705
	546.65	0.0018293	-0.6863	0.2437	-1.4118
	548.57	0.0018229	-0.8035	0.2858	-1.2524
	550.51	0.0018165	-0.9377	0.3342	-1.0961
	552.49	0.0018100	-1.0939	0.3905	-0.9403
	Δm / mg	23.89	W / Hz·mg^{-1}	639.3	
3	544.66	0.0018360	-0.6077	0.2118	-1.5523
	546.58	0.0018296	-0.7099	0.2478	-1.3951
	548.53	0.0018230	-0.8277	0.2894	-1.2399
	550.47	0.0018166	-0.9665	0.3385	-1.0831
	552.41	0.0018103	-1.1276	0.3957	-0.9271
	554.38	0.0018038	-1.3143	0.4620	-0.7721
	556.31	0.0017976	-1.5322	0.5396	-0.6170
	558.26	0.0017913	-1.7932	0.6326	-0.4580
	Δm / mg	30.56	W / Hz·mg^{-1}	650.4	

[a] Standard uncertainty of the temperature is $u(T/\mathrm{K}) = 0.02$ and of the Knudsen vapor pressures are $u(p/\mathrm{Pa}) = 0.005$.

Table S6. Experimental results for the C_1 polymorph of decaphenylbiphenyl (**1**), where a and b are from the Clausius-Clapeyron equation $\ln\left(p/\mathrm{Pa}\right) = a - b\cdot\left(\mathrm{K}/T\right)$, and $b = \Delta^{g}_{cr}H_m\left(\langle T\rangle\right)/R$.

Exp.	a	b / K	R^2	$\langle T\rangle$ / K	$p\left(\langle T\rangle\right)$ / Pa	$\Delta^{g}_{cr}H^{0}_{m}\left(\langle T\rangle\right)$ / kJ·mol^{-1}	$\Delta^{g}_{cr}S^{0}_{m}\left(\langle T\rangle\right)$ / J·K^{-1}·mol^{-1}
1	44.31 ± 0.12	-24994 ± 69	0.99996	552.91	0.4081	207.8 ± 0.6	272.7 ± 1.0
2	43.17 ± 0.09	-24371 ± 50	0.99998	547.61	0.2640	202.6 ± 0.4	263.2 ± 0.8
3	43.27 ± 0.13	-24413 ± 71	0.9999	551.45	0.3669	203.0 ± 0.6	264.0 ± 1.1
Global results				550.66		204.5 ± 0.5	266.6 ± 1.0

Table S7. Experimental results obtained for the sublimation of hexaphenylbiphenyl (**2**) in the Knudsen/Quartz crystal effusion apparatus.

Exp.	T / K	T^{-1} / K^{-1}	$(df/dt)_{corr}$ / Hz·s^{-1}	p / Pa	ln (p / p*)
1	524.09	0.0019081	-0.3779	0.1376	-1.9836
	526.02	0.0019011	-0.4477	0.1632	-1.8125
	527.97	0.0018940	-0.5286	0.1931	-1.6444
	529.94	0.0018870	-0.6228	0.2279	-1.4786
	531.90	0.0018800	-0.7343	0.2693	-1.3120
	533.89	0.0018730	-0.8636	0.3173	-1.1479
	535.88	0.0018661	-1.0155	0.3738	-0.9841
	Δm / mg	14.30	W / Hz·mg^{-1}	747.5	
2	522.85	0.0019126	-0.3178	0.1142	-2.1700
	525.75	0.0019020	-0.4061	0.1463	-1.9221
	528.66	0.0018916	-0.5191	0.1876	-1.6736
	531.61	0.0018811	-0.6636	0.2404	-1.4254
	534.57	0.0018707	-0.8462	0.3074	-1.1795
	537.53	0.0018604	-1.0780	0.3927	-0.9346
	540.50	0.0018501	-1.3746	0.5022	-0.6888
	543.51	0.0018399	-1.7559	0.6433	-0.4412
	Δm / mg	19.95	W / Hz·mg^{-1}	756.4	
3	525.75	0.0019020	-0.3716	0.1346	-2.0057
	528.66	0.0018916	-0.4755	0.1727	-1.7563
	531.61	0.0018811	-0.6068	0.2210	-1.5098
	534.57	0.0018707	-0.7705	0.2814	-1.2681
	537.53	0.0018604	-0.9802	0.3589	-1.0246
	540.50	0.0018501	-1.2487	0.4585	-0.7798
	543.51	0.0018399	-1.5922	0.5862	-0.5340
	546.50	0.0018298	-2.0263	0.7481	-0.2902
	Δm / mg	23.40	W / Hz·mg^{-1}	752.6	

[a] Standard uncertainty of the temperature is $u(T/\mathrm{K}) = 0.02$ and of the Knudsen vapor pressures are $u(p/\mathrm{Pa}) = 0.005$.

Table S8. Experimental results for hexaphenylbiphenyl (**2**), where a and b are from the Clausius-Clapeyron equation $\ln\left(p/\mathrm{Pa}\right) = a - b\cdot\left(\mathrm{K}/T\right)$, and $b = \Delta_{cr}^{g}H_{m}\left(\langle T\rangle\right)/R$.

Exp.	a	b / K	R^2	$\langle T\rangle$ / K	$p\left(\langle T\rangle\right)$ / Pa	$\Delta_{cr}^{g}H_{m}^{0}\left(\langle T\rangle\right)$ / kJ·mol^{-1}	$\Delta_{cr}^{g}S_{m}^{0}\left(\langle T\rangle\right)$ / J·K^{-1}·mol^{-1}
1	43.39 ± 0.12	-23777 ± 61	0.99997	529.96	0.2281	197.7 ± 0.5	265.0 ± 1.0
2	43.27 ± 0.08	-23757 ± 44	0.99998	533.12	0.2733	197.5 ± 0.4	264.0 ± 0.7
3	43.09 ± 0.11	-23708 ± 61	0.99996	536.08	0.3202	197.1 ± 0.5	262.5 ± 1.0
Global results				533.05		197.4 ± 0.5	263.8 ± 0.9

Table S9. Experimental results obtained for the sublimation of 1,2,3,5-tetraphenylbenzene (**7**) in the Knudsen/Quartz crystal effusion apparatus.

Exp.	T / K	T^{-1} / K^{-1}	$(df/dt)_{corr}$ / Hz·s^{-1}	p / Pa	ln (p / p*)
1	429.84	0.0023264	-0.2379	0.1016	-2.2869
	432.78	0.0023106	-0.3221	0.1380	-1.9806
	435.71	0.0022951	-0.4293	0.1845	-1.6899
	438.65	0.0022797	-0.5739	0.2475	-1.3963
	441.61	0.0022644	-0.7654	0.3312	-1.1050
	444.56	0.0022494	-1.0135	0.4400	-0.8209
	447.50	0.0022347	-1.3365	0.5822	-0.5410
	450.42	0.0022202	-1.7564	0.7676	-0.2645
	453.33	0.0022059	-2.2924	1.0050	0.005022
	Δm / mg	24.40	W / Hz·mg^{-1}	729.4	
2	428.93	0.0023314	-0.2196	0.0936	-2.3691
	431.83	0.0023157	-0.2947	0.1260	-2.0715
	434.77	0.0023001	-0.3935	0.1688	-1.7789
	437.68	0.0022848	-0.5239	0.2255	-1.4894
	440.61	0.0022696	-0.6973	0.3011	-1.2002
	443.55	0.0022545	-0.9281	0.4022	-0.9109
	Δm / mg	17.35	W / Hz·mg^{-1}	730.0	
3	432.63	0.0023114	-0.2940	0.1255	-2.0757
	434.64	0.0023008	-0.3580	0.1531	-1.8765
	436.63	0.0022903	-0.4347	0.1864	-1.6800
	438.62	0.0022799	-0.5296	0.2276	-1.4803
	440.61	0.0022696	-0.6424	0.2767	-1.2849
	442.62	0.0022593	-0.7796	0.3365	-1.0891
	444.58	0.0022493	-0.9377	0.4057	-0.9022
	446.54	0.0022394	-1.1340	0.4917	-0.7099
	448.51	0.0022296	-1.3716	0.5960	-0.5175
	Δm / mg	27.13	W / Hz·mg^{-1}	732.0	

[a] Standard uncertainty of the temperature is $u(T/\mathrm{K}) = 0.02$ and of the Knudsen vapor pressures are $u(p/\mathrm{Pa}) = 0.005$.

Table S10. Experimental results for 1,2,3,5-tetraphenylbenzene (**7**), where a and b are from the Clausius-Clapeyron equation $\ln\left(p / \mathrm{Pa}\right) = a - b \cdot \left(\mathrm{K} / T\right)$, and $b = \Delta_{cr}^{g} H_{m}\left(\langle T \rangle\right) / R$.

Exp.	a	b / K	R^2	$\langle T \rangle$ / K	$p\left(\langle T \rangle\right)$ / Pa	$\Delta_{cr}^{g} H_{m}^{0}\left(\langle T \rangle\right)$ / kJ·mol^{-1}	$\Delta_{cr}^{g} S_{m}^{0}\left(\langle T \rangle\right)$ / J·K^{-1}·mol^{-1}
1	41.92 ± 0.03	-19001 ± 15	0.999996	441.60	0.3304	158.0 ± 0.1	252.8 ± 0.3
2	41.82 ± 0.09	-18953 ± 37	0.99998	436.23	0.1957	157.6 ± 0.3	252.0 ± 0.7
3	41.90 ± 0.09	-19027 ± 41	0.99997	440.60	0.2767	158.2 ± 0.3	252.7 ± 0.8
Global results				439.47		157.9 ± 0.3	252.5 ± 0.6

Standard molar quantities of sublimation at T = 298.15 K

The standard molar enthalpy of sublimation, $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{0}$, at T = 298.15 K is determined by equation S14:

$$\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}^{0}(298.15\ \mathrm{K}) = \Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}(\langle T\rangle) + (298.15 - \langle T\rangle)\cdot \Delta_{\mathrm{cr}}^{\mathrm{g}}C_{p,\mathrm{m}}^{0} \quad \text{(S14)}$$

since the dependence of $\Delta_{\mathrm{cr}}^{\mathrm{g}}H_{\mathrm{m}}$ on pressure is negligible, and where:

$$\Delta_{\mathrm{cr}}^{\mathrm{g}}C_{p,\mathrm{m}}^{0} = C_{p,\mathrm{m}}^{\mathrm{o}}(\mathrm{g}) - C_{p,\mathrm{m}}^{\mathrm{o}}(\mathrm{cr}) \quad \text{(S15)}$$

The values of $\Delta_{\mathrm{cr}}^{\mathrm{g}}C_{p,\mathrm{m}}^{0}$ are presented in Table 4 of the main manuscript. The standard molar entropy of sublimation, $\Delta_{\mathrm{cr}}^{\mathrm{g}}S_{\mathrm{m}}^{0}$, at T = 298.15 K, was calculated according to equation S16:

$$\Delta_{cr}^{g}S_{m}^{0}(298.15K) = \Delta_{cr}^{g}S_{m}(\langle T\rangle, p(\langle T\rangle)) + \Delta_{cr}^{g}C_{p,m}^{\ 0}\cdot \ln(298.15/\langle T\rangle) - R\cdot \ln\{p^{0}/p(\langle T\rangle)\} \quad \text{(S16)}$$

where p^{o} = 10^5 Pa. The standard molar Gibbs energy of sublimation, $\Delta_{\mathrm{cr}}^{\mathrm{g}}G_{\mathrm{m}}^{0}$, at T = 298.15 K, was calculated using equation S17:

$$\Delta_{cr}^{g}G_{m}^{0}(298.15K) = \Delta_{cr}^{g}H_{m}^{0}(298.15K) - 298.15\cdot \Delta_{cr}^{g}S_{m}^{0}(298.15K) \quad \text{(S17)}$$

4. Mini-bomb combustion calorimetry

The samples were pressed in the form of pellets and placed into the platinum crucible, and their apparent mass weighed on a Mettler Toledo, model UMT2, micro-balance with a resolution of 1 ± 10^{-7} g and estimated uncertainty of 5 ± 10^{-7} g. The electrical discharge for the ignition was made via a 2 cm long platinum wire (Goodfellow, mass fraction 0.999, $\Phi = 0.080$ mm) tied on both electrodes terminals and bent down to a "V" shape towards the pellets. A platinum sheet with an inverted U shape was placed above the crucible assemble to concentrate the heat, thus helping to prevent the formation of carbon residues. Ultra-pure water (0.050 cm^3) was added to the bomb before adjusting the head with an O-ring to the body of the mini-bomb by means of a retaining screw-ring. The bomb was purged four times and filled with ultra-pure oxygen up to a pressure of 3.04 MPa. The bomb was then placed in its support, equipped with an electrical contact for electrical discharge, and introduced into the cylindrical copper block, which contains a bean type thermistor ($R^0 = 4$ kΩ, at $T = 298.15$ K) for temperature measurement. Helium (mass fraction 0.9999) was used to fill the block up to 0.2 MPa, after purging, in order to improve heat conduction between the bomb and the block. The calorimetric system is surrounded by a thermostatic water bath, maintained at a constant temperature of (298.150 ± 0.001) K by a TRONAC temperature controller, model PTC-40. For data acquisition, a 6 ½ digits multimeter (Keithley, model 2000) interfaced to a PC was used to measure the resistance of the thermistor every 10 s, in four-wire measurement mode. The charging, firing circuit and voltage measurement across the 2000 μF discharger condenser, are done automatically by means of a set of Advantech data acquisition/automation modules, series 4000. Real time recording and displaying of data is achieved with a modified version of the LABTERMO software.[S4] The amount of carbon soot, when formed, is determined gravimetrically, and this is considered for the total energy involved in the combustion process based on the value of $\Delta_c u^0(C) = -33$ kJ·g^{-1}.[S5] The energy equivalent of the calorimeter, ε(calor) / J·K^{-1}, was obtained from calibration experiments made with benzoic acid (Calorimetric Standard NIST 39j).[S5]

Results

The products of combustion in the experiments consist of a gaseous phase and an aqueous mixture for which the thermodynamic properties are known. The values of $^{\Delta_c U_m^0}$ refer to the combustion reactions of the compounds, represented by the general equation:

$$C_aH_b\,(cr) + (a+b/4)\,O_2\,(g) \rightarrow a\,CO_2(g) + (b/2)\,H_2O(l) \qquad (S18)$$

The internal energy for the isothermal bomb process, ΔU(IBP), was calculated according to equation (S19):

$$\Delta U(\text{IBP}) = -\varepsilon(\text{calor})\cdot\Delta T_{ad} + (T_i - 298.15)\cdot\varepsilon_i + (298.15 - T_i - \Delta T_{ad})\cdot\varepsilon_f - \Delta U(\text{ign}) \qquad (S19)$$

where ΔT_{ad} is the calorimeter adiabatic temperature change corrected for the heat exchange and the work of stirring, calculated with the LABTERMO program using the Regnault-Pfaundler method, and applying a second order fitting for the initial and final periods as reported by Santos *et al.*[S4] The general combustion results for the compounds studied by combustion calorimetry are presented in tables S11 to S13. In these tables ΔU(IBP) does not include ΔU(ignition); m(cpd.) is the mass of compound burnt in each experiment; m(aux.) is the mass of the pellet of benzoic acid used as combustion auxiliary; T_i is the initial temperature; T_f is the final temperature; ε_i(cont.) is the energy equivalent of the contents in the initial state; ε_f(cont.) is the energy equivalent of the contents in the final state; ΔT_{ad} is the corrected adiabatic temperature rise; ΔU(IBP) is the energy change for the isothermal bomb process; ΔU(ignition) is the electric energy for the ignition; ΔU(aux.) is the energy of combustion of the auxiliary; ΔU_Σ represents the standard state, or Washburn, corrections; ΔU(carbon) is the energy of combustion of the carbon residue formed, and $\Delta_c u^o$ is the standard massic energy of combustion. The final result of $\Delta_c u^o$ is presented as $\langle\Delta_c u^o\rangle \pm \sigma_m(\Delta_c u^o)$; % error is calculated as: % error = $\sigma_m(\Delta_c u^o) / \langle\Delta_c u^o\rangle$, where σ_m is the standard deviation of the mean.

Table S11. Experimental results for the combustion of decaphenylbiphenyl (**1**), C_1 polymorph, at T = 298.15 K.

	1	2	3	4	5	6	7	8	9	10	11
m(cpd.) / mg	16.7225	17.6478	13.4329	11.8274	13.7139	15.7563	23.9207	10.0910	16.9253	15.0557	12.1256
m(aux.) / mg	---	---	---	---	---	---	---	6.9694	---	---	---
T_i / K	298.0626	298.0631	298.0608	298.0590	298.0609	298.0617	298.0626	298.0677	298.0685	298.0757	298.0718
T_f / K	298.3682	298.3852	298.3105	298.2795	298.3127	298.3486	298.4889	298.3388	298.3764	298.3533	298.3022
ΔT_{ad} / K	0.342241	0.361384	0.274473	0.242014	0.280401	0.322058	0.489052	0.301159	0.345978	0.307282	0.248183
ε_i (cont.) / (J·K^{-1})	1.011	1.012	1.007	0.973	0.975	0.978	0.986	0.980	0.979	0.977	0.974
ε_f (cont.) / (J·K^{-1})	1.035	1.038	1.027	0.991	0.995	1.001	1.022	1.002	1.004	0.999	0.991
$-\Delta U$(IBP) / J	666.055	703.340	533.955	470.648	545.425	626.672	952.017	585.912	673.242	597.775	482.649
ΔU(ignition) / J	0.735	0.748	0.800	0.858	0.871	0.784	0.802	0.828	0.819	0.894	0.876
$-\Delta U$(aux.) / J	---	---	---	---	---	---	---	184.371	---	---	---
ΔU_{Σ} / J	0.368	0.390	0.290	0.253	0.297	0.345	0.543	0.347	0.372	0.328	0.260
$-\Delta U$(carbon) / J	0.419	0.158	1.188	0.637	0.964	1.356	1.304	0.518	0.884	1.841	0.561
$-\Delta_c u^o$(cpd.) / J.g^{-1}	**39799.46**	**39807.65**	**39783.11**	**39791.91**	**39786.80**	**39803.49**	**39797.14**	**39775.46**	**39774.01**	**39771.24**	**39795.45**
$\langle\Delta_c u^o\rangle$ / J·g^{-1} = –39789.6 ± 3.7 (0.009 %)											

Table S12. Experimental results for the combustion of hexaphenylbiphenyl (**2**), at T = 298.15 K.

	1	2	3	4	5	6	7	8	9	10
m(cpd.) / mg	23.0097	22.8385	24.2918	20.9489	11.7312	16.8118	13.1366	21.5171	16.0390	15.9147
m(aux.) / mg	---	---	---	---	13.7415	---	---	---	---	---
T_i / K	298.0658	298.0652	298.0591	298.0661	298.0706	298.0693	298.0810	298.0725	298.0779	298.0730
T_f/ K	298.4787	298.4739	298.4940	298.4447	298.4481	298.3789	298.3260	298.4618	298.3740	298.3678
ΔT_{ad} / K	0.470654	0.467054	0.496537	0.428055	0.426992	0.343233	0.268673	0.440094	0.328061	0.325161
ε_i (cont.) / (J·K^{-1})	0.986	0.985	0.987	0.983	0.990	0.979	0.975	0.984	0.978	0.978
ε_f (cont.) / (J·K^{-1})	1.020	1.019	1.023	1.015	1.023	1.004	0.994	1.016	1.002	1.002
–ΔU(IBP) / J	915.646	908.597	966.071	832.640	830.600	667.380	522.078	856.092	637.806	632.162
ΔU(ignition) / J	1.326	1.360	1.328	1.335	1.306	1.333	1.369	1.338	1.347	1.341
–ΔU(aux.) / J	---	---	---	---	363.523	---	---	---	---	---
ΔU_Σ / J	0.518	0.513	0.550	0.467	0.521	0.368	0.282	0.481	0.349	0.347
–ΔU(carbon) / J	0.610	0.544	0.561	1.320	0.248	1.459	1.013	0.690	0.769	1.122
–$\Delta_c u^o$(cpd.) / J.g^{-1}	**39764.14**	**39751.14**	**39736.14**	**39753.14**	**39757.92**	**39728.26**	**39764.09**	**39762.49**	**39758.30**	**39736.86**
$\langle\Delta_c u^o\rangle$ / J·g^{-1} = –39751.2 ± 4.1 (0.010 %)										

Table S13. Experimental results for the combustion of 1,2,3,5-tetraphenylbenzene (**7**), at T = 298.15 K.

	1	2	3	4	5	6	7	8	9
m(cpd.) / mg	16.7537	13.4583	11.5199	19.1316	16.5581	16.3658	14.1550	20.0835	24.4392
m(aux.) / mg	---	---	---	---	---	---	---	---	---
T_i / K	298.0706	298.0724	298.0759	298.0657	298.0743	298.0714	298.0740	298.0756	298.0713
T_f/ K	298.3790	298.3261	298.2945	298.4154	298.3816	298.3751	298.3401	298.4431	298.5133
ΔT_{ad} / K	0.343931	0.276431	0.236435	0.392858	0.340152	0.336099	0.290952	0.412409	0.501760
ε_i (cont.) / (J·K^{-1})	0.979	0.975	0.973	0.982	0.979	0.979	0.976	0.983	0.988
ε_f (cont.) / (J·K^{-1})	1.005	0.996	0.991	1.011	1.004	1.004	0.998	1.014	1.025
$-\Delta U$(IBP) / J	668.742	537.189	459.304	764.094	661.464	653.353	565.559	802.213	976.259
ΔU(ignition) / J	1.332	1.374	1.334	1.304	1.247	1.461	1.294	1.279	1.319
$-\Delta U$(aux.) / J	---	---	---	---	---	---	---	---	---
$\Delta U_{\sum}$ / J	0.363	0.286	0.243	0.419	0.358	0.354	0.302	0.442	0.548
$-\Delta U$(carbon) / J	0.290	0.327	0.591	0.155	0.188	0.267	0.132	0.422	0.271
$-\Delta_c u^o$(cpd.) / J.g^{-1}	**39877.85**	**39884.13**	**39866.84**	**39891.16**	**39903.85**	**39882.69**	**39908.77**	**39908.99**	**39901.18**
$\langle\Delta_c u^o\rangle$ / J·g^{-1} = –39891.7 ± 5.0 (0.012 %)									

5. UV-Vis spectroscopy

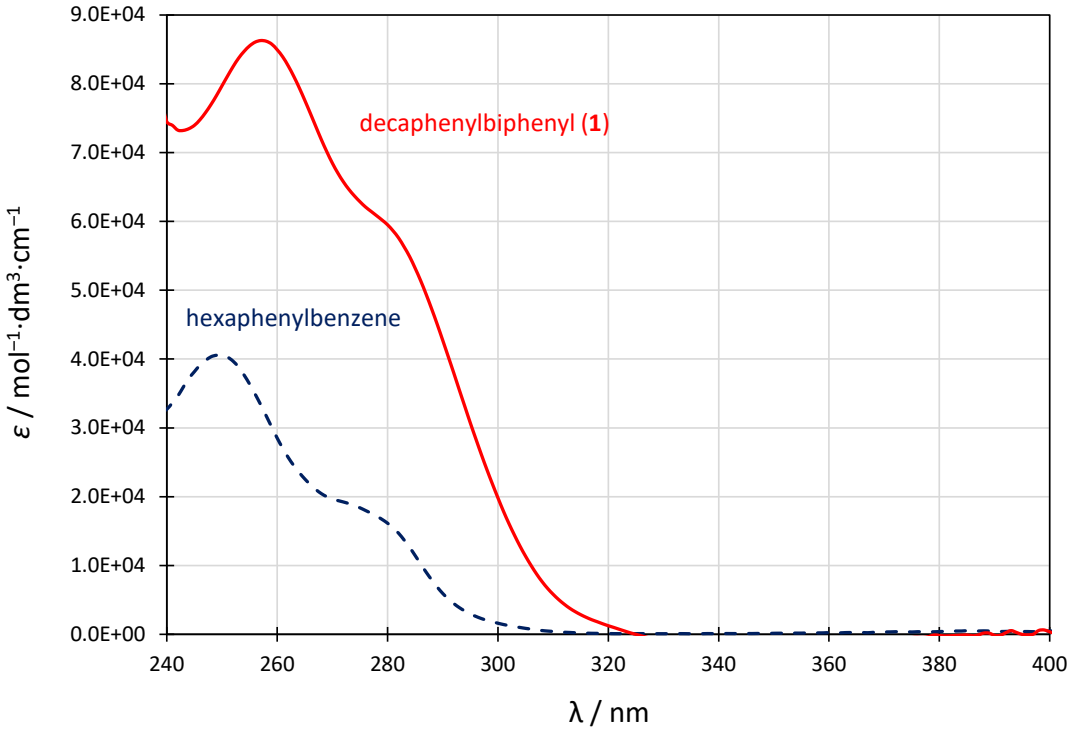
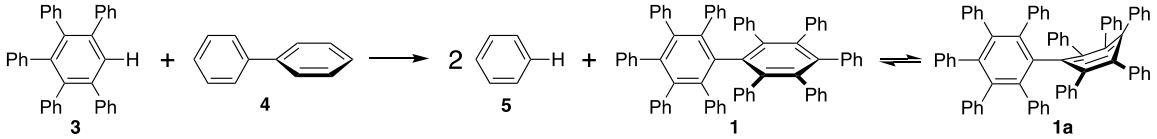


Figure S1. UV-Vis spectra of decaphenylbiphenyl (**1**) (red full line) and hexaphenylbenzene (blue dotted line) in CH_2Cl_2 at T = 298.1 K. The spectrum of compound **1** does not reveal significant bathochromic shifts relative to that of hexaphenylbenzene, thus supporting that there is no significant inter-ring electronic conjugation in **1**. Compound **1** has greater ε owing to the larger number of absorbing phenyl rings. Hexaphenylbenzene was commercially obtained from Sigma-Aldrich, washed with boiling acetone, and sublimed under reduced pressure.

6. Computational details: Full tabulation of computational data

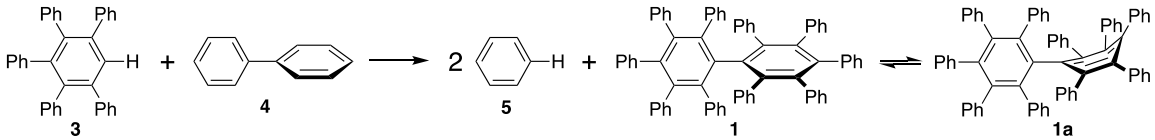
Table S14. Computationally Estimated Strain in Decaphenylbiphenyl.



Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)	nI[b]
At the B3PW91/6-311G(d,p) level								
5	D_{6h}	-232.213605		-232.113194		-232.107849		0
4	D_2	-463.230608		-463.049324		-463.039451		0
3	C_2	-1387.275064		-1386.771912		-1386.742718		0
1	D_2	-2773.316143		-2772.330237		-2772.272294		0
1a	C_1	-2773.311177		-2772.325541		-2772.267345		0
2 **3** + **4**		-3237.780736	0.0	-3236.593148	0.0	-3236.524887	0.0	
2 **5** + **1**		-3237.743353	+98.1	-3236.556625	+95.9	-3236.487992	**+96.9**	
2 **5** + **1a**		-3237.738387	+111.2	-3236.551929	+108.2	-3236.483043	+109.9	
At the B3PW91/6-311++G(2d,p) level								
5	D_{6h}	-232.222093		-232.121873		-232.116514		0
4	D_2	-463.247589		-463.066580		-463.056686		0
3	C_2	-1387.324868		-1386.822291		-1386.793069		0
1	D_2	-2773.413583		-2772.431651		-2772.373660		0
1a	C_1	-2773.409130		-2772.424288		-2772.366123		0
2 **3** + **4**		-3237.897325	0.0	-3236.711162	0.0	-3236.642824	0.0	
2 **5** + **1**		-3237.857769	+103.9	-3236.675397	+93.9	-3236.606688	**+94.9**	
2 **5** + **1a**		-3237.853316	+115.5	-3236.668034	+113.2	-3236.599151	+114.7	
At the M052X-D3/6-311G(d,p) level								
5	D_{6h}	-232.273771		-232.171780		-232.166479		0
4	D_2	-463.364930		-463.180581		-463.170844		0
3	C_2	-1387.724114		-1387.212502		-1387.183777		0
1	D_2	-2774.267924		-2773.265624		-2773.208576		0
1a	C_1	-2774.260689		-2773.258308		-2773.201017		0
2 **3** + **4**		-3238.813158	0.0	-3237.605585	0.0	-3237.538398	0.0	
2 **5** + **1**		-3238.815466	-6.1	-3237.609184	-9.4	-3237.541534	**-8.2**	
2 **5** + **1a**		-3238.808231	+12.9	-3237.601868	+9.8	-3237.533975	+11.6	

[a] 1 au = 2625.5 kJ/mol. [b] nI = number of imaginary frequencies.

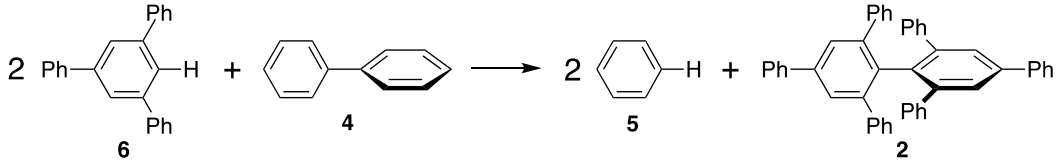
Table S14. (Continued)



Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)	nI[b]
At the M052X-D3/6-311++G(2d,p) level								
5	D_{6h}	-232.285170		-232.183150		-232.177850		0
4	D_2	-463.387612		-463.203156		-463.193427		0
3	C_2	-1387.789770		-1387.277759		-1387.249073		0
1	D_2	-2774.395513		-2773.392276		-2773.335316		0
1a	C_1	-2774.389017		-2773.385850		-2773.328622		0
2 **3** + **4**		-3238.967152	0.0	-3237.758674	0.0	-3237.691573	0.0	
2 **5** + **1**		-3238.965853	+3.4	-3237.758576	+0.3	-3237.691016	**+1.5**	
2 **5** + **1a**		-3238.959357	+20.5	-3237.752150	+17.1	-3237..684322	+19.0	
At the PW6B95-D3(BJ)/6-311G(d,p) level								
5	D_{6h}	-232.613888		-232.512672		-232.507347		0
4	D_2	-464.039883		-463.857169		-463.847363		0
3	C_2	1389.737312		-1389.230254		-1389.201217		0
1	D_2	-2778.292255		-2777.297771		-2777.240556		0
1a	C_1	-2778.284495		-2777.290215		-2777.232651		0
2 **3** + **4**		-3243.514507	0.0	-3242.317677	0.0	-3242.249797	0.0	
2 **5** + **1**		-3243.520031	-14.5	-3242.323115	-14.3	-3242.255250	**-14.3**	
2 **5** + **1a**		-3243.512271	+5.9	-3242.315559	+5.6	-3242.247345	+6.4	
At the PW6B95-D3(BJ)/6-311++G(2d,p) level								
5	D_{6h}	-232.622729		-232.521693		-232.516356		0
4	D_2	-464.057201		-463.874747		-463.864916		0
3	C_2	-1389.786780		-1389.279836		-1389.250882		0
1	D_2	-2778.387089		-2777.393356		-2777.336014		0
1a	C_1	-2778.379887		-2777.386217		-2777.328655		0
2 **3** + **4**		-3243.630761	0.0	-3242.434419	0.0	-3242.366680	0.0	
2 **5** + **1**		-3243.632547	-4.7	-3242.436742	-6.1	-3242.368726	**-5.4**	
2 **5** + **1a**		-3243.625345	+14.2	-3242.429603	+12.6	-3242.361367	+13.9	

[a] 1 au = 2625.5 kJ/mol. [b] nI = number of imaginary frequencies.

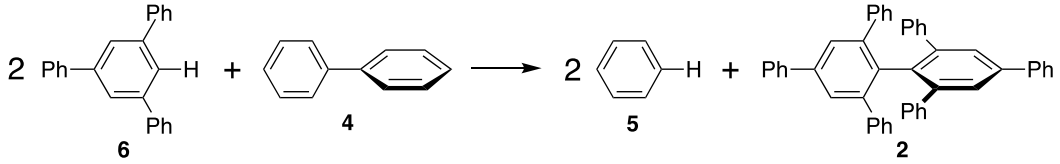
Table S15. Computationally Estimated Strain in Hexaphenylbiphenyl.



Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)	*n*I[b]
At the B3PW91/6-311G(d,p) level								
5	D_{6h}	-232.213605		-232.113194		-232.107849		0
4	D_2	-463.230608		-463.049324		-463.039451		0
6	D_3	-925.264467		-924.921895		-924.902488		0
2	D_2	-1849.307383		-1848.642415		-1848.603910		0
2 **6** + **4**		-2313.759542	0.0	-2312.893114	0.0	-2312.844427	0.0	
2 **5** + **2**		-2313.734593	+65.5	-2312.868803	+63.8	-2312.819608	+65.2	
At the B3PW91/6-311++G(2d,p) level								
5	D_{6h}	-232.222093		-232.121873		-232.116514		0
4	D_2	-463.247589		-463.066580		-463.056686		0
6	D_3	-925.298328		-924.956235		-924.936791		0
2	D_2	-1849.373202		-1848.709005		-1848.670439		0
2 **6** + **4**		-2313.844245	0.0	-2312.979050	0.0	-2312.930268	0.0	
2 **5** + **2**		-2313.817388	+70.5	-2312.952751	+69.0	-2312.903467	+70.4	
At the M052X-D3/6-311G(d,p) level								
5	D_{6h}	-232.273771		-232.171780		-232.166479		0
4	D_2	-463.364930		-463.180581		-463.170844		0
6	D_3	-925.547899		-925.199779		-925.180610		0
2	D_2	-1849.919125		-1849.242511		-1849.204839		0
2 **6** + **4**		-2314.460728	0.0	-2313.580139	0.0	-2313.532064	0.0	
2 **5** + **2**		-2314.466667	-15.6	-2313.586071	-15.6	-2313.537797	-15.1	

[a] 1 au = 2625.5 kJ/mol. [b] *n*I = number of imaginary frequencies.

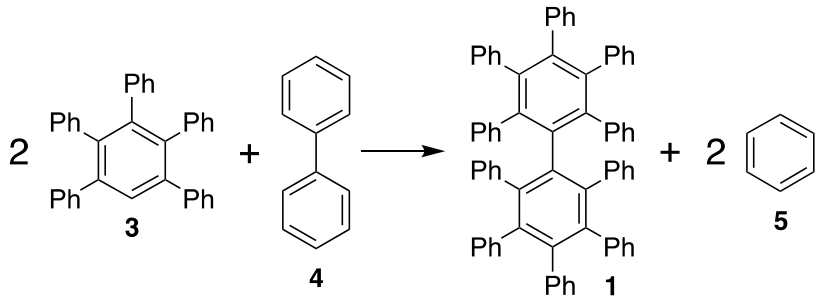
Table S15. (Continued)



Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)	*n*I[b]
At the M052X-D3/6-311++G(2d,p) level								
5	D_{6h}	-232.285170		-232.183150		-232.177850		0
4	D_2	-463.387612		-463.203156		-463.193427		0
6	D_3	-925.593101		-925.244634		-925.225515		0
2	D_2	-1850.005618		-1849.328581		-1849.290886		0
2 **6** + **4**		-2314.573814	0.0	-2313.692424	0.0	-2313.644457	0.0	
2 **5** + **2**		-2314.575958	-5.6	-2313.694881	-6.5	-2313.646586	-5.6	
At the PW6B95-D3(BJ)/6-311G(d,p) level								
5	D_{6h}	-232.613888		-232.512672		-232.507347		0
4	D_2	-464.039883		-463.857169		-463.847363		0
6	D_3	-926.892684		-926.547173		-926.527959		0
2	D_2	-1852.605644		-1851.935219		-1851.897122		0
2 **6** + **4**		-2317.825251	0.0	-2316.951515	0.0	-2316.903281	0.0	
2 **5** + **2**		-2317.833420	-21.4	-2316.960563	-23.8	-2316.911816	-22.4	
At the PW6B95-D3(BJ)/6-311++G(2d,p) level								
5	D_{6h}	-232.622729		-232.521693		-232.516356		0
4	D_2	-464.057201		-463.874747		-463.864916		0
6	D_3	-926.926843		-926.581857		-926.562583		0
2	D_2	-1852.670073		-1851.999556		-1851.961768		0
2 **6** + **4**		-2317.910887	0.0	-2317.038461	0.0	-2316.989992	0.0	
2 **5** + **2**		-2317.915531	-12.2	-2317.042942	-11.8	-2316.994480	-11.8	

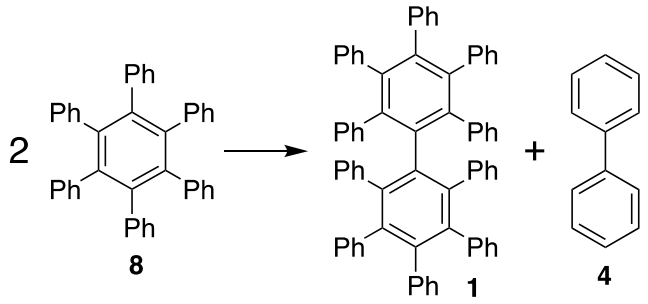
[a] 1 au = 2625.5 kJ/mol. [b] *n*I = number of imaginary frequencies.

Table S16. PW6B95-D3(BJ)/6-311++G(2d,p)-Calculated Enthalpies of Reaction for Homodesmotic Reactions R1-R6.



Reaction R1

Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
3	C_2	-1389.786780		-1389.279836		-1389.250882	
4	D_2	-464.057201		-463.874747		-463.864916	
1	D_2	-2778.387089		-2777.393356		-2777.336014	
5	D_{6h}	-232.622729		-232.521693		-232.516356	
2 **3** + **4**		-3243.630761	0.0	-3242.434419	0.0	-3242.366680	0.0
2 **5** + **1**		-3243.632547	-4.7	-3242.436742	-6.1	-3242.368726	**-5.4**

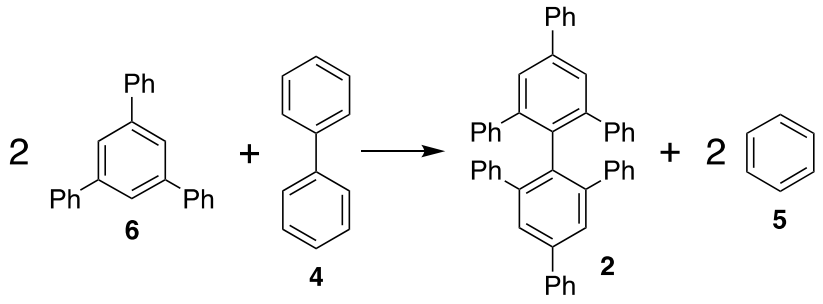


Reaction R2

Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
8	D_6	-1621.217197		-1620.629101		-1620.595372	
1	D_2	-2778.387089		-2777.393356		-2777.336014	
4	D_2	-464.057201		-463.874747		-463.864916	
2 **8**		-3242.434394	0.0	-3241.258202	0.0	-3241.190744	0.0
1 + **4**		-3242.444290	-26.0	-3241.268103	-26.0	-3241.200930	**-26.7**

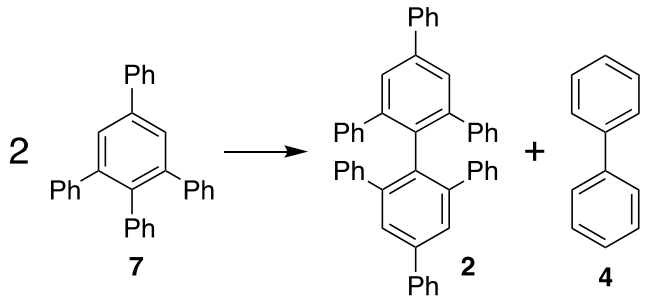
[a] 1 au = 2625.5 kJ/mol.

Table S16. PW6B95-D3(BJ)/6-311++G(2d,p)-Calculated Enthalpies of Reaction for Homodesmotic Reactions R1-R6 (continued).



Reaction R3

Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
6	D_3	-926.926843		-926.581857		-926.562583	
4	D_2	-464.057201		-463.874747		-463.864916	
2	D_2	-1852.670073		-1851.999556		-1851.961768	
5	D_{6h}	-232.622729		-232.521693		-232.516356	
2 **6** + **4**		-2317.910887	0.0	-2317.038461	0.0	-2316.989992	0.0
2 **5** + **2**		-2317.915531	-12.2	-2317.042942	-11.8	-2316.994480	**-11.8**

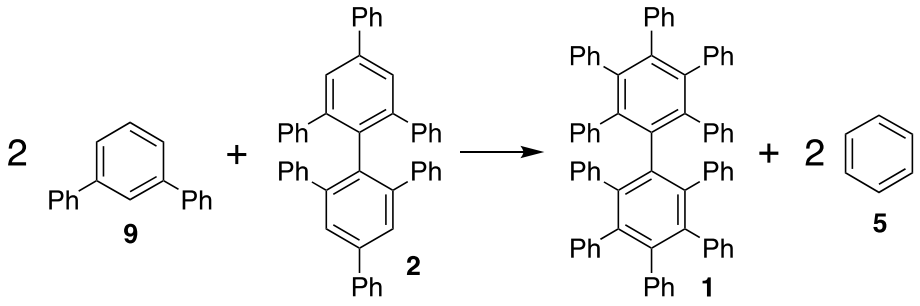


Reaction R4

Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
7	C_2	-1158.356794		-1157.930938		-1157.906802	
2	D_2	-1852.670073		-1851.999556		-1851.961768	
4	D_2	-464.057201		-463.874747		-463.864916	
2 **7**		-2316.713588	0.0	-2315.861876	0.0	-2315.813604	0.0
2 + **4**		-2316.727274	-35.9	-2315.874303	-32.6	-2315.826684	**-34.3**

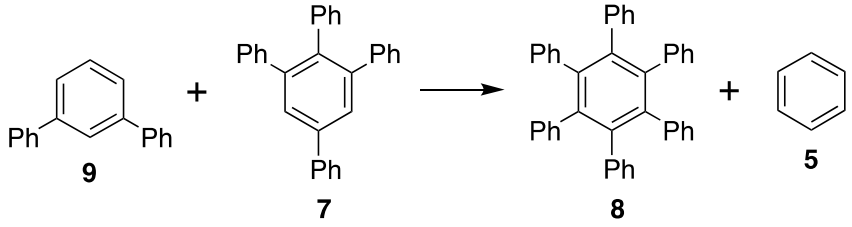
[a] 1 au = 2625.5 kJ/mol.

Table S16. PW6B95-D3(BJ)/6-311++G(2d,p)-Calculated Enthalpies of Reaction for Homodesmotic Reactions R1-R6 (continued).



Reaction R5

Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
9	C_2	-695.491929		-695.228156		-695.213666	
2	D_2	-1852.670073		-1851.999556		-1851.961768	
1	D_2	-2778.387089		-2777.393356		-2777.336014	
5	D_{6h}	-232.622729		-232.521693		-232.516356	
2 **9** + **2**		-3243.653931	0.0	-3242.455868	0.0	-3242.389100	0.0
2 **5** + **1**		-3243.632547	+56.1	-3242.436742	+50.2	-3242.368726	**+53.5**

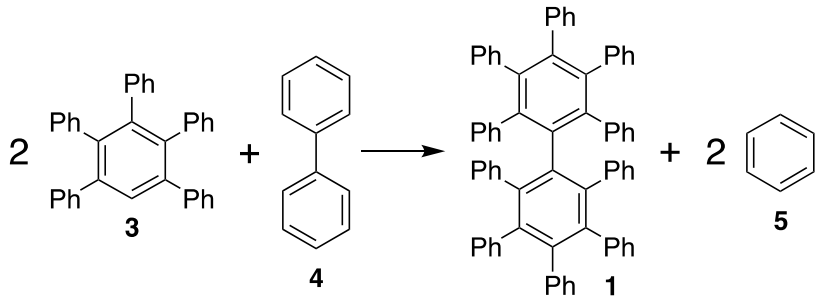


Reaction R6

Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
9	C_2	-695.491929		-695.228156		-695.213666	
7	C_2	-1158.356794		-1157.930938		-1157.906802	
8	D_6	-1621.217197		-1620.629101		-1620.595372	
5	D_{6h}	-232.622729		-232.521693		-232.516356	
9 + **7**		-1853.848723	0.0	-1853.159094	0.0	-1853.120468	0.0
8 + **5**		-1853.839926	+23.1	-1853.150794	+21.8	-1853.111728	**+22.9**

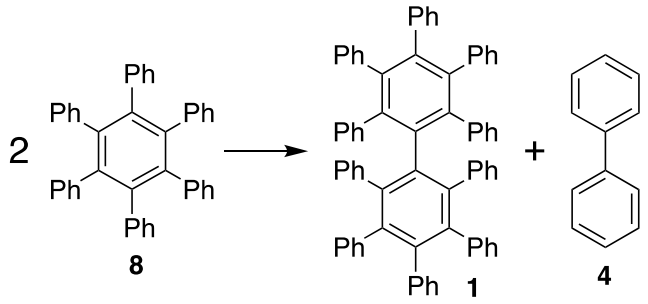
[a] 1 au = 2625.5 kJ/mol.

Table S17. M052X-D3/6-311++G(2d,p)-Calculated Enthalpies of Reaction for Homodesmotic Reactions R1-R6.



Reaction R1

Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
3	C_2	-1387.789770		-1387.277759		-1387.249073	
4	D_2	-463.387612		-463.203156		-463.193427	
1	D_2	-2774.395513		-2773.392276		-2773.335316	
5	D_{6h}	-232.285170		-232.183150		-232.177850	
2 **3** + **4**		-3238.967152	0.0	-3237.758674	0.0	-3237.691573	0.0
2 **5** + **1**		-3238.965853	+3.4	-3237.758576	+0.3	-3237.691016	**+1.5**

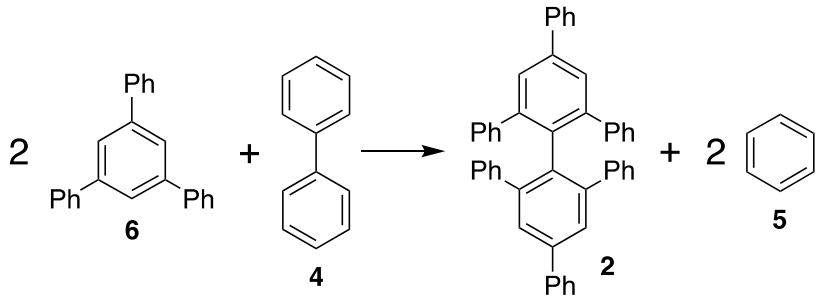


Reaction R2

Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
8	D_6	-1618.888222		-1618.294980		-1618.261375	
1	D_2	-2774.395513		-2773.392276		-2773.335316	
4	D_2	-463.387612		-463.203156		-463.193427	
2 **8**		-3237.776444	0.0	-3236.589960	0.0	-3236.522750	0.0
1 + **4**		-3237.783125	-17.5	-3236.595432	-14.4	-3236.528743	**-15.7**

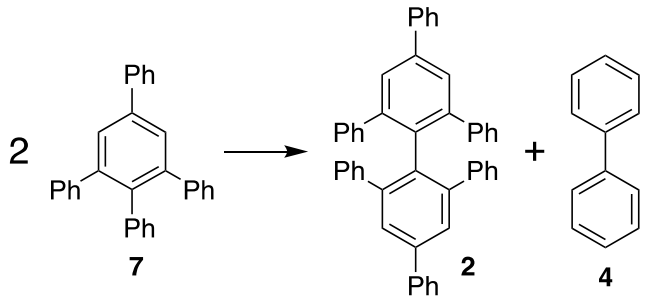
[a] 1 au = 2625.5 kJ/mol.

Table S17. M052X-D3/6-311++G(2d,p)-Calculated Enthalpies of Reaction for Homodesmotic Reactions R1-R6 (continued).



Reaction R3

Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
6	D_3	-925.593101		-925.244634		-925.225515	
4	D_2	-463.387612		-463.203156		-463.193427	
2	D_2	-1850.005618		-1849.328581		-1849.290886	
5	D_{6h}	-232.285170		-232.183150		-232.177850	
2 **6** + **4**		-2314.573814	0.0	-2313.692424	0.0	-2313.644457	0.0
2 **5** + **2**		-2314.575958	-5.6	-2313.694881	-6.5	-2313.646586	**-5.6**

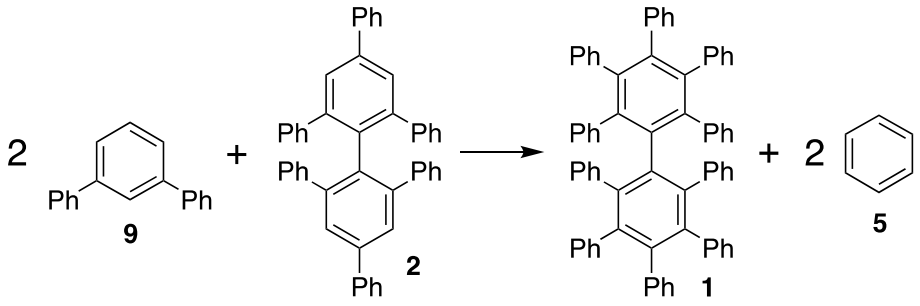


Reaction R4

Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
7	C_2	-1156.691462		-1156.261071		-1156.237204	
2	D_2	-1850.005618		-1849.328581		-1849.290886	
4	D_2	-463.387612		-463.203156		-463.193427	
2 **7**		-2313.382924	0.0	-2312.522142	0.0	-2312.474408	0.0
2 + **4**		-2313.393230	-27.1	-2312.531737	-25.2	-2312.484313	**-26.0**

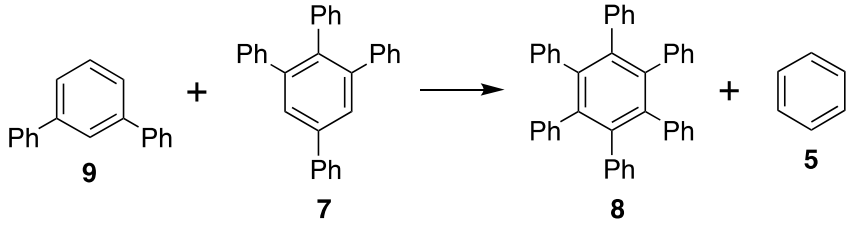
[a] 1 au = 2625.5 kJ/mol.

Table S17. M052X-D3/6-311++G(2d,p)-Calculated Enthalpies of Reaction for Homodesmotic Reactions R1-R6 (continued).



Reaction R5

Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
9	C_2	-694.490248		-694.223779		-694.209387	
2	D_2	-1850.005618		-1849.328581		-1849.290886	
1	D_2	-2774.395513		-2773.392276		-2773.335316	
5	D_{6h}	-232.285170		-232.183150		-232.177850	
2 **9** + **2**		-3238.986114	0.0	-3237.776139	0.0	-3237.709660	0.0
2 **5** + **1**		-3238.965853	+53.2	-3237.758576	+46.1	-3237.691016	**+48.9**

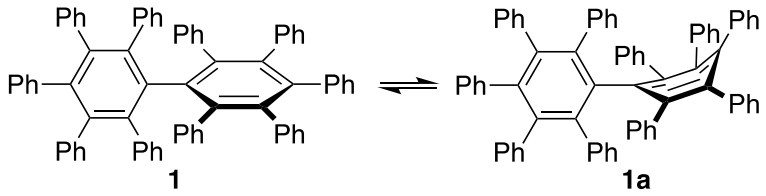


Reaction R6

Cmpd	Symm	*E* (au)[a]	Δ*E* (kJ/mol)	*E*+ZPE (au)[a]	Δ(*E*+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)
9	C_2	-694.490248		-694.223779		-694.209387	
7	C_2	-1156.691462		-1156.261071		-1156.237204	
8	D_6	-1618.888222		-1618.294980		-1618.261375	
5	D_{6h}	-232.285170		-232.183150		-232.177850	
9 + **7**		-1851.181710	0.0	-1850.484850	0.0	-1850.446591	0.0
8 + **5**		-1851.173392	+21.8	-1850.478130	+17.6	-1850.439225	**+19.3**

[a] 1 au = 2625.5 kJ/mol.

Table S18. Effect of a Continuum Solvent Model on the Calculated Relative Energies of the D_2 (**1**) and C_1 (**1a**) Conformations of Decaphenylbiphenyl.



1 **1a**

Cmpd	Symm	E (au)[a]	ΔE (kJ/mol)	E+ZPE (au)[a]	$\Delta(E$+ZPE) (kJ/mol)	H_{298} (au)[a]	ΔH_{298} (kJ/mol)	nI[b]
At the B3PW91/6-311G(d,p) level								
1	D_2	-2773.316143		-2772.330237		-2772.272294		0
1a	C_1	-2773.311177	+13.0	-2772.325541	+12.3	-2772.267345	+13.0	0
At the B3PW91/6-311G(d,p) level with PCM[c]								
1	D_2	-2773.324801		-2772.338914		-2772.281013		0
1a	C_1	-2773.320340	+11.7	-2772.334778	+10.9	-2772.276611	+11.6	0
At the M052X-D3/6-311G(d,p) level								
1	D_2	-2774.267924		-2773.265624		-2773.208576		0
1a	C_1	-2774.260689	+19.0	-2773.258308	+19.2	-2773.201017	+19.8	0
At the M052X-D3/6-311G(d,p) level with PCM[c]								
1	D_2	-2774.277698		-2773.275622		-2773.218517		0
1a	C_1	-2774.271204	+17.0	-2773.269198	+16.9	-2773.211800	+17.6	0
At the PW6B95-D3(BJ)/6-311G(d,p) level								
1	D_2	-2778.292255		-2777.297771		-2777.240556		0
1a	C_1	-2778.284495	+20.4	-2777.290215	+19.8	-2777.232651	+20.8	0
At the PW6B95-D3(BJ)/6-311G(d,p) level with PCM[c]								
1	D_2	-2778.299785		-2777.305691		-2777.248332		0
1a	C_1	-2778.292587	+18.9	-2777.298560	+18.7	-2777.240904	+19.5	0

[a] 1 au = 2625.5 kJ/mol. [b] nI = number of imaginary frequencies. [c] The polarizable continuum model in Gaussian 16 was used with keywords: SCRF=(PCM,SOLVENT=BENZENE).

7. Computational details: Atomic coordinates of calculated structures

D2 Decaphenylbiphenyl (1)
B3PW91/6-311++G(2d,p)-optimized
E = -2773.413583 au
E + ZPE = -2772.431651 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.481759	2.064278	0.743064
2	6	0	-0.746872	0.967582	1.449535
3	6	0	0.783769	-0.930569	2.857163
4	6	0	-0.000000	0.000000	0.750036
5	6	0	-0.783769	0.930569	2.857163
6	6	0	-0.000000	0.000000	3.557553
7	6	0	0.746872	-0.967582	1.449535
8	6	0	0.000000	0.000000	-0.750036
9	6	0	-1.674668	1.858049	3.617511
10	6	0	-0.000000	0.000000	5.051784
11	6	0	1.481759	-2.064278	0.743064
12	6	0	1.674668	-1.858049	3.617511
13	6	0	0.000000	0.000000	-3.557553
14	6	0	0.746872	0.967582	-1.449535
15	6	0	-0.746872	-0.967582	-1.449535
16	6	0	-0.783769	-0.930569	-2.857163
17	6	0	0.783769	0.930569	-2.857163
18	6	0	1.481759	2.064278	-0.743064
19	6	0	-1.481759	-2.064278	-0.743064
20	6	0	-1.674668	-1.858049	-3.617511
21	6	0	1.674668	1.858049	-3.617511
22	6	0	0.000000	0.000000	-5.051784
23	6	0	-0.000000	0.000000	7.852908
24	6	0	1.129280	0.401158	5.765134
25	6	0	-1.129280	-0.401158	5.765134
26	6	0	-1.129405	-0.404839	7.153196
27	6	0	1.129405	0.404839	7.153196
28	1	0	2.017385	0.711738	5.225676
29	1	0	-2.017385	-0.711738	5.225676
30	1	0	-2.017174	-0.722693	7.689687
31	1	0	2.017174	0.722693	7.689687
32	1	0	-0.000000	0.000000	8.937616
33	6	0	0.000000	0.000000	-7.852908
34	6	0	1.129280	-0.401158	-5.765134
35	6	0	-1.129280	0.401158	-5.765134
36	6	0	-1.129405	0.404839	-7.153196
37	6	0	1.129405	-0.404839	-7.153196
38	1	0	2.017385	-0.711738	-5.225676
39	1	0	-2.017385	0.711738	-5.225676
40	1	0	-2.017174	0.722693	-7.689687
41	1	0	2.017174	-0.722693	-7.689687
42	1	0	0.000000	0.000000	-8.937616
43	6	0	3.378277	-3.556358	5.055916
44	6	0	3.060324	-1.754479	3.492747
45	6	0	1.157766	-2.826705	4.478135
46	6	0	2.000168	-3.671102	5.187224
47	6	0	3.905677	-2.592588	4.206519
48	1	0	3.479955	-1.008169	2.826886
49	1	0	0.083624	-2.921346	4.590938
50	1	0	1.577135	-4.420872	5.847397
51	1	0	4.980347	-2.493168	4.096076
52	1	0	4.037118	-4.214211	5.612450
53	6	0	3.378277	3.556358	-5.055916
54	6	0	3.060324	1.754479	-3.492747
55	6	0	1.157766	2.826705	-4.478135
56	6	0	2.000168	3.671102	-5.187224
57	6	0	3.905677	2.592588	-4.206519
58	1	0	3.479955	1.008169	-2.826886
59	1	0	0.083624	2.921346	-4.590938
60	1	0	1.577135	4.420872	-5.847397

61	1	0	4.980347	2.493168	-4.096076
62	1	0	4.037118	4.214211	-5.612450
63	6	0	-3.378277	3.556358	5.055916
64	6	0	-1.157766	2.826705	4.478135
65	6	0	-3.060324	1.754479	3.492747
66	6	0	-3.905677	2.592588	4.206519
67	6	0	-2.000168	3.671102	5.187224
68	1	0	-0.083624	2.921346	4.590938
69	1	0	-3.479955	1.008169	2.826886
70	1	0	-4.980347	2.493168	4.096076
71	1	0	-1.577135	4.420872	5.847397
72	1	0	-4.037118	4.214211	5.612450
73	6	0	-3.378277	-3.556358	-5.055916
74	6	0	-1.157766	-2.826705	-4.478135
75	6	0	-3.060324	-1.754479	-3.492747
76	6	0	-3.905677	-2.592588	-4.206519
77	6	0	-2.000168	-3.671102	-5.187224
78	1	0	-0.083624	-2.921346	-4.590938
79	1	0	-3.479955	-1.008169	-2.826886
80	1	0	-4.980347	-2.493168	-4.096076
81	1	0	-1.577135	-4.420872	-5.847397
82	1	0	-4.037118	-4.214211	-5.612450
83	6	0	2.877511	-4.193323	-0.457677
84	6	0	2.452904	-1.832467	-0.232963
85	6	0	1.213189	-3.393073	1.084729
86	6	0	1.901075	-4.443451	0.497433
87	6	0	3.145398	-2.881878	-0.823822
88	1	0	2.683001	-0.822614	-0.543429
89	1	0	0.444477	-3.605390	1.816886
90	1	0	1.668336	-5.462804	0.786129
91	1	0	3.901535	-2.668312	-1.572036
92	1	0	3.421852	-5.012795	-0.914851
93	6	0	2.877511	4.193323	0.457677
94	6	0	2.452904	1.832467	0.232963
95	6	0	1.213189	3.393073	-1.084729
96	6	0	1.901075	4.443451	-0.497433
97	6	0	3.145398	2.881878	0.823822
98	1	0	2.683001	0.822614	0.543429
99	1	0	0.444477	3.605390	-1.816886
100	1	0	1.668336	5.462804	-0.786129
101	1	0	3.901535	2.668312	1.572036
102	1	0	3.421852	5.012795	0.914851
103	6	0	-2.877511	4.193323	-0.457677
104	6	0	-1.213189	3.393073	1.084729
105	6	0	-2.452904	1.832467	-0.232963
106	6	0	-3.145398	2.881878	-0.823822
107	6	0	-1.901075	4.443451	0.497433
108	1	0	-0.444477	3.605390	1.816886
109	1	0	-2.683001	0.822614	-0.543429
110	1	0	-3.901535	2.668312	-1.572036
111	1	0	-1.668336	5.462804	0.786129
112	1	0	-3.421852	5.012795	-0.914851
113	6	0	-2.877511	-4.193323	0.457677
114	6	0	-1.213189	-3.393073	-1.084729
115	6	0	-2.452904	-1.832467	0.232963
116	6	0	-3.145398	-2.881878	0.823822
117	6	0	-1.901075	-4.443451	-0.497433
118	1	0	-0.444477	-3.605390	-1.816886
119	1	0	-2.683001	-0.822614	0.543429
120	1	0	-3.901535	-2.668312	1.572036
121	1	0	-1.668336	-5.462804	-0.786129
122	1	0	-3.421852	-5.012795	0.914851

D2 Decaphenylbiphenyl (1)
M052X-D3/6-311++G(2d,p)-optimized
E = -2774.395513 au
E + ZPE = -2773.392276 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.431955	2.077950	0.717199
2	6	0	-0.725782	0.977025	1.438317
3	6	0	0.761115	-0.944128	2.839214
4	6	0	0.000000	-0.000000	0.746450
5	6	0	-0.761115	0.944128	2.839214
6	6	0	0.000000	-0.000000	3.536556
7	6	0	0.725782	-0.977025	1.438317
8	6	0	0.000000	-0.000000	-0.746450
9	6	0	-1.625643	1.894930	3.593670
10	6	0	0.000000	-0.000000	5.027253
11	6	0	1.431955	-2.077950	0.717199
12	6	0	1.625643	-1.894930	3.593670
13	6	0	0.000000	-0.000000	-3.536556
14	6	0	0.725782	0.977025	-1.438317
15	6	0	-0.725782	-0.977025	-1.438317
16	6	0	-0.761115	-0.944128	-2.839214
17	6	0	0.761115	0.944128	-2.839214
18	6	0	1.431955	2.077950	-0.717199
19	6	0	-1.431955	-2.077950	-0.717199
20	6	0	-1.625643	-1.894930	-3.593670
21	6	0	1.625643	1.894930	-3.593670
22	6	0	0.000000	-0.000000	-5.027253
23	6	0	0.000000	-0.000000	7.814874
24	6	0	1.158222	0.306704	5.732491
25	6	0	-1.158222	-0.306704	5.732491
26	6	0	-1.158582	-0.309882	7.118091
27	6	0	1.158582	0.309882	7.118091
28	1	0	2.063175	0.537653	5.188193
29	1	0	-2.063175	-0.537653	5.188193
30	1	0	-2.065317	-0.551001	7.653430
31	1	0	2.065317	0.551001	7.653430
32	1	0	0.000000	-0.000000	8.895041
33	6	0	0.000000	-0.000000	-7.814874
34	6	0	1.158222	-0.306704	-5.732491
35	6	0	-1.158222	0.306704	-5.732491
36	6	0	-1.158582	0.309882	-7.118091
37	6	0	1.158582	-0.309882	-7.118091
38	1	0	2.063175	-0.537653	-5.188193
39	1	0	-2.063175	0.537653	-5.188193
40	1	0	-2.065317	0.551001	-7.653430
41	1	0	2.065317	-0.551001	-7.653430
42	1	0	0.000000	-0.000000	-8.895041
43	6	0	3.276685	-3.644600	5.003573
44	6	0	3.004660	-1.860525	3.419046
45	6	0	1.082284	-2.815101	4.483502
46	6	0	1.901394	-3.687214	5.181293
47	6	0	3.826826	-2.727311	4.120937
48	1	0	3.430951	-1.152659	2.721331
49	1	0	0.011457	-2.844956	4.626459
50	1	0	1.465074	-4.399035	5.866702
51	1	0	4.896472	-2.688737	3.975179
52	1	0	3.915714	-4.322963	5.549649
53	6	0	3.276685	3.644600	-5.003573
54	6	0	3.004660	1.860525	-3.419046
55	6	0	1.082284	2.815101	-4.483502
56	6	0	1.901394	3.687214	-5.181293
57	6	0	3.826826	2.727311	-4.120937
58	1	0	3.430951	1.152659	-2.721331
59	1	0	0.011457	2.844956	-4.626459
60	1	0	1.465074	4.399035	-5.866702
61	1	0	4.896472	2.688737	-3.975179
62	1	0	3.915714	4.322963	-5.549649
63	6	0	-3.276685	3.644600	5.003573

64	6	0	-1.082284	2.815101	4.483502
65	6	0	-3.004660	1.860525	3.419046
66	6	0	-3.826826	2.727311	4.120937
67	6	0	-1.901394	3.687214	5.181293
68	1	0	-0.011457	2.844956	4.626459
69	1	0	-3.430951	1.152659	2.721331
70	1	0	-4.896472	2.688737	3.975179
71	1	0	-1.465074	4.399035	5.866702
72	1	0	-3.915714	4.322963	5.549649
73	6	0	-3.276685	-3.644600	-5.003573
74	6	0	-1.082284	-2.815101	-4.483502
75	6	0	-3.004660	-1.860525	-3.419046
76	6	0	-3.826826	-2.727311	-4.120937
77	6	0	-1.901394	-3.687214	-5.181293
78	1	0	-0.011457	-2.844956	-4.626459
79	1	0	-3.430951	-1.152659	-2.721331
80	1	0	-4.896472	-2.688737	-3.975179
81	1	0	-1.465074	-4.399035	-5.866702
82	1	0	-3.915714	-4.322963	-5.549649
83	6	0	2.735643	-4.209495	-0.545852
84	6	0	2.357915	-1.847329	-0.296844
85	6	0	1.159009	-3.397438	1.072482
86	6	0	1.806233	-4.452476	0.454489
87	6	0	3.003991	-2.903073	-0.923135
88	1	0	2.579030	-0.840483	-0.613090
89	1	0	0.415568	-3.594362	1.830373
90	1	0	1.573992	-5.465915	0.747808
91	1	0	3.720330	-2.699275	-1.705835
92	1	0	3.242362	-5.031094	-1.030827
93	6	0	2.735643	4.209495	0.545852
94	6	0	2.357915	1.847329	0.296844
95	6	0	1.159009	3.397438	-1.072482
96	6	0	1.806233	4.452476	-0.454489
97	6	0	3.003991	2.903073	0.923135
98	1	0	2.579030	0.840483	0.613090
99	1	0	0.415568	3.594362	-1.830373
100	1	0	1.573992	5.465915	-0.747808
101	1	0	3.720330	2.699275	1.705835
102	1	0	3.242362	5.031094	1.030827
103	6	0	-2.735643	4.209495	-0.545852
104	6	0	-1.159009	3.397438	1.072482
105	6	0	-2.357915	1.847329	-0.296844
106	6	0	-3.003991	2.903073	-0.923135
107	6	0	-1.806233	4.452476	0.454489
108	1	0	-0.415568	3.594362	1.830373
109	1	0	-2.579030	0.840483	-0.613090
110	1	0	-3.720330	2.699275	-1.705835
111	1	0	-1.573992	5.465915	0.747808
112	1	0	-3.242362	5.031094	-1.030827
113	6	0	-2.735643	-4.209495	0.545852
114	6	0	-1.159009	-3.397438	-1.072482
115	6	0	-2.357915	-1.847329	0.296844
116	6	0	-3.003991	-2.903073	0.923135
117	6	0	-1.806233	-4.452476	-0.454489
118	1	0	-0.415568	-3.594362	-1.830373
119	1	0	-2.579030	-0.840483	0.613090
120	1	0	-3.720330	-2.699275	1.705835
121	1	0	-1.573992	-5.465915	-0.747808
122	1	0	-3.242362	-5.031094	1.030827

D2 Decaphenylbiphenyl (1)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -2778.387089 au
E + ZPE = -2777.393356 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.415227	2.080007	0.721831
2	6	0	-0.720649	0.977874	1.439736
3	6	0	0.760124	-0.942939	2.839799
4	6	0	0.000000	-0.000000	0.745720
5	6	0	-0.760124	0.942939	2.839799
6	6	0	0.000000	-0.000000	3.537629
7	6	0	0.720649	-0.977874	1.439736
8	6	0	0.000000	-0.000000	-0.745720
9	6	0	-1.630001	1.888356	3.586396
10	6	0	0.000000	-0.000000	5.024171
11	6	0	1.415227	-2.080007	0.721831
12	6	0	1.630001	-1.888356	3.586396
13	6	0	0.000000	-0.000000	-3.537629
14	6	0	0.720649	0.977874	-1.439736
15	6	0	-0.720649	-0.977874	-1.439736
16	6	0	-0.760124	-0.942939	-2.839799
17	6	0	0.760124	0.942939	-2.839799
18	6	0	1.415227	2.080007	-0.721831
19	6	0	-1.415227	-2.080007	-0.721831
20	6	0	-1.630001	-1.888356	-3.586396
21	6	0	1.630001	1.888356	-3.586396
22	6	0	0.000000	-0.000000	-5.024171
23	6	0	0.000000	-0.000000	7.811076
24	6	0	1.161713	0.282019	5.731565
25	6	0	-1.161713	-0.282019	5.731565
26	6	0	-1.162058	-0.286354	7.114578
27	6	0	1.162058	0.286354	7.114578
28	1	0	2.072028	0.492771	5.189989
29	1	0	-2.072028	-0.492771	5.189989
30	1	0	-2.073166	-0.509753	7.649179
31	1	0	2.073166	0.509753	7.649179
32	1	0	0.000000	-0.000000	8.890698
33	6	0	0.000000	-0.000000	-7.811076
34	6	0	1.161713	-0.282019	-5.731565
35	6	0	-1.161713	0.282019	-5.731565
36	6	0	-1.162058	0.286354	-7.114578
37	6	0	1.162058	-0.286354	-7.114578
38	1	0	2.072028	-0.492771	-5.189989
39	1	0	-2.072028	0.492771	-5.189989
40	1	0	-2.073166	0.509753	-7.649179
41	1	0	2.073166	-0.509753	-7.649179
42	1	0	0.000000	-0.000000	-8.890698
43	6	0	3.300897	-3.634331	4.976232
44	6	0	3.003115	-1.875881	3.374023
45	6	0	1.105617	-2.788091	4.506118
46	6	0	1.933030	-3.657654	5.192182
47	6	0	3.834140	-2.738175	4.065352
48	1	0	3.418346	-1.187262	2.652360
49	1	0	0.040651	-2.804149	4.682826
50	1	0	1.508327	-4.353923	5.899740
51	1	0	4.899040	-2.713285	3.888783
52	1	0	3.947253	-4.311260	5.514333
53	6	0	3.300897	3.634331	-4.976232
54	6	0	3.003115	1.875881	-3.374023
55	6	0	1.105617	2.788091	-4.506118
56	6	0	1.933030	3.657654	-5.192182
57	6	0	3.834140	2.738175	-4.065352
58	1	0	3.418346	1.187262	-2.652360
59	1	0	0.040651	2.804149	-4.682826
60	1	0	1.508327	4.353923	-5.899740
61	1	0	4.899040	2.713285	-3.888783
62	1	0	3.947253	4.311260	-5.514333
63	6	0	-3.300897	3.634331	4.976232

64	6	0	-1.105617	2.788091	4.506118
65	6	0	-3.003115	1.875881	3.374023
66	6	0	-3.834140	2.738175	4.065352
67	6	0	-1.933030	3.657654	5.192182
68	1	0	-0.040651	2.804149	4.682826
69	1	0	-3.418346	1.187262	2.652360
70	1	0	-4.899040	2.713285	3.888783
71	1	0	-1.508327	4.353923	5.899740
72	1	0	-3.947253	4.311260	5.514333
73	6	0	-3.300897	-3.634331	-4.976232
74	6	0	-1.105617	-2.788091	-4.506118
75	6	0	-3.003115	-1.875881	-3.374023
76	6	0	-3.834140	-2.738175	-4.065352
77	6	0	-1.933030	-3.657654	-5.192182
78	1	0	-0.040651	-2.804149	-4.682826
79	1	0	-3.418346	-1.187262	-2.652360
80	1	0	-4.899040	-2.713285	-3.888783
81	1	0	-1.508327	-4.353923	-5.899740
82	1	0	-3.947253	-4.311260	-5.514333
83	6	0	2.684138	-4.217325	-0.559555
84	6	0	2.322837	-1.857217	-0.307782
85	6	0	1.149257	-3.396388	1.087666
86	6	0	1.777806	-4.453370	0.460425
87	6	0	2.950433	-2.914653	-0.943659
88	1	0	2.544868	-0.851214	-0.624575
89	1	0	0.418355	-3.588376	1.857921
90	1	0	1.547649	-5.464713	0.760191
91	1	0	3.652962	-2.715992	-1.739351
92	1	0	3.176163	-5.041669	-1.053726
93	6	0	2.684138	4.217325	0.559555
94	6	0	2.322837	1.857217	0.307782
95	6	0	1.149257	3.396388	-1.087666
96	6	0	1.777806	4.453370	-0.460425
97	6	0	2.950433	2.914653	0.943659
98	1	0	2.544868	0.851214	0.624575
99	1	0	0.418355	3.588376	-1.857921
100	1	0	1.547649	5.464713	-0.760191
101	1	0	3.652962	2.715992	1.739351
102	1	0	3.176163	5.041669	1.053726
103	6	0	-2.684138	4.217325	-0.559555
104	6	0	-1.149257	3.396388	1.087666
105	6	0	-2.322837	1.857217	-0.307782
106	6	0	-2.950433	2.914653	-0.943659
107	6	0	-1.777806	4.453370	0.460425
108	1	0	-0.418355	3.588376	1.857921
109	1	0	-2.544868	0.851214	-0.624575
110	1	0	-3.652962	2.715992	-1.739351
111	1	0	-1.547649	5.464713	0.760191
112	1	0	-3.176163	5.041669	-1.053726
113	6	0	-2.684138	-4.217325	0.559555
114	6	0	-1.149257	-3.396388	-1.087666
115	6	0	-2.322837	-1.857217	0.307782
116	6	0	-2.950433	-2.914653	0.943659
117	6	0	-1.777806	-4.453370	-0.460425
118	1	0	-0.418355	-3.588376	-1.857921
119	1	0	-2.544868	-0.851214	0.624575
120	1	0	-3.652962	-2.715992	1.739351
121	1	0	-1.547649	-5.464713	-0.760191
122	1	0	-3.176163	-5.041669	1.053726

C1 Decaphenylbiphenyl (1a)
B3PW91/6-311++G(2d,p)-optimized
E = -2773.409130 au
E + ZPE = -2772.424288 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.738895	0.133400	0.225403
2	6	0	-1.548144	-0.609525	1.107433
3	6	0	-2.947760	-0.602018	0.941942
4	6	0	-3.539623	0.212754	-0.032773
5	6	0	-2.741382	1.061773	-0.813435
6	6	0	-1.339221	1.028643	-0.684694
7	6	0	0.753817	-0.049659	0.177589
8	6	0	1.286904	-1.096171	-0.610762
9	6	0	2.682364	-1.191262	-0.785184
10	6	0	3.540771	-0.292513	-0.130348
11	6	0	3.008931	0.709723	0.693608
12	6	0	1.616595	0.845269	0.829766
13	6	0	-0.991410	-1.319259	2.301669
14	6	0	-0.050970	-2.344473	2.243918
15	1	0	0.296824	-2.694627	1.284782
16	6	0	0.422025	-2.953035	3.400756
17	1	0	1.148068	-3.755651	3.322572
18	6	0	-0.034695	-2.547861	4.646050
19	1	0	0.333666	-3.024034	5.548385
20	6	0	-0.974753	-1.527336	4.723111
21	1	0	-1.344607	-1.197578	5.688218
22	6	0	-1.445179	-0.925291	3.566595
23	1	0	-2.170461	-0.123648	3.640320
24	6	0	-3.797753	-1.542105	1.732019
25	6	0	-3.658644	-2.918194	1.545077
26	1	0	-2.924754	-3.285350	0.835954
27	6	0	-4.448512	-3.815804	2.249908
28	1	0	-4.326958	-4.881417	2.086520
29	6	0	-5.389550	-3.353123	3.160358
30	1	0	-6.005976	-4.053617	3.713494
31	6	0	-5.536071	-1.986068	3.356590
32	1	0	-6.267448	-1.613530	4.066054
33	6	0	-4.749948	-1.090342	2.645334
34	1	0	-4.871753	-0.025335	2.807147
35	6	0	-5.008800	0.115067	-0.294553
36	6	0	-5.495258	-0.887685	-1.132245
37	1	0	-4.799162	-1.588092	-1.580800
38	6	0	-6.854532	-1.001326	-1.391891
39	1	0	-7.212757	-1.788633	-2.046710
40	6	0	-7.752276	-0.113378	-0.814667
41	1	0	-8.814434	-0.201531	-1.016053
42	6	0	-7.280099	0.887501	0.023998
43	1	0	-7.973109	1.585332	0.482173
44	6	0	-5.920255	0.999402	0.279883
45	1	0	-5.561548	1.781915	0.939863
46	6	0	-3.386709	1.904998	-1.866516
47	6	0	-3.287737	1.543308	-3.209708
48	1	0	-2.728067	0.655170	-3.482007
49	6	0	-3.895382	2.301956	-4.200848
50	1	0	-3.806993	2.000173	-5.239127
51	6	0	-4.612762	3.442240	-3.865186
52	1	0	-5.087069	4.037260	-4.638135
53	6	0	-4.718059	3.814718	-2.531549
54	1	0	-5.274684	4.704773	-2.257638
55	6	0	-4.113090	3.050602	-1.543423
56	1	0	-4.195781	3.353855	-0.505611
57	6	0	-0.534907	1.992937	-1.502702
58	6	0	0.421607	1.610157	-2.444640
59	1	0	0.646599	0.563811	-2.598359
60	6	0	1.100142	2.554213	-3.205563
61	1	0	1.832024	2.224908	-3.935653
62	6	0	0.841640	3.907483	-3.040406
63	1	0	1.368155	4.643821	-3.638136

64	6	0	-0.098296	4.306961	-2.099524
65	1	0	-0.307327	5.360908	-1.950170
66	6	0	-0.772229	3.361435	-1.341831
67	1	0	-1.490401	3.687609	-0.600081
68	6	0	0.419612	-2.147612	-1.240648
69	6	0	-0.615868	-1.865123	-2.133953
70	1	0	-0.844816	-0.841482	-2.392994
71	6	0	-1.368603	-2.879638	-2.712015
72	1	0	-2.158623	-2.624365	-3.410433
73	6	0	-1.115234	-4.208251	-2.403838
74	1	0	-1.705110	-4.999398	-2.853901
75	6	0	-0.093341	-4.511124	-1.514079
76	1	0	0.123243	-5.543372	-1.260819
77	6	0	0.663175	-3.495457	-0.949799
78	1	0	1.468661	-3.755141	-0.273249
79	6	0	3.267827	-2.221688	-1.695718
80	6	0	3.005648	-2.184527	-3.065408
81	1	0	2.358710	-1.410241	-3.463160
82	6	0	3.559571	-3.123767	-3.924243
83	1	0	3.344216	-3.073935	-4.986357
84	6	0	4.383943	-4.124266	-3.426322
85	1	0	4.815719	-4.860565	-4.095590
86	6	0	4.652267	-4.173416	-2.064276
87	1	0	5.295995	-4.949580	-1.664151
88	6	0	4.103146	-3.228104	-1.209576
89	1	0	4.325122	-3.270411	-0.149025
90	6	0	5.019619	-0.394241	-0.314310
91	6	0	5.608068	-0.097118	-1.543408
92	1	0	4.980925	0.204537	-2.375113
93	6	0	6.982932	-0.183723	-1.713232
94	1	0	7.421549	0.054631	-2.676444
95	6	0	7.793982	-0.576038	-0.656236
96	1	0	8.868296	-0.646150	-0.788559
97	6	0	7.219211	-0.876499	0.571887
98	1	0	7.843442	-1.182393	1.404784
99	6	0	5.844693	-0.782395	0.741139
100	1	0	5.404102	-1.010837	1.705418
101	6	0	3.924722	1.645787	1.411373
102	6	0	4.690009	2.579480	0.713189
103	1	0	4.613604	2.630264	-0.367215
104	6	0	5.543924	3.443067	1.385016
105	1	0	6.128083	4.165083	0.824279
106	6	0	5.652419	3.382760	2.768336
107	1	0	6.321525	4.055728	3.293761
108	6	0	4.896965	2.455336	3.473995
109	1	0	4.973185	2.400215	4.554808
110	6	0	4.038334	1.597287	2.800687
111	1	0	3.447394	0.878968	3.358346
112	6	0	1.090154	1.981201	1.646926
113	6	0	1.239511	3.294606	1.199740
114	1	0	1.704130	3.480360	0.239156
115	6	0	0.800042	4.362573	1.969349
116	1	0	0.925663	5.375505	1.601600
117	6	0	0.208170	4.137819	3.205556
118	1	0	-0.130613	4.972823	3.809817
119	6	0	0.065163	2.835866	3.665870
120	1	0	-0.381989	2.646450	4.636263
121	6	0	0.505579	1.768660	2.893661
122	1	0	0.410341	0.759414	3.272428

C1 Decaphenylbiphenyl (1a)
M052X-D3/6-311++G(2d,p)-optimized
E = -2774.389017 au
E + ZPE = -2773.385850 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.705830	0.277990	0.359196
2	6	0	-1.530276	-0.458931	1.217758
3	6	0	-2.912362	-0.483184	0.985323
4	6	0	-3.471434	0.329437	-0.005373
5	6	0	-2.661251	1.220473	-0.714920
6	6	0	-1.270237	1.187344	-0.544630
7	6	0	0.757872	-0.006971	0.261887
8	6	0	1.142661	-1.111513	-0.518241
9	6	0	2.500699	-1.337807	-0.769594
10	6	0	3.466977	-0.477968	-0.229693
11	6	0	3.077175	0.595523	0.575850
12	6	0	1.719319	0.831379	0.820162
13	6	0	-0.993665	-1.094395	2.457606
14	6	0	0.083235	-1.971961	2.507581
15	1	0	0.557701	-2.293226	1.599261
16	6	0	0.559316	-2.445878	3.722673
17	1	0	1.396577	-3.128706	3.733459
18	6	0	-0.029674	-2.049706	4.911354
19	1	0	0.344861	-2.417153	5.855489
20	6	0	-1.106566	-1.174546	4.876754
21	1	0	-1.575770	-0.852282	5.794872
22	6	0	-1.579589	-0.705346	3.664973
23	1	0	-2.403766	-0.007751	3.645434
24	6	0	-3.763493	-1.464978	1.710805
25	6	0	-3.463036	-2.820153	1.609932
26	1	0	-2.611997	-3.127754	1.016831
27	6	0	-4.247433	-3.763774	2.252991
28	1	0	-4.005275	-4.812812	2.163552
29	6	0	-5.339935	-3.362822	3.007659
30	1	0	-5.951688	-4.097584	3.510408
31	6	0	-5.645243	-2.013631	3.112544
32	1	0	-6.495518	-1.694249	3.697312
33	6	0	-4.863473	-1.071216	2.464541
34	1	0	-5.105892	-0.020962	2.541462
35	6	0	-4.907902	0.165869	-0.370174
36	6	0	-5.303812	-0.990149	-1.035166
37	1	0	-4.562498	-1.743783	-1.262620
38	6	0	-6.630118	-1.182760	-1.385695
39	1	0	-6.923331	-2.086060	-1.900498
40	6	0	-7.579073	-0.221452	-1.071232
41	1	0	-8.614018	-0.370941	-1.341924
42	6	0	-7.193270	0.931091	-0.404290
43	1	0	-7.927171	1.682623	-0.151993
44	6	0	-5.864844	1.122958	-0.057376
45	1	0	-5.568971	2.017483	0.470791
46	6	0	-3.264819	2.072024	-1.781835
47	6	0	-3.209637	1.649173	-3.104334
48	1	0	-2.726870	0.710258	-3.338631
49	6	0	-3.765989	2.416512	-4.115769
50	1	0	-3.715413	2.074352	-5.139081
51	6	0	-4.384789	3.619635	-3.814105
52	1	0	-4.817539	4.219791	-4.600957
53	6	0	-4.445165	4.049072	-2.496795
54	1	0	-4.924587	4.986231	-2.253921
55	6	0	-3.889712	3.278039	-1.488604
56	1	0	-3.930037	3.617850	-0.463040
57	6	0	-0.419806	2.130640	-1.333234
58	6	0	0.573184	1.717846	-2.218293
59	1	0	0.775292	0.668270	-2.359997
60	6	0	1.328760	2.645124	-2.921088
61	1	0	2.095140	2.300208	-3.600240
62	6	0	1.101583	4.002537	-2.757602
63	1	0	1.688703	4.723323	-3.307684

64	6	0	0.116135	4.426502	-1.878719
65	1	0	-0.065828	5.481348	-1.732696
66	6	0	-0.628674	3.498785	-1.171447
67	1	0	-1.370616	3.833555	-0.462667
68	6	0	0.126436	-2.074132	-1.053499
69	6	0	-0.871451	-1.689117	-1.945367
70	1	0	-0.930948	-0.665731	-2.278057
71	6	0	-1.798353	-2.605142	-2.417866
72	1	0	-2.562837	-2.279346	-3.109107
73	6	0	-1.746686	-3.928310	-2.007929
74	1	0	-2.472704	-4.640856	-2.371039
75	6	0	-0.748744	-4.329890	-1.133122
76	1	0	-0.687110	-5.359969	-0.813888
77	6	0	0.178812	-3.412476	-0.667108
78	1	0	0.964514	-3.743445	-0.003544
79	6	0	2.923768	-2.477308	-1.631440
80	6	0	2.525951	-2.535163	-2.962643
81	1	0	1.898653	-1.750194	-3.362146
82	6	0	2.920472	-3.588268	-3.771875
83	1	0	2.604785	-3.619082	-4.804436
84	6	0	3.715374	-4.600981	-3.255914
85	1	0	4.022136	-5.423816	-3.884817
86	6	0	4.115383	-4.551782	-1.928675
87	1	0	4.736173	-5.335796	-1.520317
88	6	0	3.724583	-3.494356	-1.123323
89	1	0	4.045660	-3.449964	-0.092176
90	6	0	4.910729	-0.702201	-0.520410
91	6	0	5.389653	-0.604317	-1.822184
92	1	0	4.701101	-0.372956	-2.622774
93	6	0	6.732885	-0.805760	-2.095424
94	1	0	7.091671	-0.724738	-3.111083
95	6	0	7.612913	-1.113631	-1.068492
96	1	0	8.659974	-1.272843	-1.280696
97	6	0	7.142459	-1.214736	0.232312
98	1	0	7.822123	-1.451433	1.037831
99	6	0	5.799787	-1.006918	0.504259
100	1	0	5.434478	-1.073693	1.519309
101	6	0	4.100171	1.511594	1.151502
102	6	0	4.890801	2.296728	0.319994
103	1	0	4.758533	2.232038	-0.750949
104	6	0	5.838295	3.153760	0.855877
105	1	0	6.444884	3.760635	0.199659
106	6	0	6.008168	3.231172	2.230331
107	1	0	6.747857	3.898000	2.648681
108	6	0	5.222543	2.450861	3.065604
109	1	0	5.346569	2.508933	4.137096
110	6	0	4.271351	1.598381	2.528484
111	1	0	3.649877	0.997465	3.177592
112	6	0	1.306790	2.004359	1.638365
113	6	0	1.536438	3.295054	1.174596
114	1	0	1.996002	3.435983	0.206619
115	6	0	1.172193	4.389488	1.941460
116	1	0	1.352289	5.387361	1.568223
117	6	0	0.578849	4.205013	3.182177
118	1	0	0.298147	5.059344	3.781054
119	6	0	0.354361	2.919957	3.653013
120	1	0	-0.099087	2.765416	4.621618
121	6	0	0.719155	1.824712	2.885006
122	1	0	0.562406	0.824241	3.259890

C1 Decaphenylbiphenyl (1a)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -2778.379887 au
E + ZPE = -2777.386217 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.693153	0.302601	0.366836
2	6	0	-1.485639	-0.484205	1.210599
3	6	0	-2.870469	-0.527814	1.001986
4	6	0	-3.463186	0.306329	0.050319
5	6	0	-2.685426	1.241790	-0.635123
6	6	0	-1.292441	1.236217	-0.485842
7	6	0	0.765832	0.031911	0.229627
8	6	0	1.130980	-1.061979	-0.572683
9	6	0	2.482685	-1.309676	-0.828598
10	6	0	3.464018	-0.479407	-0.272133
11	6	0	3.093243	0.598890	0.535235
12	6	0	1.739857	0.858889	0.779892
13	6	0	-0.918579	-1.152362	2.414696
14	6	0	0.186073	-1.994344	2.429719
15	1	0	0.672615	-2.263275	1.512372
16	6	0	0.675373	-2.508946	3.619647
17	1	0	1.532649	-3.165466	3.598231
18	6	0	0.077025	-2.189337	4.823673
19	1	0	0.462694	-2.589187	5.749323
20	6	0	-1.023385	-1.347343	4.827567
21	1	0	-1.501888	-1.081439	5.758240
22	6	0	-1.510874	-0.839864	3.640341
23	1	0	-2.359492	-0.173483	3.654212
24	6	0	-3.686272	-1.545039	1.709422
25	6	0	-3.339546	-2.886606	1.596310
26	1	0	-2.476741	-3.155869	1.004357
27	6	0	-4.089394	-3.863728	2.224515
28	1	0	-3.809723	-4.901785	2.122803
29	6	0	-5.194857	-3.512345	2.981043
30	1	0	-5.780167	-4.273912	3.474147
31	6	0	-5.547286	-2.178134	3.099990
32	1	0	-6.408354	-1.895994	3.687239
33	6	0	-4.801079	-1.202880	2.464461
34	1	0	-5.083984	-0.164593	2.552344
35	6	0	-4.896708	0.122073	-0.297878
36	6	0	-5.288871	-1.042196	-0.947982
37	1	0	-4.544432	-1.791147	-1.174775
38	6	0	-6.613321	-1.251354	-1.285356
39	1	0	-6.900235	-2.161278	-1.791029
40	6	0	-7.569420	-0.300710	-0.969692
41	1	0	-8.604493	-0.463513	-1.229905
42	6	0	-7.190427	0.857705	-0.313984
43	1	0	-7.929898	1.601799	-0.058025
44	6	0	-5.863242	1.066801	0.017335
45	1	0	-5.575285	1.967444	0.537430
46	6	0	-3.317664	2.101988	-1.673081
47	6	0	-3.267077	1.710818	-3.004127
48	1	0	-2.765463	0.789924	-3.264661
49	6	0	-3.851663	2.482889	-3.992475
50	1	0	-3.803661	2.162075	-5.022303
51	6	0	-4.494949	3.662619	-3.661628
52	1	0	-4.950528	4.267349	-4.431139
53	6	0	-4.549816	4.063019	-2.337390
54	1	0	-5.047564	4.983279	-2.070179
55	6	0	-3.966623	3.286477	-1.352884
56	1	0	-4.004657	3.606466	-0.321668
57	6	0	-0.478185	2.224031	-1.246714
58	6	0	0.533131	1.869408	-2.133950
59	1	0	0.763984	0.831385	-2.308007
60	6	0	1.265869	2.836814	-2.800625
61	1	0	2.046211	2.534820	-3.483367
62	6	0	0.999259	4.179686	-2.599431
63	1	0	1.570645	4.932699	-3.121117

64	6	0	-0.004808	4.547052	-1.719861
65	1	0	-0.217653	5.590648	-1.542826
66	6	0	-0.727855	3.579336	-1.050422
67	1	0	-1.483981	3.873232	-0.339966
68	6	0	0.093943	-1.988666	-1.116812
69	6	0	-0.900713	-1.557799	-1.988161
70	1	0	-0.923938	-0.529169	-2.306408
71	6	0	-1.865839	-2.429635	-2.458275
72	1	0	-2.630061	-2.065197	-3.129292
73	6	0	-1.851774	-3.759638	-2.074606
74	1	0	-2.607560	-4.440105	-2.436733
75	6	0	-0.851556	-4.210581	-1.230644
76	1	0	-0.817416	-5.248290	-0.934551
77	6	0	0.109614	-3.334342	-0.760892
78	1	0	0.892829	-3.703262	-0.116159
79	6	0	2.876799	-2.444770	-1.702222
80	6	0	2.455890	-2.490011	-3.025555
81	1	0	1.833218	-1.694807	-3.409214
82	6	0	2.818883	-3.541240	-3.847401
83	1	0	2.485090	-3.558909	-4.874049
84	6	0	3.603830	-4.569554	-3.353645
85	1	0	3.885257	-5.392798	-3.992821
86	6	0	4.026110	-4.535510	-2.035201
87	1	0	4.639268	-5.332520	-1.642052
88	6	0	3.668829	-3.478619	-1.218158
89	1	0	4.010731	-3.448057	-0.194233
90	6	0	4.901078	-0.746020	-0.538767
91	6	0	5.406387	-0.692201	-1.831811
92	1	0	4.740566	-0.461358	-2.650230
93	6	0	6.745158	-0.937319	-2.076821
94	1	0	7.122375	-0.888173	-3.087314
95	6	0	7.597795	-1.248988	-1.031180
96	1	0	8.642439	-1.443551	-1.222012
97	6	0	7.102799	-1.308781	0.260706
98	1	0	7.760423	-1.549676	1.082457
99	6	0	5.765541	-1.054703	0.504177
100	1	0	5.384033	-1.088898	1.513889
101	6	0	4.131134	1.485202	1.120181
102	6	0	4.981973	2.217311	0.301856
103	1	0	4.886638	2.132223	-0.770488
104	6	0	5.942431	3.048555	0.848301
105	1	0	6.593209	3.614562	0.198727
106	6	0	6.070583	3.153289	2.223153
107	1	0	6.821955	3.800163	2.650514
108	6	0	5.228188	2.425643	3.046783
109	1	0	5.319155	2.503453	4.119842
110	6	0	4.262533	1.601489	2.498325
111	1	0	3.596667	1.044931	3.141235
112	6	0	1.346598	2.047898	1.575571
113	6	0	1.667408	3.321414	1.122039
114	1	0	2.177850	3.431214	0.176400
115	6	0	1.319119	4.437761	1.857853
116	1	0	1.568675	5.420955	1.487695
117	6	0	0.648277	4.296011	3.061623
118	1	0	0.379624	5.168129	3.639054
119	6	0	0.326289	3.030390	3.521506
120	1	0	-0.191642	2.908730	4.461306
121	6	0	0.673633	1.913099	2.782017
122	1	0	0.437609	0.927701	3.150941

D2 2,2',4,4',6,6'-hexaphenylbiphenyl (2)
B3PW91/6-311++G(2d,p)-optimized
E = -1849.373202 au
E + ZPE = -1848.709005 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.428690	2.124836	-0.824996
2	6	0	-0.679602	1.007406	-1.463830
3	6	0	0.670492	-0.982507	-2.858289
4	6	0	0.000000	-0.000000	-0.746768
5	6	0	-0.670492	0.982507	-2.858289
6	6	0	0.000000	-0.000000	-3.578843
7	6	0	0.679602	-1.007406	-1.463830
8	6	0	-0.000000	-0.000000	0.746768
9	1	0	-1.202181	1.762140	-3.391992
10	6	0	0.000000	-0.000000	-5.057956
11	6	0	1.428690	-2.124836	-0.824996
12	1	0	1.202181	-1.762140	-3.391992
13	6	0	-0.000000	-0.000000	3.578843
14	6	0	0.679602	1.007406	1.463830
15	6	0	-0.679602	-1.007406	1.463830
16	6	0	-0.670492	-0.982507	2.858289
17	6	0	0.670492	0.982507	2.858289
18	6	0	1.428690	2.124836	0.824996
19	6	0	-1.428690	-2.124836	0.824996
20	1	0	-1.202181	-1.762140	3.391992
21	1	0	1.202181	1.762140	3.391992
22	6	0	-0.000000	-0.000000	5.057956
23	6	0	-2.900422	4.276791	0.224033
24	6	0	-1.244317	3.427308	-1.300778
25	6	0	-2.364370	1.927364	0.193535
26	6	0	-3.093271	2.990216	0.709695
27	6	0	-1.969368	4.490770	-0.783890
28	1	0	-0.502920	3.609488	-2.070880
29	1	0	-2.536600	0.933961	0.587296
30	1	0	-3.819970	2.807719	1.494232
31	1	0	-1.798890	5.491917	-1.165351
32	1	0	-3.470098	5.106114	0.629397
33	6	0	0.000000	-0.000000	-7.863585
34	6	0	1.150069	-0.340309	-5.775805
35	6	0	-1.150069	0.340309	-5.775805
36	6	0	-1.150642	0.339685	-7.163286
37	6	0	1.150642	-0.339685	-7.163286
38	1	0	2.060833	-0.584694	-5.239570
39	1	0	-2.060833	0.584694	-5.239570
40	1	0	-2.057206	0.598327	-7.700067
41	1	0	2.057206	-0.598327	-7.700067
42	1	0	0.000000	-0.000000	-8.948113
43	6	0	2.900422	-4.276791	0.224033
44	6	0	2.364370	-1.927364	0.193535
45	6	0	1.244317	-3.427308	-1.300778
46	6	0	1.969368	-4.490770	-0.783890
47	6	0	3.093271	-2.990216	0.709695
48	1	0	2.536600	-0.933961	0.587296
49	1	0	0.502920	-3.609488	-2.070880
50	1	0	1.798890	-5.491917	-1.165351
51	1	0	3.819970	-2.807719	1.494232
52	1	0	3.470098	-5.106114	0.629397
53	6	0	-2.900422	-4.276791	-0.224033
54	6	0	-1.244317	-3.427308	1.300778
55	6	0	-2.364370	-1.927364	-0.193535
56	6	0	-3.093271	-2.990216	-0.709695
57	6	0	-1.969368	-4.490770	0.783890
58	1	0	-0.502920	-3.609488	2.070880
59	1	0	-2.536600	-0.933961	-0.587296
60	1	0	-3.819970	-2.807719	-1.494232
61	1	0	-1.798890	-5.491917	1.165351
62	1	0	-3.470098	-5.106114	-0.629397
63	6	0	-0.000000	-0.000000	7.863585

64	6	0	1.150069	0.340309	5.775805
65	6	0	-1.150069	-0.340309	5.775805
66	6	0	-1.150642	-0.339685	7.163286
67	6	0	1.150642	0.339685	7.163286
68	1	0	2.060833	0.584694	5.239570
69	1	0	-2.060833	-0.584694	5.239570
70	1	0	-2.057206	-0.598327	7.700067
71	1	0	2.057206	0.598327	7.700067
72	1	0	-0.000000	-0.000000	8.948113
73	6	0	2.900422	4.276791	-0.224033
74	6	0	2.364370	1.927364	-0.193535
75	6	0	1.244317	3.427308	1.300778
76	6	0	1.969368	4.490770	0.783890
77	6	0	3.093271	2.990216	-0.709695
78	1	0	2.536600	0.933961	-0.587296
79	1	0	0.502920	3.609488	2.070880
80	1	0	1.798890	5.491917	1.165351
81	1	0	3.819970	2.807719	-1.494232
82	1	0	3.470098	5.106114	-0.629397

D2 2,2',4,4',6,6'-hexaphenylbiphenyl (2)
M052X-D3/6-311++G(2d,p)-optimized
E = -1850.005618 au
E + ZPE = -1849.328581 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.347275	2.155474	-0.797529
2	6	0	-0.652001	1.019345	-1.457233
3	6	0	0.646612	-0.999399	-2.847642
4	6	0	0.000000	0.000000	-0.745806
5	6	0	-0.646612	0.999399	-2.847642
6	6	0	0.000000	0.000000	-3.560916
7	6	0	0.652001	-1.019345	-1.457233
8	6	0	-0.000000	0.000000	0.745806
9	1	0	-1.153859	1.790921	-3.380165
10	6	0	0.000000	0.000000	-5.039738
11	6	0	1.347275	-2.155474	-0.797529
12	1	0	1.153859	-1.790921	-3.380165
13	6	0	-0.000000	0.000000	3.560916
14	6	0	0.652001	1.019345	1.457233
15	6	0	-0.652001	-1.019345	1.457233
16	6	0	-0.646612	-0.999399	2.847642
17	6	0	0.646612	0.999399	2.847642
18	6	0	1.347275	2.155474	0.797529
19	6	0	-1.347275	-2.155474	0.797529
20	1	0	-1.153859	-1.790921	3.380165
21	1	0	1.153859	1.790921	3.380165
22	6	0	-0.000000	0.000000	5.039738
23	6	0	-2.639136	4.348036	0.358776
24	6	0	-1.104764	3.449447	-1.254781
25	6	0	-2.251166	1.976611	0.247467
26	6	0	-2.890526	3.064286	0.820677
27	6	0	-1.744776	4.536659	-0.683647
28	1	0	-0.376087	3.603257	-2.038201
29	1	0	-2.456903	0.984789	0.620195
30	1	0	-3.588622	2.905840	1.629674
31	1	0	-1.530663	5.532837	-1.042732
32	1	0	-3.135922	5.194573	0.809911
33	6	0	0.000000	0.000000	-7.832989
34	6	0	1.146144	-0.350381	-5.749967
35	6	0	-1.146144	0.350381	-5.749967
36	6	0	-1.146374	0.350114	-7.135304
37	6	0	1.146374	-0.350114	-7.135304
38	1	0	2.048397	-0.601544	-5.210728
39	1	0	-2.048397	0.601544	-5.210728
40	1	0	-2.045914	0.616498	-7.670916
41	1	0	2.045914	-0.616498	-7.670916
42	1	0	0.000000	0.000000	-8.913031
43	6	0	2.639136	-4.348036	0.358776
44	6	0	2.251166	-1.976611	0.247467
45	6	0	1.104764	-3.449447	-1.254781
46	6	0	1.744776	-4.536659	-0.683647
47	6	0	2.890526	-3.064286	0.820677
48	1	0	2.456903	-0.984789	0.620195
49	1	0	0.376087	-3.603257	-2.038201
50	1	0	1.530663	-5.532837	-1.042732
51	1	0	3.588622	-2.905840	1.629674
52	1	0	3.135922	-5.194573	0.809911
53	6	0	-2.639136	-4.348036	-0.358776
54	6	0	-1.104764	-3.449447	1.254781
55	6	0	-2.251166	-1.976611	-0.247467
56	6	0	-2.890526	-3.064286	-0.820677
57	6	0	-1.744776	-4.536659	0.683647
58	1	0	-0.376087	-3.603257	2.038201
59	1	0	-2.456903	-0.984789	-0.620195
60	1	0	-3.588622	-2.905840	-1.629674
61	1	0	-1.530663	-5.532837	1.042732
62	1	0	-3.135922	-5.194573	-0.809911
63	6	0	-0.000000	0.000000	7.832989

64	6	0	1.146144	0.350381	5.749967
65	6	0	-1.146144	-0.350381	5.749967
66	6	0	-1.146374	-0.350114	7.135304
67	6	0	1.146374	0.350114	7.135304
68	1	0	2.048397	0.601544	5.210728
69	1	0	-2.048397	-0.601544	5.210728
70	1	0	-2.045914	-0.616498	7.670916
71	1	0	2.045914	0.616498	7.670916
72	1	0	-0.000000	0.000000	8.913031
73	6	0	2.639136	4.348036	-0.358776
74	6	0	2.251166	1.976611	-0.247467
75	6	0	1.104764	3.449447	1.254781
76	6	0	1.744776	4.536659	0.683647
77	6	0	2.890526	3.064286	-0.820677
78	1	0	2.456903	0.984789	-0.620195
79	1	0	0.376087	3.603257	2.038201
80	1	0	1.530663	5.532837	1.042732
81	1	0	3.588622	2.905840	-1.629674
82	1	0	3.135922	5.194573	-0.809911

D2 2,2',4,4',6,6'-hexaphenylbiphenyl (2)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -1852.670073 au
E + ZPE = -1851.999556 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.337113	2.155019	-0.804950
2	6	0	-0.646923	1.020371	-1.459018
3	6	0	0.638347	-0.999625	-2.847304
4	6	0	0.000000	0.000000	-0.744556
5	6	0	-0.638347	0.999625	-2.847304
6	6	0	0.000000	0.000000	-3.564383
7	6	0	0.646923	-1.020371	-1.459018
8	6	0	-0.000000	0.000000	0.744556
9	1	0	-1.140661	1.795259	-3.376808
10	6	0	0.000000	0.000000	-5.038131
11	6	0	1.337113	-2.155019	-0.804950
12	1	0	1.140661	-1.795259	-3.376808
13	6	0	-0.000000	0.000000	3.564383
14	6	0	0.646923	1.020371	1.459018
15	6	0	-0.646923	-1.020371	1.459018
16	6	0	-0.638347	-0.999625	2.847304
17	6	0	0.638347	0.999625	2.847304
18	6	0	1.337113	2.155019	0.804950
19	6	0	-1.337113	-2.155019	0.804950
20	1	0	-1.140661	-1.795259	3.376808
21	1	0	1.140661	1.795259	3.376808
22	6	0	-0.000000	0.000000	5.038131
23	6	0	-2.599336	4.352326	0.369225
24	6	0	-1.111728	3.445476	-1.276934
25	6	0	-2.217855	1.984015	0.258710
26	6	0	-2.840657	3.072768	0.841494
27	6	0	-1.735503	4.533972	-0.697138
28	1	0	-0.402520	3.595578	-2.077904
29	1	0	-2.419626	0.993685	0.635810
30	1	0	-3.520139	2.918871	1.666377
31	1	0	-1.531284	5.527465	-1.067369
32	1	0	-3.082456	5.201182	0.829403
33	6	0	0.000000	0.000000	-7.831990
34	6	0	1.119021	-0.421083	-5.751656
35	6	0	-1.119021	0.421083	-5.751656
36	6	0	-1.119724	0.420630	-7.134359
37	6	0	1.119724	-0.420630	-7.134359
38	1	0	2.004581	-0.729042	-5.215576
39	1	0	-2.004581	0.729042	-5.215576
40	1	0	-2.000848	0.742655	-7.668972
41	1	0	2.000848	-0.742655	-7.668972
42	1	0	0.000000	0.000000	-8.911459
43	6	0	2.599336	-4.352326	0.369225
44	6	0	2.217855	-1.984015	0.258710
45	6	0	1.111728	-3.445476	-1.276934
46	6	0	1.735503	-4.533972	-0.697138
47	6	0	2.840657	-3.072768	0.841494
48	1	0	2.419626	-0.993685	0.635810
49	1	0	0.402520	-3.595578	-2.077904
50	1	0	1.531284	-5.527465	-1.067369
51	1	0	3.520139	-2.918871	1.666377
52	1	0	3.082456	-5.201182	0.829403
53	6	0	-2.599336	-4.352326	-0.369225
54	6	0	-1.111728	-3.445476	1.276934
55	6	0	-2.217855	-1.984015	-0.258710
56	6	0	-2.840657	-3.072768	-0.841494
57	6	0	-1.735503	-4.533972	0.697138
58	1	0	-0.402520	-3.595578	2.077904
59	1	0	-2.419626	-0.993685	-0.635810
60	1	0	-3.520139	-2.918871	-1.666377
61	1	0	-1.531284	-5.527465	1.067369
62	1	0	-3.082456	-5.201182	-0.829403
63	6	0	-0.000000	0.000000	7.831990

64	6	0	1.119021	0.421083	5.751656
65	6	0	-1.119021	-0.421083	5.751656
66	6	0	-1.119724	-0.420630	7.134359
67	6	0	1.119724	0.420630	7.134359
68	1	0	2.004581	0.729042	5.215576
69	1	0	-2.004581	-0.729042	5.215576
70	1	0	-2.000848	-0.742655	7.668972
71	1	0	2.000848	0.742655	7.668972
72	1	0	-0.000000	0.000000	8.911459
73	6	0	2.599336	4.352326	-0.369225
74	6	0	2.217855	1.984015	-0.258710
75	6	0	1.111728	3.445476	1.276934
76	6	0	1.735503	4.533972	0.697138
77	6	0	2.840657	3.072768	-0.841494
78	1	0	2.419626	0.993685	-0.635810
79	1	0	0.402520	3.595578	2.077904
80	1	0	1.531284	5.527465	1.067369
81	1	0	3.520139	2.918871	-1.666377
82	1	0	3.082456	5.201182	-0.829403

C2 Pentaphenylbenzene (3)
B3PW91/6-311++G(2d,p)-optimized
E = -1387.324868 au
E + ZPE = -1386.822291 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.243721
2	6	0	0.000000	0.000000	0.750152
3	6	0	-0.000000	-0.000000	-2.017393
4	6	0	0.000000	1.225407	0.054846
5	6	0	-0.000000	-1.225407	0.054846
6	6	0	0.005208	-1.220304	-1.350692
7	6	0	-0.005208	1.220304	-1.350692
8	6	0	0.020361	2.519048	0.796404
9	6	0	-0.020361	-2.519048	0.796404
10	6	0	0.031848	-2.456121	-2.177141
11	6	0	-0.031848	2.456121	-2.177141
12	1	0	-0.000000	-0.000000	-3.102130
13	6	0	0.069693	4.964025	2.163582
14	6	0	-1.044832	2.902355	1.612045
15	6	0	1.109458	3.382997	0.676128
16	6	0	1.137152	4.592549	1.356475
17	6	0	-1.022839	4.115050	2.286848
18	1	0	-1.899390	2.243309	1.717704
19	1	0	1.943431	3.102416	0.041762
20	1	0	1.995387	5.248002	1.252930
21	1	0	-1.862533	4.396321	2.913504
22	1	0	0.088741	5.910209	2.693596
23	6	0	0.000000	0.000000	5.044936
24	6	0	-1.101896	-0.471458	2.957279
25	6	0	1.101896	0.471458	2.957279
26	6	0	1.104650	0.468398	4.345346
27	6	0	-1.104650	-0.468398	4.345346
28	1	0	-1.965373	-0.845390	2.417945
29	1	0	1.965373	0.845390	2.417945
30	1	0	1.972799	0.836364	4.881857
31	1	0	-1.972799	-0.836364	4.881857
32	1	0	0.000000	0.000000	6.129623
33	6	0	-0.069693	-4.964025	2.163582
34	6	0	-1.109458	-3.382997	0.676128
35	6	0	1.044832	-2.902355	1.612045
36	6	0	1.022839	-4.115050	2.286848
37	6	0	-1.137152	-4.592549	1.356475
38	1	0	-1.943431	-3.102416	0.041762
39	1	0	1.899390	-2.243309	1.717704
40	1	0	1.862533	-4.396321	2.913504
41	1	0	-1.995387	-5.248002	1.252930
42	1	0	-0.088741	-5.910209	2.693596
43	6	0	0.108955	-4.715402	-3.835061
44	6	0	-0.929662	-2.648397	-3.171869
45	6	0	1.036327	-3.415059	-2.031638
46	6	0	1.076104	-4.531374	-2.854438
47	6	0	-0.895324	-3.769374	-3.990654
48	1	0	-1.720306	-1.915191	-3.294752
49	1	0	1.797224	-3.280366	-1.271851
50	1	0	1.869038	-5.261088	-2.729605
51	1	0	-1.657385	-3.903649	-4.751076
52	1	0	0.139172	-5.590784	-4.474776
53	6	0	-0.108955	4.715402	-3.835061
54	6	0	0.929662	2.648397	-3.171869
55	6	0	-1.036327	3.415059	-2.031638
56	6	0	-1.076104	4.531374	-2.854438
57	6	0	0.895324	3.769374	-3.990654
58	1	0	1.720306	1.915191	-3.294752
59	1	0	-1.797224	3.280366	-1.271851
60	1	0	-1.869038	5.261088	-2.729605
61	1	0	1.657385	3.903649	-4.751076
62	1	0	-0.139172	5.590784	-4.474776

C2 Pentaphenylbenzene (3)
M052X-D3/6-311++G(2d,p)-optimized
E = -1387.789770 au
E + ZPE = -1387.277759 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	2.218462
2	6	0	0.000000	0.000000	0.727701
3	6	0	-0.000000	-0.000000	-2.037098
4	6	0	-0.000000	1.219030	0.034079
5	6	0	-0.000000	-1.219030	0.034079
6	6	0	0.006507	-1.214588	-1.366070
7	6	0	-0.006507	1.214588	-1.366070
8	6	0	0.019951	2.508970	0.777403
9	6	0	-0.019951	-2.508970	0.777403
10	6	0	0.032485	-2.459647	-2.175735
11	6	0	-0.032485	2.459647	-2.175735
12	1	0	-0.000000	-0.000000	-3.118339
13	6	0	0.069203	4.935060	2.151615
14	6	0	-1.018690	2.855763	1.635328
15	6	0	1.082202	3.391869	0.614347
16	6	0	1.109508	4.596031	1.299443
17	6	0	-0.996392	4.062221	2.316042
18	1	0	-1.844434	2.171944	1.770911
19	1	0	1.887122	3.131615	-0.058829
20	1	0	1.942116	5.270889	1.164534
21	1	0	-1.810395	4.318788	2.978178
22	1	0	0.088535	5.874411	2.684532
23	6	0	0.000000	0.000000	5.006615
24	6	0	-1.073250	-0.532589	2.924235
25	6	0	1.073250	0.532589	2.924235
26	6	0	1.075731	0.530150	4.309851
27	6	0	-1.075731	-0.530150	4.309851
28	1	0	-1.906398	-0.955413	2.380687
29	1	0	1.906398	0.955413	2.380687
30	1	0	1.916809	0.945959	4.845155
31	1	0	-1.916809	-0.945959	4.845155
32	1	0	0.000000	0.000000	6.086780
33	6	0	-0.069203	-4.935060	2.151615
34	6	0	-1.082202	-3.391869	0.614347
35	6	0	1.018690	-2.855763	1.635328
36	6	0	0.996392	-4.062221	2.316042
37	6	0	-1.109508	-4.596031	1.299443
38	1	0	-1.887122	-3.131615	-0.058829
39	1	0	1.844434	-2.171944	1.770911
40	1	0	1.810395	-4.318788	2.978178
41	1	0	-1.942116	-5.270889	1.164534
42	1	0	-0.088535	-5.874411	2.684532
43	6	0	0.082442	-4.758155	-3.758018
44	6	0	-0.914960	-2.651739	-3.177080
45	6	0	1.011373	-3.430909	-1.981677
46	6	0	1.036968	-4.569947	-2.768328
47	6	0	-0.893452	-3.795277	-3.961321
48	1	0	-1.681909	-1.904645	-3.328151
49	1	0	1.753346	-3.290479	-1.209581
50	1	0	1.804203	-5.313199	-2.607823
51	1	0	-1.641614	-3.934102	-4.728156
52	1	0	0.100717	-5.649795	-4.367391
53	6	0	-0.082442	4.758155	-3.758018
54	6	0	0.914960	2.651739	-3.177080
55	6	0	-1.011373	3.430909	-1.981677
56	6	0	-1.036968	4.569947	-2.768328
57	6	0	0.893452	3.795277	-3.961321
58	1	0	1.681909	1.904645	-3.328151
59	1	0	-1.753346	3.290479	-1.209581
60	1	0	-1.804203	5.313199	-2.607823
61	1	0	1.641614	3.934102	-4.728156
62	1	0	-0.100717	5.649795	-4.367391

C2 Pentaphenylbenzene (3)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -1389.786780 au
E + ZPE = -1389.279836 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-0.000000	2.223898
2	6	0	0.000000	-0.000000	0.737224
3	6	0	-0.000000	0.000000	-2.020385
4	6	0	0.000000	1.219407	0.045172
5	6	0	-0.000000	-1.219407	0.045172
6	6	0	0.000968	-1.215096	-1.354446
7	6	0	-0.000968	1.215096	-1.354446
8	6	0	0.010807	2.505481	0.786516
9	6	0	-0.010807	-2.505481	0.786516
10	6	0	0.010571	-2.450611	-2.170740
11	6	0	-0.010571	2.450611	-2.170740
12	1	0	-0.000000	0.000000	-3.100685
13	6	0	0.032909	4.936093	2.152003
14	6	0	-1.021922	2.839644	1.654546
15	6	0	1.053733	3.407180	0.611723
16	6	0	1.068388	4.611129	1.292202
17	6	0	-1.013888	4.046765	2.329100
18	1	0	-1.834683	2.144331	1.802195
19	1	0	1.855402	3.161330	-0.069184
20	1	0	1.888347	5.298439	1.147131
21	1	0	-1.825982	4.291871	2.997099
22	1	0	0.041253	5.877090	2.681166
23	6	0	0.000000	-0.000000	5.011502
24	6	0	-1.058170	-0.556013	2.931995
25	6	0	1.058170	0.556013	2.931995
26	6	0	1.061379	0.552886	4.314970
27	6	0	-1.061379	-0.552886	4.314970
28	1	0	-1.881419	-0.998714	2.391071
29	1	0	1.881419	0.998714	2.391071
30	1	0	1.893167	0.986762	4.849452
31	1	0	-1.893167	-0.986762	4.849452
32	1	0	0.000000	-0.000000	6.091114
33	6	0	-0.032909	-4.936093	2.152003
34	6	0	-1.053733	-3.407180	0.611723
35	6	0	1.021922	-2.839644	1.654546
36	6	0	1.013888	-4.046765	2.329100
37	6	0	-1.068388	-4.611129	1.292202
38	1	0	-1.855402	-3.161330	-0.069184
39	1	0	1.834683	-2.144331	1.802195
40	1	0	1.825982	-4.291871	2.997099
41	1	0	-1.888347	-5.298439	1.147131
42	1	0	-0.041253	-5.877090	2.681166
43	6	0	0.024127	-4.725309	-3.787846
44	6	0	-0.921684	-2.604456	-3.191604
45	6	0	0.955621	-3.453287	-1.976952
46	6	0	0.963952	-4.577904	-2.780529
47	6	0	-0.919485	-3.733882	-3.991294
48	1	0	-1.663906	-1.834730	-3.346827
49	1	0	1.688459	-3.347824	-1.191882
50	1	0	1.708160	-5.343298	-2.618983
51	1	0	-1.658054	-3.839666	-4.771839
52	1	0	0.028954	-5.607418	-4.410222
53	6	0	-0.024127	4.725309	-3.787846
54	6	0	0.921684	2.604456	-3.191604
55	6	0	-0.955621	3.453287	-1.976952
56	6	0	-0.963952	4.577904	-2.780529
57	6	0	0.919485	3.733882	-3.991294
58	1	0	1.663906	1.834730	-3.346827
59	1	0	-1.688459	3.347824	-1.191882
60	1	0	-1.708160	5.343298	-2.618983
61	1	0	1.658054	3.839666	-4.771839
62	1	0	-0.028954	5.607418	-4.410222

D2 Biphenyl (4)
B3PW91/6-311++G(2d,p)-optimized
E = -463.247589 au
E + ZPE = -463.066580 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.739715
2	6	0	-0.415160	1.125114	-1.457548
3	6	0	-0.415813	1.125419	-2.845105
4	6	0	0.000000	0.000000	-3.545343
5	6	0	0.415813	-1.125419	-2.845105
6	6	0	0.415160	-1.125114	-1.457548
7	6	0	-0.000000	0.000000	0.739715
8	6	0	0.415160	1.125114	1.457548
9	6	0	0.415813	1.125419	2.845105
10	6	0	-0.000000	0.000000	3.545343
11	6	0	-0.415813	-1.125419	2.845105
12	6	0	-0.415160	-1.125114	1.457548
13	1	0	-0.764907	2.000457	-0.920582
14	1	0	-0.751066	2.006496	-3.381991
15	1	0	0.000000	0.000000	-4.629872
16	1	0	0.751066	-2.006496	-3.381991
17	1	0	0.764907	-2.000457	-0.920582
18	1	0	0.764907	2.000457	0.920582
19	1	0	0.751066	2.006496	3.381991
20	1	0	-0.000000	0.000000	4.629872
21	1	0	-0.751066	-2.006496	3.381991
22	1	0	-0.764907	-2.000457	0.920582

D2 Biphenyl (4)
M052X-D3/6-311++G(2d,p)-optimized
E = -463.3876118 au
E + ZPE = -463.203156 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	0.000000	-0.739782
2	6	0	-0.426389	1.119806	-1.450402
3	6	0	-0.426599	1.120107	-2.835826
4	6	0	-0.000000	0.000000	-3.533524
5	6	0	0.426599	-1.120107	-2.835826
6	6	0	0.426389	-1.119806	-1.450402
7	6	0	-0.000000	0.000000	0.739782
8	6	0	0.426389	1.119806	1.450402
9	6	0	0.426599	1.120107	2.835826
10	6	0	-0.000000	0.000000	3.533524
11	6	0	-0.426599	-1.120107	2.835826
12	6	0	-0.426389	-1.119806	1.450402
13	1	0	-0.782673	1.985678	-0.910704
14	1	0	-0.768400	1.993695	-3.371555
15	1	0	-0.000000	0.000000	-4.613545
16	1	0	0.768400	-1.993695	-3.371555
17	1	0	0.782673	-1.985678	-0.910704
18	1	0	0.782673	1.985678	0.910704
19	1	0	0.768400	1.993695	3.371555
20	1	0	-0.000000	0.000000	4.613545
21	1	0	-0.768400	-1.993695	3.371555
22	1	0	-0.782673	-1.985678	0.910704

D2 Biphenyl (4)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -464.057201 au
E + ZPE = -463.874747 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.737292
2	6	0	-0.389701	1.130054	-1.451145
3	6	0	-0.390197	1.130622	-2.833867
4	6	0	0.000000	0.000000	-3.531424
5	6	0	0.390197	-1.130622	-2.833867
6	6	0	0.389701	-1.130054	-1.451145
7	6	0	-0.000000	0.000000	0.737292
8	6	0	0.389701	1.130054	1.451145
9	6	0	0.390197	1.130622	2.833867
10	6	0	-0.000000	0.000000	3.531424
11	6	0	-0.390197	-1.130622	2.833867
12	6	0	-0.389701	-1.130054	1.451145
13	1	0	-0.718171	2.007929	-0.914563
14	1	0	-0.704807	2.014317	-3.368658
15	1	0	0.000000	0.000000	-4.610897
16	1	0	0.704807	-2.014317	-3.368658
17	1	0	0.718171	-2.007929	-0.914563
18	1	0	0.718171	2.007929	0.914563
19	1	0	0.704807	2.014317	3.368658
20	1	0	-0.000000	0.000000	4.610897
21	1	0	-0.704807	-2.014317	3.368658
22	1	0	-0.718171	-2.007929	0.914563

D6h Benzene (5)
B3PW91/6-311++G(2d,p)-optimized
E = -232.222093 au
E + ZPE = -232.121873 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.389745	0.000000
2	6	0	1.203555	0.694873	0.000000
3	6	0	1.203555	-0.694873	0.000000
4	6	0	-0.000000	-1.389745	0.000000
5	6	0	-1.203555	-0.694873	0.000000
6	6	0	-1.203555	0.694873	0.000000
7	1	0	0.000000	2.474552	0.000000
8	1	0	2.143025	1.237276	0.000000
9	1	0	2.143025	-1.237276	0.000000
10	1	0	-0.000000	-2.474552	0.000000
11	1	0	-2.143025	-1.237276	0.000000
12	1	0	-2.143025	1.237276	0.000000

D6h Benzene (5)
M052X-D3/6-311++G(2d,p)-optimized
E = -232.285170 au
E + ZPE = -232.183150 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.387187	0.000000
2	6	0	1.201339	0.693594	0.000000
3	6	0	1.201339	-0.693594	0.000000
4	6	0	-0.000000	-1.387187	0.000000
5	6	0	-1.201339	-0.693594	0.000000
6	6	0	-1.201339	0.693594	0.000000
7	1	0	0.000000	2.467494	0.000000
8	1	0	2.136913	1.233747	0.000000
9	1	0	2.136913	-1.233747	0.000000
10	1	0	-0.000000	-2.467494	0.000000
11	1	0	-2.136913	-1.233747	0.000000
12	1	0	-2.136913	1.233747	0.000000

D6h Benzene (5)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -232.622729 au
E + ZPE = -232.521693 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.385093	0.000000
2	6	0	1.199526	0.692546	0.000000
3	6	0	1.199526	-0.692546	0.000000
4	6	0	-0.000000	-1.385093	0.000000
5	6	0	-1.199526	-0.692546	0.000000
6	6	0	-1.199526	0.692546	0.000000
7	1	0	0.000000	2.464870	0.000000
8	1	0	2.134640	1.232435	0.000000
9	1	0	2.134640	-1.232435	0.000000
10	1	0	-0.000000	-2.464870	0.000000
11	1	0	-2.134640	-1.232435	0.000000
12	1	0	-2.134640	1.232435	0.000000

D3 1,3,5-triphenylbenzene (6)
B3PW91/6-311++G(2d,p)-optimized
E = -925.298328 au
E + ZPE = -924.956235 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.469556	-0.000000
2	6	0	0.000000	1.385072	-0.000000
3	6	0	-0.000000	-1.404233	0.000000
4	6	0	-1.216101	0.702116	-0.000000
5	6	0	1.216101	0.702116	0.000000
6	6	0	1.199508	-0.692536	0.000000
7	6	0	-1.199508	-0.692536	-0.000000
8	6	0	-2.498141	1.442302	-0.000000
9	6	0	2.498141	1.442302	0.000000
10	1	0	2.138698	-1.234778	0.000000
11	1	0	-2.138698	-1.234778	-0.000000
12	6	0	-0.000000	-2.884604	-0.000000
13	6	0	-4.927333	2.844797	-0.000000
14	6	0	-2.666618	2.585063	0.786695
15	6	0	-3.572039	1.016828	-0.786695
16	6	0	-4.773546	1.710932	-0.787659
17	6	0	-3.868484	3.278546	0.787659
18	1	0	-1.853985	2.918757	1.423222
19	1	0	-3.454710	0.146220	-1.423222
20	1	0	-5.591037	1.368665	-1.413299
21	1	0	-3.980817	4.157648	1.413299
22	1	0	-5.866561	3.387061	-0.000000
23	6	0	-0.000000	-5.689594	-0.000000
24	6	0	-0.905421	-3.601891	0.786695
25	6	0	0.905421	-3.601891	-0.786695
26	6	0	0.905062	-4.989478	-0.787659
27	6	0	-0.905062	-4.989478	0.787659
28	1	0	-1.600725	-3.064977	1.423222
29	1	0	1.600725	-3.064977	-1.423222
30	1	0	1.610220	-5.526312	-1.413299
31	1	0	-1.610220	-5.526312	1.413299
32	1	0	-0.000000	-6.774121	-0.000000
33	6	0	4.927333	2.844797	0.000000
34	6	0	3.572039	1.016828	0.786695
35	6	0	2.666618	2.585063	-0.786695
36	6	0	3.868484	3.278546	-0.787659
37	6	0	4.773546	1.710932	0.787659
38	1	0	3.454710	0.146220	1.423222
39	1	0	1.853985	2.918757	-1.423222
40	1	0	3.980817	4.157648	-1.413299
41	1	0	5.591037	1.368665	1.413299
42	1	0	5.866561	3.387061	0.000000

D3 1,3,5-triphenylbenzene (6)
M052X-D3/6-311++G(2d,p)-optimized
E = -925.593101 au
E + ZPE = -925.244634 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.464476	0.000000
2	6	0	0.000000	1.383687	0.000000
3	6	0	-0.000000	-1.397830	-0.000000
4	6	0	-1.210556	0.698915	-0.000000
5	6	0	1.210556	0.698915	-0.000000
6	6	0	1.198308	-0.691843	0.000000
7	6	0	-1.198308	-0.691843	0.000000
8	6	0	-2.492326	1.438945	-0.000000
9	6	0	2.492326	1.438945	0.000000
10	1	0	2.134299	-1.232238	0.000000
11	1	0	-2.134299	-1.232238	0.000000
12	6	0	-0.000000	-2.877890	-0.000000
13	6	0	-4.911060	2.835402	-0.000000
14	6	0	-2.658515	2.570955	0.794545
15	6	0	-3.555770	1.016864	-0.794545
16	6	0	-4.755478	1.709730	-0.794975
17	6	0	-3.858409	3.263500	0.794975
18	1	0	-1.848893	2.894289	1.433279
19	1	0	-3.430974	0.154044	-1.433279
20	1	0	-5.567520	1.374251	-1.423491
21	1	0	-3.973896	4.134488	1.423491
22	1	0	-5.846406	3.375424	-0.000000
23	6	0	-0.000000	-5.670803	-0.000000
24	6	0	-0.897255	-3.587819	0.794545
25	6	0	0.897255	-3.587819	-0.794545
26	6	0	0.897070	-4.973230	-0.794975
27	6	0	-0.897070	-4.973230	0.794975
28	1	0	-1.582081	-3.048333	1.433279
29	1	0	1.582081	-3.048333	-1.433279
30	1	0	1.593624	-5.508739	-1.423491
31	1	0	-1.593624	-5.508739	1.423491
32	1	0	-0.000000	-6.750848	-0.000000
33	6	0	4.911060	2.835402	0.000000
34	6	0	3.555770	1.016864	0.794545
35	6	0	2.658515	2.570955	-0.794545
36	6	0	3.858409	3.263500	-0.794975
37	6	0	4.755478	1.709730	0.794975
38	1	0	3.430974	0.154044	1.433279
39	1	0	1.848893	2.894289	-1.433279
40	1	0	3.973896	4.134488	-1.423491
41	1	0	5.567520	1.374251	1.423491
42	1	0	5.846406	3.375424	0.000000

D3 1,3,5-triphenylbenzene (6)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -926.926843 au
E + ZPE = -926.581857 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.463276	0.000000
2	6	0	0.000000	1.382784	0.000000
3	6	0	-0.000000	-1.400417	-0.000000
4	6	0	-1.212797	0.700208	-0.000000
5	6	0	1.212797	0.700208	-0.000000
6	6	0	1.197526	-0.691392	0.000000
7	6	0	-1.197526	-0.691392	0.000000
8	6	0	-2.491583	1.438516	0.000000
9	6	0	2.491583	1.438516	0.000000
10	1	0	2.133259	-1.231638	0.000000
11	1	0	-2.133259	-1.231638	0.000000
12	6	0	-0.000000	-2.877032	0.000000
13	6	0	-4.913480	2.836799	0.000000
14	6	0	-2.643107	2.603793	0.750901
15	6	0	-3.576504	0.987101	-0.750901
16	6	0	-4.775609	1.679281	-0.751036
17	6	0	-3.842104	3.296158	0.751036
18	1	0	-1.820537	2.952928	1.358441
19	1	0	-3.467579	0.100167	-1.358441
20	1	0	-5.601925	1.318512	-1.346030
21	1	0	-3.942827	4.192154	1.346030
22	1	0	-5.848781	3.376795	0.000000
23	6	0	-0.000000	-5.673598	0.000000
24	6	0	-0.933397	-3.590894	0.750901
25	6	0	0.933397	-3.590894	-0.750901
26	6	0	0.933505	-4.975439	-0.751036
27	6	0	-0.933505	-4.975439	0.751036
28	1	0	-1.647042	-3.053095	1.358441
29	1	0	1.647042	-3.053095	-1.358441
30	1	0	1.659098	-5.510665	-1.346030
31	1	0	-1.659098	-5.510665	1.346030
32	1	0	-0.000000	-6.753591	0.000000
33	6	0	4.913480	2.836799	0.000000
34	6	0	3.576504	0.987101	0.750901
35	6	0	2.643107	2.603793	-0.750901
36	6	0	3.842104	3.296158	-0.751036
37	6	0	4.775609	1.679281	0.751036
38	1	0	3.467579	0.100167	1.358441
39	1	0	1.820537	2.952928	-1.358441
40	1	0	3.942827	4.192154	-1.346030
41	1	0	5.601925	1.318512	1.346030
42	1	0	5.848781	3.376795	0.000000

C2 1,2,3,5-triphenylbenzene (7)
M052X-D3/6-311++G(2d,p)-optimized
E = -1156.691462 au
E + ZPE = -1156.261071 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	-0.000000	-2.095520
2	6	0	-0.000000	-0.000000	-0.608031
3	6	0	0.000000	0.000000	2.208459
4	6	0	1.207878	-0.001392	0.105136
5	6	0	-1.207878	0.001392	0.105136
6	6	0	-1.191296	-0.006162	1.495119
7	6	0	1.191296	0.006162	1.495119
8	6	0	2.531809	-0.029047	-0.569633
9	6	0	-2.531809	0.029047	-0.569633
10	1	0	-2.133230	-0.013740	2.025502
11	1	0	2.133230	0.013740	2.025502
12	6	0	0.000000	0.000000	3.687499
13	6	0	0.000000	0.000000	6.480463
14	6	0	0.916641	-0.772260	4.397567
15	6	0	-0.916641	0.772260	4.397567
16	6	0	-0.916582	0.772498	5.782932
17	6	0	0.916582	-0.772498	5.782932
18	1	0	1.617221	-1.393774	3.858294
19	1	0	-1.617221	1.393774	3.858294
20	1	0	-1.628578	1.383310	6.318607
21	1	0	1.628578	-1.383310	6.318607
22	1	0	0.000000	0.000000	7.560512
23	6	0	-5.047948	0.082419	-1.774796
24	6	0	-3.488282	-0.931669	-0.255383
25	6	0	-2.854029	1.023145	-1.489862
26	6	0	-4.103336	1.050415	-2.086006
27	6	0	-4.737767	-0.908490	-0.856794
28	1	0	-3.241350	-1.710040	0.453433
29	1	0	-2.119005	1.774600	-1.738469
30	1	0	-4.339947	1.829114	-2.796254
31	1	0	-5.466308	-1.666991	-0.609906
32	1	0	-6.020269	0.101938	-2.244791
33	6	0	-0.000000	-0.000000	-4.884369
34	6	0	-0.613983	-1.029325	-2.802073
35	6	0	0.613983	1.029325	-2.802073
36	6	0	0.611385	1.031896	-4.187603
37	6	0	-0.611385	-1.031896	-4.187603
38	1	0	-1.099190	-1.827887	-2.258587
39	1	0	1.099190	1.827887	-2.258587
40	1	0	1.090137	1.838749	-4.722946
41	1	0	-1.090137	-1.838749	-4.722946
42	1	0	-0.000000	-0.000000	-5.964531
43	6	0	5.047948	-0.082419	-1.774796
44	6	0	2.854029	-1.023145	-1.489862
45	6	0	3.488282	0.931669	-0.255383
46	6	0	4.737767	0.908490	-0.856794
47	6	0	4.103336	-1.050415	-2.086006
48	1	0	2.119005	-1.774600	-1.738469
49	1	0	3.241350	1.710040	0.453433
50	1	0	5.466308	1.666991	-0.609906
51	1	0	4.339947	-1.829114	-2.796254
52	1	0	6.020269	-0.101938	-2.244791

C2 1,2,3,5-triphenylbenzene (7)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -1158.356794 au
E + ZPE = -1157.930938 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-2.102202
2	6	0	0.000000	0.000000	-0.619569
3	6	0	-0.000000	-0.000000	2.199437
4	6	0	1.207217	0.000836	0.094773
5	6	0	-1.207217	-0.000836	0.094773
6	6	0	-1.187499	-0.009507	1.482833
7	6	0	1.187499	0.009507	1.482833
8	6	0	2.531109	-0.027850	-0.570161
9	6	0	-2.531109	0.027850	-0.570161
10	1	0	-2.129367	-0.019211	2.011418
11	1	0	2.129367	0.019211	2.011418
12	6	0	-0.000000	-0.000000	3.673416
13	6	0	-0.000000	-0.000000	6.467019
14	6	0	0.956938	-0.716958	4.386787
15	6	0	-0.956938	0.716958	4.386787
16	6	0	-0.956923	0.717729	5.769508
17	6	0	0.956923	-0.717729	5.769508
18	1	0	1.692628	-1.298048	3.850561
19	1	0	-1.692628	1.298048	3.850561
20	1	0	-1.702057	1.287666	6.304123
21	1	0	1.702057	-1.287666	6.304123
22	1	0	-0.000000	-0.000000	7.546494
23	6	0	-5.062017	0.089362	-1.744311
24	6	0	-3.503306	-0.901114	-0.214814
25	6	0	-2.849913	0.994214	-1.518960
26	6	0	-4.104401	1.026187	-2.098065
27	6	0	-4.757526	-0.874691	-0.799555
28	1	0	-3.264614	-1.659812	0.516606
29	1	0	-2.107739	1.724854	-1.801895
30	1	0	-4.335415	1.786334	-2.829200
31	1	0	-5.495748	-1.610803	-0.518294
32	1	0	-6.039510	0.112457	-2.201970
33	6	0	0.000000	0.000000	-4.890618
34	6	0	-0.634377	-1.013709	-2.811171
35	6	0	0.634377	1.013709	-2.811171
36	6	0	0.631000	1.017083	-4.194046
37	6	0	-0.631000	-1.017083	-4.194046
38	1	0	-1.136508	-1.802208	-2.270212
39	1	0	1.136508	1.802208	-2.270212
40	1	0	1.125194	1.814419	-4.728637
41	1	0	-1.125194	-1.814419	-4.728637
42	1	0	0.000000	0.000000	-5.970217
43	6	0	5.062017	-0.089362	-1.744311
44	6	0	2.849913	-0.994214	-1.518960
45	6	0	3.503306	0.901114	-0.214814
46	6	0	4.757526	0.874691	-0.799555
47	6	0	4.104401	-1.026187	-2.098065
48	1	0	2.107739	-1.724854	-1.801895
49	1	0	3.264614	1.659812	0.516606
50	1	0	5.495748	1.610803	-0.518294
51	1	0	4.335415	-1.786334	-2.829200
52	1	0	6.039510	-0.112457	-2.201970

D6 hexaphenylbenzene (8)
M052X-D3/6-311++G(2d,p)-optimized
E = -1618.888222 au
E + ZPE = -1618.294980 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000000	-1.399684	-0.000000
2	6	0	0.000000	1.399684	-0.000000
3	6	0	-1.212162	-0.699842	-0.000000
4	6	0	1.212162	-0.699842	-0.000000
5	6	0	1.212162	0.699842	0.000000
6	6	0	-1.212162	0.699842	-0.000000
7	6	0	2.502688	-1.444927	0.000000
8	6	0	4.917489	-2.839114	0.000000
9	6	0	3.384349	-1.329871	1.069201
10	6	0	2.843877	-2.265996	-1.069201
11	6	0	4.044902	-2.956896	-1.071597
12	6	0	4.583198	-2.024540	1.071597
13	6	0	2.502688	1.444927	-0.000000
14	6	0	4.917489	2.839114	-0.000000
15	6	0	2.843877	2.265996	1.069201
16	6	0	3.384349	1.329871	-1.069201
17	6	0	4.583198	2.024540	-1.071597
18	6	0	4.044902	2.956896	1.071597
19	6	0	0.000000	2.889855	0.000000
20	6	0	0.000000	5.678227	0.000000
21	6	0	-0.540472	3.595868	1.069201
22	6	0	0.540472	3.595868	-1.069201
23	6	0	0.538296	4.981436	-1.071597
24	6	0	-0.538296	4.981436	1.071597
25	6	0	-2.502688	1.444927	0.000000
26	6	0	-4.917489	2.839114	0.000000
27	6	0	-3.384349	1.329871	1.069201
28	6	0	-2.843877	2.265996	-1.069201
29	6	0	-4.044902	2.956896	-1.071597
30	6	0	-4.583198	2.024540	1.071597
31	6	0	-2.502688	-1.444927	0.000000
32	6	0	-4.917489	-2.839114	0.000000
33	6	0	-2.843877	-2.265996	1.069201
34	6	0	-3.384349	-1.329871	-1.069201
35	6	0	-4.583198	-2.024540	-1.071597
36	6	0	-4.044902	-2.956896	1.071597
37	6	0	-0.000000	-2.889855	0.000000
38	6	0	-0.000000	-5.678227	0.000000
39	6	0	0.540472	-3.595868	1.069201
40	6	0	-0.540472	-3.595868	-1.069201
41	6	0	-0.538296	-4.981436	-1.071597
42	6	0	0.538296	-4.981436	1.071597
43	1	0	5.852942	-3.379198	0.000000
44	1	0	3.128283	-0.686893	1.899374
45	1	0	2.159008	-2.365726	-1.899374
46	1	0	4.297374	-3.590166	-1.909507
47	1	0	5.257862	-1.926551	1.909507
48	1	0	5.852942	3.379198	-0.000000
49	1	0	2.159008	2.365726	1.899374
50	1	0	3.128283	0.686893	-1.899374
51	1	0	5.257862	1.926551	-1.909507
52	1	0	4.297374	3.590166	1.909507
53	1	0	0.000000	6.758395	0.000000
54	1	0	-0.969274	3.052619	1.899374
55	1	0	0.969274	3.052619	-1.899374
56	1	0	0.960488	5.516718	-1.909507
57	1	0	-0.960488	5.516718	1.909507
58	1	0	-5.852942	3.379198	0.000000
59	1	0	-3.128283	0.686893	1.899374
60	1	0	-2.159008	2.365726	-1.899374
61	1	0	-4.297374	3.590166	-1.909507
62	1	0	-5.257862	1.926551	1.909507
63	1	0	-5.852942	-3.379198	0.000000

64	1	0	-2.159008	-2.365726	1.899374
65	1	0	-3.128283	-0.686893	-1.899374
66	1	0	-5.257862	-1.926551	-1.909507
67	1	0	-4.297374	-3.590166	1.909507
68	1	0	-0.000000	-6.758395	0.000000
69	1	0	0.969274	-3.052619	1.899374
70	1	0	-0.969274	-3.052619	-1.899374
71	1	0	-0.960488	-5.516718	-1.909507
72	1	0	0.960488	-5.516718	1.909507

D6 hexaphenylbenzene (8)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -1621.217197 au
E + ZPE = -1620.629101 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.398854	-0.000000
2	6	0	-0.000000	1.398854	-0.000000
3	6	0	-1.211443	-0.699427	-0.000000
4	6	0	1.211443	-0.699427	-0.000000
5	6	0	1.211443	0.699427	-0.000000
6	6	0	-1.211443	0.699427	-0.000000
7	6	0	2.498389	-1.442446	-0.000000
8	6	0	4.912656	-2.836323	-0.000000
9	6	0	3.391307	-1.312381	1.056486
10	6	0	2.832208	-2.280767	-1.056486
11	6	0	4.031362	-2.969637	-1.059634
12	6	0	4.587462	-2.006443	1.059634
13	6	0	2.498389	1.442446	-0.000000
14	6	0	4.912656	2.836323	-0.000000
15	6	0	2.832208	2.280767	1.056486
16	6	0	3.391307	1.312381	-1.056486
17	6	0	4.587462	2.006443	-1.059634
18	6	0	4.031362	2.969637	1.059634
19	6	0	0.000000	2.884891	-0.000000
20	6	0	0.000000	5.672646	-0.000000
21	6	0	-0.559098	3.593148	1.056486
22	6	0	0.559098	3.593148	-1.056486
23	6	0	0.556101	4.976080	-1.059634
24	6	0	-0.556101	4.976080	1.059634
25	6	0	-2.498389	1.442446	-0.000000
26	6	0	-4.912656	2.836323	-0.000000
27	6	0	-3.391307	1.312381	1.056486
28	6	0	-2.832208	2.280767	-1.056486
29	6	0	-4.031362	2.969637	-1.059634
30	6	0	-4.587462	2.006443	1.059634
31	6	0	-2.498389	-1.442446	0.000000
32	6	0	-4.912656	-2.836323	0.000000
33	6	0	-2.832208	-2.280767	1.056486
34	6	0	-3.391307	-1.312381	-1.056486
35	6	0	-4.587462	-2.006443	-1.059634
36	6	0	-4.031362	-2.969637	1.059634
37	6	0	-0.000000	-2.884891	-0.000000
38	6	0	-0.000000	-5.672646	-0.000000
39	6	0	0.559098	-3.593148	1.056486
40	6	0	-0.559098	-3.593148	-1.056486
41	6	0	-0.556101	-4.976080	-1.059634
42	6	0	0.556101	-4.976080	1.059634
43	1	0	5.847632	-3.376132	-0.000000
44	1	0	3.145621	-0.656623	1.878570
45	1	0	2.141463	-2.395877	-1.878570
46	1	0	4.276038	-3.614761	-1.890149
47	1	0	5.268494	-1.895777	1.890149
48	1	0	5.847632	3.376132	-0.000000
49	1	0	2.141463	2.395877	1.878570
50	1	0	3.145621	0.656623	-1.878570
51	1	0	5.268494	1.895777	-1.890149
52	1	0	4.276038	3.614761	1.890149
53	1	0	0.000000	6.752263	-0.000000
54	1	0	-1.004159	3.052499	1.878570
55	1	0	1.004159	3.052499	-1.878570
56	1	0	0.992456	5.510538	-1.890149
57	1	0	-0.992456	5.510538	1.890149
58	1	0	-5.847632	3.376132	-0.000000
59	1	0	-3.145621	0.656623	1.878570
60	1	0	-2.141463	2.395877	-1.878570
61	1	0	-4.276038	3.614761	-1.890149
62	1	0	-5.268494	1.895777	1.890149
63	1	0	-5.847632	-3.376132	0.000000

64	1	0	-2.141463	-2.395877	1.878570
65	1	0	-3.145621	-0.656623	-1.878570
66	1	0	-5.268494	-1.895777	-1.890149
67	1	0	-4.276038	-3.614761	1.890149
68	1	0	-0.000000	-6.752263	-0.000000
69	1	0	1.004159	-3.052499	1.878570
70	1	0	-1.004159	-3.052499	-1.878570
71	1	0	-0.992456	-5.510538	-1.890149
72	1	0	0.992456	-5.510538	1.890149

C2 1,3-diphenylbenzene (9)
M052X-D3/6-311++G(2d,p)-optimized
E = -694.490248 au
E + ZPE = -694.223779 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005725	4.905122	-1.405332
2	6	0	-0.000000	0.000000	0.066044
3	6	0	-0.000000	0.000000	2.827476
4	6	0	-0.004670	1.213205	0.746471
5	6	0	0.004670	-1.213205	0.746471
6	6	0	0.004957	-1.201786	2.139064
7	6	0	-0.004957	1.201786	2.139064
8	6	0	-0.000000	2.491694	0.000874
9	6	0	-0.000000	-2.491694	0.000874
10	1	0	-0.016838	-2.136573	2.680083
11	1	0	0.016838	2.136573	2.680083
12	1	0	-0.000000	0.000000	3.907603
13	6	0	0.801515	3.850394	-1.826424
14	1	0	1.438381	1.842851	-1.446891
15	6	0	-0.792789	4.754430	-0.281606
16	1	0	0.007972	5.838153	-1.949029
17	1	0	-1.436833	3.436255	1.276661
18	6	0	0.798372	2.653371	-1.129025
19	1	0	-1.421948	5.567980	0.048519
20	6	0	-0.795014	3.557471	0.415848
21	1	0	0.000000	-0.000000	-1.014803
22	1	0	1.433021	3.962367	-2.695522
23	6	0	-0.005725	-4.905122	-1.405332
24	6	0	0.795014	-3.557471	0.415848
25	6	0	-0.798372	-2.653371	-1.129025
26	6	0	-0.801515	-3.850394	-1.826424
27	6	0	0.792789	-4.754430	-0.281606
28	1	0	1.436833	-3.436255	1.276661
29	1	0	-1.438381	-1.842851	-1.446891
30	1	0	-1.433021	-3.962367	-2.695522
31	1	0	1.421948	-5.567980	0.048519
32	1	0	-0.007972	-5.838153	-1.949029

C2 1,3-diphenylbenzene (9)
PW6B95-D3(BJ)/6-311++G(2d,p)-optimized
E = -695.491929 au
E + ZPE = -695.228156 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.001932	4.904639	-1.402299
2	6	0	0.000000	0.000000	0.068095
3	6	0	0.000000	0.000000	2.822202
4	6	0	-0.003858	1.214456	0.744005
5	6	0	0.003858	-1.214456	0.744005
6	6	0	0.003913	-1.199893	2.135837
7	6	0	-0.003913	1.199893	2.135837
8	6	0	-0.000000	2.488704	0.001240
9	6	0	-0.000000	-2.488704	0.001240
10	1	0	-0.018110	-2.132579	2.679313
11	1	0	0.018110	2.132579	2.679313
12	1	0	0.000000	0.000000	3.901968
13	6	0	0.738897	3.827907	-1.865775
14	1	0	1.334285	1.805286	-1.526366
15	6	0	-0.735834	4.775080	-0.237698
16	1	0	0.002811	5.837977	-1.944633
17	1	0	-1.332917	3.479324	1.350991
18	6	0	0.737457	2.632333	-1.170999
19	1	0	-1.320610	5.606073	0.127519
20	6	0	-0.735892	3.579397	0.456560
21	1	0	-0.000000	-0.000000	-1.012142
22	1	0	1.324872	3.921578	-2.767858
23	6	0	-0.001932	-4.904639	-1.402299
24	6	0	0.735892	-3.579397	0.456560
25	6	0	-0.737457	-2.632333	-1.170999
26	6	0	-0.738897	-3.827907	-1.865775
27	6	0	0.735834	-4.775080	-0.237698
28	1	0	1.332917	-3.479324	1.350991
29	1	0	-1.334285	-1.805286	-1.526366
30	1	0	-1.324872	-3.921578	-2.767858
31	1	0	1.320610	-5.606073	0.127519
32	1	0	-0.002811	-5.837977	-1.944633

C1 Decaphenylbiphenyl (1a)
B3PW91/6-31G(d)-optimized
E = -2772.722598 au
E + ZPE = -2771.732108 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.424012	-2.161401	-1.241285
2	6	0	-1.292589	-1.108453	-0.610620
3	6	0	-3.015476	0.705884	0.704873
4	6	0	-0.755089	-0.062645	0.185107
5	6	0	-2.693664	-1.199817	-0.784497
6	6	0	-3.552371	-0.295510	-0.125841
7	6	0	-1.617853	0.835439	0.843757
8	6	0	0.739238	0.125540	0.227368
9	6	0	-3.283864	-2.230487	-1.695629
10	6	0	-5.033740	-0.389457	-0.312766
11	6	0	-1.083736	1.967130	1.665743
12	6	0	-3.928032	1.649178	1.422127
13	6	0	3.547812	0.221727	-0.044425
14	6	0	1.559035	-0.623106	1.102365
15	6	0	1.332148	1.031083	-0.685760
16	6	0	2.738602	1.073593	-0.820126
17	6	0	2.962731	-0.604608	0.932014
18	6	0	1.010152	-1.343033	2.296902
19	6	0	0.516450	1.996721	-1.494667
20	6	0	3.376422	1.929229	-1.871032
21	6	0	3.822096	-1.544783	1.716051
22	6	0	5.017817	0.129232	-0.316893
23	6	0	-0.175899	4.118061	3.232894
24	6	0	-0.494343	1.743972	2.914267
25	6	0	-1.227250	3.287846	1.221622
26	6	0	-0.773725	4.352915	1.995800
27	6	0	-0.041535	2.809139	3.690722
28	1	0	-0.405083	0.730079	3.288197
29	1	0	-1.697133	3.479024	0.262306
30	1	0	-0.893869	5.370270	1.631319
31	1	0	0.409495	2.612142	4.660530
32	1	0	0.173741	4.950219	3.839340
33	6	0	-5.650387	3.406415	2.778013
34	6	0	-4.036217	1.609904	2.817561
35	6	0	-4.695776	2.583866	0.717164
36	6	0	-5.547234	3.457314	1.388938
37	6	0	-4.892448	2.478445	3.490037
38	1	0	-3.442240	0.892544	3.377566
39	1	0	-4.622584	2.624508	-0.366155
40	1	0	-6.133198	4.178352	0.824156
41	1	0	-4.964424	2.431232	4.573936
42	1	0	-6.316905	4.086536	3.302612
43	6	0	-7.817269	-0.556800	-0.661790
44	6	0	-5.867654	-0.757049	0.750344
45	6	0	-5.618086	-0.105344	-1.553089
46	6	0	-6.997608	-0.185222	-1.726137
47	6	0	-7.246842	-0.843719	0.577152
48	1	0	-5.429297	-0.972379	1.721113
49	1	0	-4.983036	0.177481	-2.388316
50	1	0	-7.432356	0.041534	-2.696601
51	1	0	-7.877193	-1.132744	1.414595
52	1	0	-8.894078	-0.621454	-0.796785
53	6	0	-4.407819	-4.142220	-3.426023
54	6	0	-4.137480	-3.227788	-1.206455
55	6	0	-3.007418	-2.207243	-3.068377
56	6	0	-3.565267	-3.151453	-3.926775
57	6	0	-4.690683	-4.177248	-2.061477
58	1	0	-4.370169	-3.256214	-0.145451
59	1	0	-2.345853	-1.441890	-3.465776
60	1	0	-3.338579	-3.113215	-4.989485
61	1	0	-5.348148	-4.944428	-1.659846
62	1	0	-4.842065	-4.881313	-4.094593
63	6	0	1.134397	-4.228225	-2.385865

64	6	0	-0.677277	-3.515021	-0.958836
65	6	0	0.630019	-1.876681	-2.120580
66	6	0	1.394726	-2.894409	-2.688718
67	6	0	0.091089	-4.533515	-1.514060
68	1	0	-1.498827	-3.774195	-0.297581
69	1	0	0.863626	-0.850174	-2.373881
70	1	0	2.198503	-2.637103	-3.374363
71	1	0	-0.132969	-5.568365	-1.267931
72	1	0	1.733834	-5.020548	-2.826907
73	6	0	0.059893	-2.586985	4.645839
74	6	0	1.456868	-0.939856	3.567259
75	6	0	0.082862	-2.386754	2.235023
76	6	0	-0.386623	-3.002696	3.394864
77	6	0	0.988733	-1.549844	4.726556
78	1	0	2.171692	-0.125579	3.640544
79	1	0	-0.251632	-2.744631	1.271223
80	1	0	-1.102057	-3.817768	3.314174
81	1	0	1.351771	-1.214045	5.694875
82	1	0	-0.306660	-3.068134	5.549209
83	6	0	5.432675	-3.356327	3.139527
84	6	0	4.778220	-1.087671	2.630723
85	6	0	3.688222	-2.926216	1.524796
86	6	0	4.487809	-3.823812	2.227830
87	6	0	5.573808	-1.984280	3.339556
88	1	0	4.893739	-0.019704	2.793403
89	1	0	2.951974	-3.294624	0.815338
90	1	0	4.370478	-4.892124	2.062823
91	1	0	6.307194	-1.608688	4.049043
92	1	0	6.055635	-4.056575	3.690501
93	6	0	7.765606	-0.094265	-0.862041
94	6	0	5.936283	1.011743	0.261943
95	6	0	5.498893	-0.869005	-1.171648
96	6	0	6.860623	-0.980118	-1.443478
97	6	0	7.298787	0.901958	-0.006757
98	1	0	5.579912	1.788684	0.933681
99	1	0	4.795577	-1.564897	-1.621511
100	1	0	7.214857	-1.762563	-2.110201
101	1	0	7.996781	1.596918	0.453906
102	1	0	8.828601	-0.180482	-1.072886
103	6	0	4.588673	3.497439	-3.866557
104	6	0	4.108265	3.075037	-1.537605
105	6	0	3.265376	1.582728	-3.222722
106	6	0	3.866252	2.357137	-4.212185
107	6	0	4.706291	3.854579	-2.524631
108	1	0	4.198484	3.364116	-0.493881
109	1	0	2.701931	0.695728	-3.500342
110	1	0	3.768161	2.068509	-5.255853
111	1	0	5.266400	4.743098	-2.243389
112	1	0	5.056810	4.103995	-4.637745
113	6	0	-0.894329	3.917656	-3.010050
114	6	0	0.750305	3.370796	-1.329053
115	6	0	-0.451354	1.611394	-2.431766
116	6	0	-1.147512	2.558996	-3.180776
117	6	0	0.059443	4.319469	-2.076538
118	1	0	1.476848	3.696322	-0.591898
119	1	0	-0.669914	0.561626	-2.588712
120	1	0	-1.888334	2.228143	-3.904723
121	1	0	0.266273	5.376037	-1.925192
122	1	0	-1.434678	4.655743	-3.597616

Decaphenylbiphenyl C1 to D2 transition state
B3PW91/6-31G(d)-optimized
E = -2772.721505 au
E + ZPE = -2771.730977 au
Number of imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.540892	-2.102569	-1.354749
2	6	0	-1.347402	-1.072063	-0.621576
3	6	0	-2.980845	0.721354	0.820664
4	6	0	-0.751926	-0.077644	0.198686
5	6	0	-2.755593	-1.118375	-0.758626
6	6	0	-3.570327	-0.223107	-0.038236
7	6	0	-1.577079	0.806686	0.928405
8	6	0	0.751909	0.077404	0.198610
9	6	0	-3.406793	-2.076409	-1.707575
10	6	0	-5.057718	-0.253394	-0.196808
11	6	0	-1.025151	1.890042	1.807971
12	6	0	-3.852565	1.673440	1.578529
13	6	0	3.570284	0.223301	-0.038419
14	6	0	1.577224	-0.806768	0.928331
15	6	0	1.347211	1.071849	-0.621759
16	6	0	2.755389	1.118427	-0.758806
17	6	0	2.980970	-0.721243	0.820496
18	6	0	1.025554	-1.890071	1.808132
19	6	0	0.540511	2.102119	-1.355061
20	6	0	3.406425	2.076551	-1.707775
21	6	0	3.852874	-1.673311	1.578183
22	6	0	5.057657	0.253691	-0.197145
23	6	0	-0.127069	3.959540	3.493631
24	6	0	-0.637673	1.629044	3.126243
25	6	0	-1.004318	3.217833	1.366014
26	6	0	-0.551110	4.240659	2.196637
27	6	0	-0.184108	2.648381	3.960991
28	1	0	-0.733954	0.620600	3.510585
29	1	0	-1.355677	3.451571	0.367363
30	1	0	-0.540065	5.263554	1.828151
31	1	0	0.109743	2.418203	4.982480
32	1	0	0.224649	4.758549	4.141717
33	6	0	-5.511104	3.451523	2.986213
34	6	0	-4.041365	1.534912	2.958310
35	6	0	-4.508264	2.717166	0.915131
36	6	0	-5.328412	3.600569	1.612571
37	6	0	-4.865369	2.414421	3.656746
38	1	0	-3.539398	0.728388	3.486264
39	1	0	-4.371570	2.834580	-0.156488
40	1	0	-5.827554	4.406382	1.079887
41	1	0	-5.001447	2.289064	4.728253
42	1	0	-6.152958	4.139449	3.530962
43	6	0	-7.852149	-0.295948	-0.492021
44	6	0	-5.882580	-0.665482	0.856716
45	6	0	-5.656526	0.138671	-1.400134
46	6	0	-7.041264	0.120331	-1.546484
47	6	0	-7.267394	-0.690181	0.710097
48	1	0	-5.432557	-0.967475	1.798599
49	1	0	-5.028675	0.456703	-2.228087
50	1	0	-7.487154	0.430313	-2.488467
51	1	0	-7.890671	-1.015656	1.539444
52	1	0	-8.933171	-0.312494	-0.606256
53	6	0	-4.662437	-3.836574	-3.506424
54	6	0	-4.273618	-3.075559	-1.246902
55	6	0	-3.184655	-1.973045	-3.086477
56	6	0	-3.807364	-2.842353	-3.978509
57	6	0	-4.891987	-3.950391	-2.136243
58	1	0	-4.463121	-3.165851	-0.180803
59	1	0	-2.512521	-1.205759	-3.461891
60	1	0	-3.621503	-2.743200	-5.045228
61	1	0	-5.558294	-4.721126	-1.756556
62	1	0	-5.147451	-4.517352	-4.201535
63	6	0	0.851514	-4.123630	-2.756180

64	6	0	-0.846181	-3.461437	-1.172100
65	6	0	0.487737	-1.785781	-2.252288
66	6	0	1.175623	-2.782492	-2.943852
67	6	0	-0.165765	-4.458291	-1.863353
68	1	0	-1.622296	-3.737584	-0.466438
69	1	0	0.760788	-0.751175	-2.423254
70	1	0	1.965215	-2.503036	-3.637255
71	1	0	-0.429974	-5.500135	-1.699808
72	1	0	1.384950	-4.899745	-3.299373
73	6	0	0.127970	-3.959493	3.494148
74	6	0	0.638874	-1.629081	3.126635
75	6	0	1.004198	-3.217830	1.366095
76	6	0	0.551238	-4.240615	2.196899
77	6	0	0.185551	-2.648382	3.961565
78	1	0	0.735556	-0.620681	3.510983
79	1	0	1.354970	-3.451581	0.367241
80	1	0	0.539772	-5.263482	1.828348
81	1	0	-0.107690	-2.418207	4.983230
82	1	0	-0.223561	-4.758471	4.142373
83	6	0	5.511773	-3.451390	2.985437
84	6	0	4.042618	-1.534327	2.957786
85	6	0	4.507802	-2.717489	0.914741
86	6	0	5.328138	-3.600886	1.611970
87	6	0	4.866797	-2.413842	3.656011
88	1	0	3.541244	-0.727452	3.485769
89	1	0	4.370358	-2.835257	-0.156743
90	1	0	5.826684	-4.407050	1.079259
91	1	0	5.003610	-2.288138	4.727384
92	1	0	6.153770	-4.139313	3.530021
93	6	0	7.852051	0.296363	-0.492683
94	6	0	5.882608	0.666091	0.856184
95	6	0	5.656356	-0.138629	-1.400442
96	6	0	7.041076	-0.120225	-1.546954
97	6	0	7.267405	0.690847	0.709404
98	1	0	5.432670	0.968300	1.798039
99	1	0	5.028433	-0.456906	-2.228247
100	1	0	7.486881	-0.430403	-2.488914
101	1	0	7.890754	1.016566	1.538601
102	1	0	8.933059	0.312956	-0.607044
103	6	0	4.661804	3.836892	-3.506635
104	6	0	4.273107	3.075827	-1.247109
105	6	0	3.184292	1.973151	-3.086675
106	6	0	3.806871	2.842546	-3.978712
107	6	0	4.891345	3.950747	-2.136456
108	1	0	4.462586	3.166162	-0.181009
109	1	0	2.512263	1.205771	-3.462084
110	1	0	3.621018	2.743364	-5.045429
111	1	0	5.557542	4.721580	-1.756774
112	1	0	5.146717	4.517737	-4.201750
113	6	0	-0.852219	4.122699	-2.756855
114	6	0	0.845430	3.461077	-1.172484
115	6	0	-0.487911	1.784991	-2.252717
116	6	0	-1.175956	2.781461	-2.944463
117	6	0	0.164847	4.457698	-1.863915
118	1	0	1.621385	3.737479	-0.466746
119	1	0	-0.760632	0.750295	-2.423666
120	1	0	-1.965379	2.501746	-3.637954
121	1	0	0.428770	5.499623	-1.700429
122	1	0	-1.385775	4.898631	-3.300192

D2 Decaphenylbiphenyl (1)
B3PW91/6-31G(d)-optimized
E = -2772.726655 au
E + ZPE = -2771.736043 au
Number of imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.477730	2.073673	-0.741424
2	6	0	-0.746898	0.973849	-1.452107
3	6	0	0.781460	-0.938881	-2.864967
4	6	0	0.000000	0.000000	-0.750977
5	6	0	-0.781460	0.938881	-2.864967
6	6	0	0.000000	0.000000	-3.567906
7	6	0	0.746898	-0.973849	-1.452107
8	6	0	0.000000	0.000000	0.750977
9	6	0	-1.664117	1.877438	-3.626162
10	6	0	0.000000	0.000000	-5.064540
11	6	0	1.477730	-2.073673	-0.741424
12	6	0	1.664117	-1.877438	-3.626162
13	6	0	0.000000	0.000000	3.567906
14	6	0	0.746898	0.973849	1.452107
15	6	0	-0.746898	-0.973849	1.452107
16	6	0	-0.781460	-0.938881	2.864967
17	6	0	0.781460	0.938881	2.864967
18	6	0	1.477730	2.073673	0.741424
19	6	0	-1.477730	-2.073673	0.741424
20	6	0	-1.664117	-1.877438	3.626162
21	6	0	1.664117	1.877438	3.626162
22	6	0	0.000000	0.000000	5.064540
23	6	0	2.861192	-4.212969	0.476853
24	6	0	2.448582	-1.842463	0.242565
25	6	0	1.203462	-3.406996	-1.083060
26	6	0	1.886221	-4.462284	-0.487315
27	6	0	3.134406	-2.897360	0.842462
28	1	0	2.680421	-0.830031	0.551774
29	1	0	0.434543	-3.616578	-1.819055
30	1	0	1.650336	-5.483400	-0.776209
31	1	0	3.888114	-2.684438	1.596786
32	1	0	3.399574	-5.035676	0.941034
33	6	0	3.352443	-3.604989	-5.065666
34	6	0	3.055919	-1.797366	-3.491982
35	6	0	1.133332	-2.837777	-4.496619
36	6	0	1.968565	-3.696273	-5.206403
37	6	0	3.893412	-2.650369	-4.206421
38	1	0	3.483549	-1.060078	-2.817482
39	1	0	0.056009	-2.911048	-4.616388
40	1	0	1.535627	-4.437329	-5.873914
41	1	0	4.971316	-2.569960	-4.088464
42	1	0	4.004769	-4.273389	-5.622106
43	6	0	0.000000	0.000000	-7.874844
44	6	0	1.143674	0.374461	-5.780313
45	6	0	-1.143674	-0.374461	-5.780313
46	6	0	-1.143494	-0.377728	-7.173028
47	6	0	1.143494	0.377728	-7.173028
48	1	0	2.040936	0.660738	-5.238111
49	1	0	-2.040936	-0.660738	-5.238111
50	1	0	-2.041140	-0.673448	-7.710625
51	1	0	2.041140	0.673448	-7.710625
52	1	0	0.000000	0.000000	-8.962013
53	6	0	-3.352443	3.604989	-5.065666
54	6	0	-1.133332	2.837777	-4.496619
55	6	0	-3.055919	1.797366	-3.491982
56	6	0	-3.893412	2.650369	-4.206421
57	6	0	-1.968565	3.696273	-5.206403
58	1	0	-0.056009	2.911048	-4.616388
59	1	0	-3.483549	1.060078	-2.817482
60	1	0	-4.971316	2.569960	-4.088464
61	1	0	-1.535627	4.437329	-5.873914
62	1	0	-4.004769	4.273389	-5.622106
63	6	0	-2.861192	4.212969	0.476853

64	6	0	-1.203462	3.406996	-1.083060
65	6	0	-2.448582	1.842463	0.242565
66	6	0	-3.134406	2.897360	0.842462
67	6	0	-1.886221	4.462284	-0.487315
68	1	0	-0.434543	3.616578	-1.819055
69	1	0	-2.680421	0.830031	0.551774
70	1	0	-3.888114	2.684438	1.596786
71	1	0	-1.650336	5.483400	-0.776209
72	1	0	-3.399574	5.035676	0.941034
73	6	0	2.861192	4.212969	-0.476853
74	6	0	2.448582	1.842463	-0.242565
75	6	0	1.203462	3.406996	1.083060
76	6	0	1.886221	4.462284	0.487315
77	6	0	3.134406	2.897360	-0.842462
78	1	0	2.680421	0.830031	-0.551774
79	1	0	0.434543	3.616578	1.819055
80	1	0	1.650336	5.483400	0.776209
81	1	0	3.888114	2.684438	-1.596786
82	1	0	3.399574	5.035676	-0.941034
83	6	0	3.352443	3.604989	5.065666
84	6	0	3.055919	1.797366	3.491982
85	6	0	1.133332	2.837777	4.496619
86	6	0	1.968565	3.696273	5.206403
87	6	0	3.893412	2.650369	4.206421
88	1	0	3.483549	1.060078	2.817482
89	1	0	0.056009	2.911048	4.616388
90	1	0	1.535627	4.437329	5.873914
91	1	0	4.971316	2.569960	4.088464
92	1	0	4.004769	4.273389	5.622106
93	6	0	0.000000	0.000000	7.874844
94	6	0	1.143674	-0.374461	5.780313
95	6	0	-1.143674	0.374461	5.780313
96	6	0	-1.143494	0.377728	7.173028
97	6	0	1.143494	-0.377728	7.173028
98	1	0	2.040936	-0.660738	5.238111
99	1	0	-2.040936	0.660738	5.238111
100	1	0	-2.041140	0.673448	7.710625
101	1	0	2.041140	-0.673448	7.710625
102	1	0	0.000000	0.000000	8.962013
103	6	0	-3.352443	-3.604989	5.065666
104	6	0	-1.133332	-2.837777	4.496619
105	6	0	-3.055919	-1.797366	3.491982
106	6	0	-3.893412	-2.650369	4.206421
107	6	0	-1.968565	-3.696273	5.206403
108	1	0	-0.056009	-2.911048	4.616388
109	1	0	-3.483549	-1.060078	2.817482
110	1	0	-4.971316	-2.569960	4.088464
111	1	0	-1.535627	-4.437329	5.873914
112	1	0	-4.004769	-4.273389	5.622106
113	6	0	-2.861192	-4.212969	-0.476853
114	6	0	-1.203462	-3.406996	1.083060
115	6	0	-2.448582	-1.842463	-0.242565
116	6	0	-3.134406	-2.897360	-0.842462
117	6	0	-1.886221	-4.462284	0.487315
118	1	0	-0.434543	-3.616578	1.819055
119	1	0	-2.680421	-0.830031	-0.551774
120	1	0	-3.888114	-2.684438	-1.596786
121	1	0	-1.650336	-5.483400	0.776209
122	1	0	-3.399574	-5.035676	-0.941034

End of Atomic Coordinates

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[S4] L. M. N. B. F. Santos, M. T. Silva, B. Schröder and L. Gomes, *J. Therm. Anal. Calorim.*, 2007, **89**, 175-180.

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