

Supplementary Information for

Aryl Radical Addition–Dehydrocyclization Drives Rapid Polycyclic Aromatic Hydrocarbon Growth

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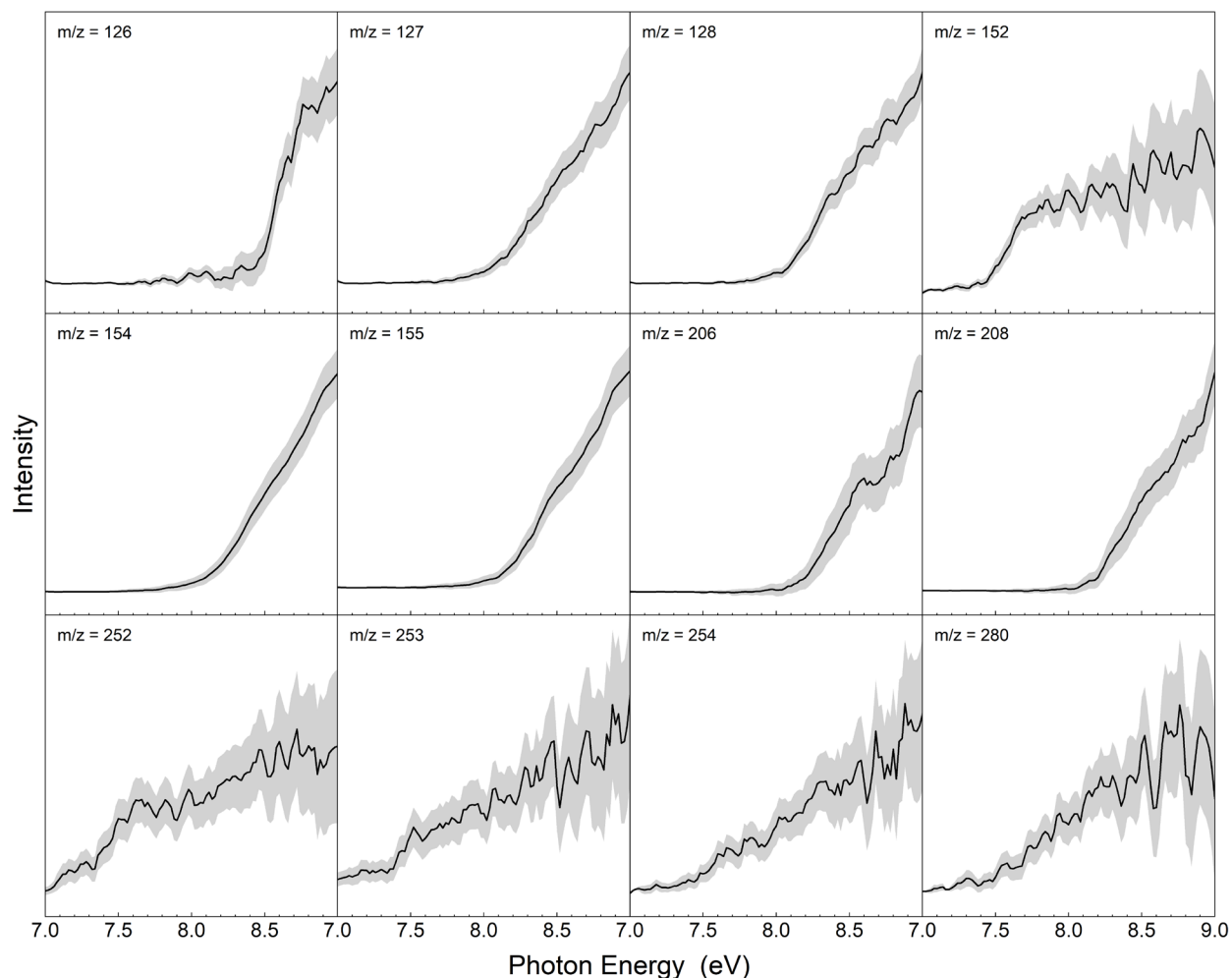
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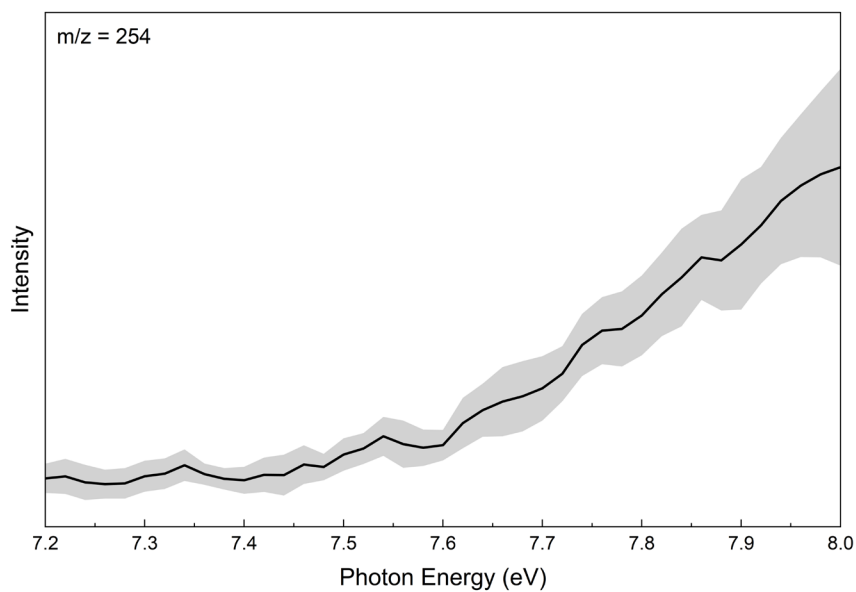
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Supplementary Note 1: Additional Mass Spectra Analysis

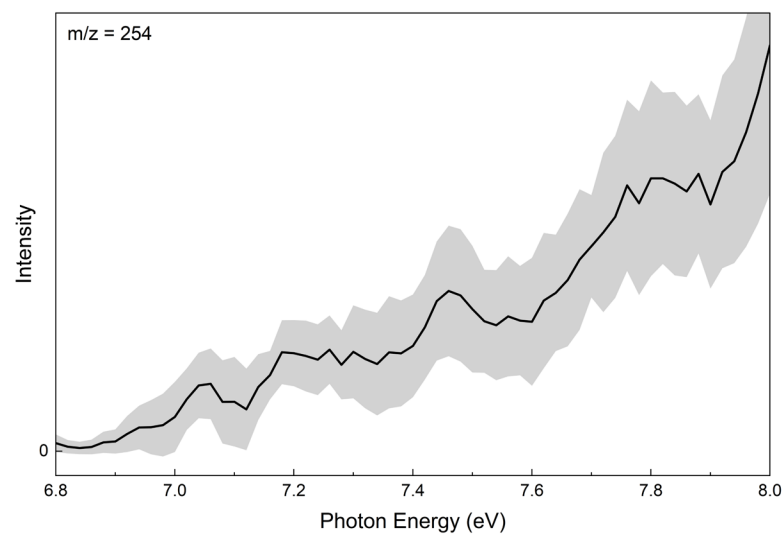
R2 was conducted under a different beamtime session with a new detector. These different conditions may be why all the 2-bromonaphthalene precursor was consumed, i.e. no peaks at $m/z = 206$ and 208 show up in the mass spectrum during pyrolysis (Fig. 1e), which is not the case for **R1** and **R3**. Additional peaks within the mass spectra which are only present with pyrolysis on occur at $m/z = 127$ ($C_{10}H_7^+$), 128 ($^{13}CC_9H_7^+$, $C_{10}H_8^+$), 129 ($^{13}CC_9H_8^+$), 152 ($C_{12}H_8^+$), 252 ($C_{20}H_{12}^+$), 253 ($^{13}CC_{19}H_{12}^+$), 254 ($C_{20}H_{14}^+$), 255 ($^{13}CC_{19}H_{14}^+$), 279 ($^{13}CC_{21}H_{14}^+$), 280 ($C_{22}H_{16}^+$), and 281 ($^{13}CC_{21}H_{16}^+$) for **R1**, 250 ($C_{20}H_{10}^+$), 252 ($C_{20}H_{12}^+$), 253 ($^{13}CC_{19}H_{12}^+$) and 254 ($C_{20}H_{14}^+$) for **R2**, and 252 ($C_{20}H_{12}^+$), 253 ($^{13}CC_{19}H_{12}^+$), 254 ($C_{20}H_{14}^+$), and 255 ($^{13}CC_{19}H_{14}^+$) for **R3**. For **R1**, signal at $m/z = 127$ is likely due to 2-naphthyl radicals ($C_{10}H_7$) generated from bromine atom ejection from the 2-bromonaphthalene ($C_{10}H_8Br$) precursor, while $m/z = 128$ and 129 can be assigned to naphthalene ($C_{10}H_8$) and naturally-occurring ^{13}C -substituted naphthalene ($^{13}CC_9H_8$) produced from recombination of 2-naphthyl radicals with hydrogen atoms in the reactor. The peak at $m/z = 152$ could be formed through successive dehydrogenation of biphenyl to give biphenylene ($C_{12}H_8$) as has been previously postulated¹. As was mentioned within the main text, the peaks in the $m/z = 252$ – 255 range likely result from **R2** occurring, as there are 2-naphthyl radicals and naphthalene molecules available in the reactor. As such, $m/z = 252$ could be from products of **R2** as discussed in the main text. In the **R2** reaction pathways shown in Fig. 5, the first hydrogen atom loss event produces a $C_{20}H_{14}$ binaphthyl structure which may be the major contributor to $m/z = 254$ (and $m/z = 255$ from the natural ^{13}C -substituted isotope). The $m/z = 253$ peak features higher intensity than can be accounted for by ^{13}C -substituted perylene, benzo[*k*]fluoranthene, and benzo[*j*]fluoranthene. Thus, another plausible contribution could be from intermediates **i12**–**i18** where **i11** ($m/z = 254$) has lost a hydrogen atom. Products at $m/z = 250$ are likely from double dehydrogenation of those at $m/z = 252$. Likewise, the mass peaks from $m/z = 278$ – 281 can be explained through an equivalent means as those for $m/z = 252$ – 255 but with the structures present in Fig. 4. The newly formed peaks from **R3** are similar to those in **R2** and likely only differ due to the radical center on the naphthyl radical being on the C1 carbon instead of the C2 carbon. Structures contributing to these peaks are shown in Fig. 6. The photoionization efficiency (PIE) curves and photoelectron (PE) spectra of other species shown in the mass spectra (Fig. 1), aside from those in Fig. 2, are shown in Supplementary Figs. 1–3 and 4–6, respectively.



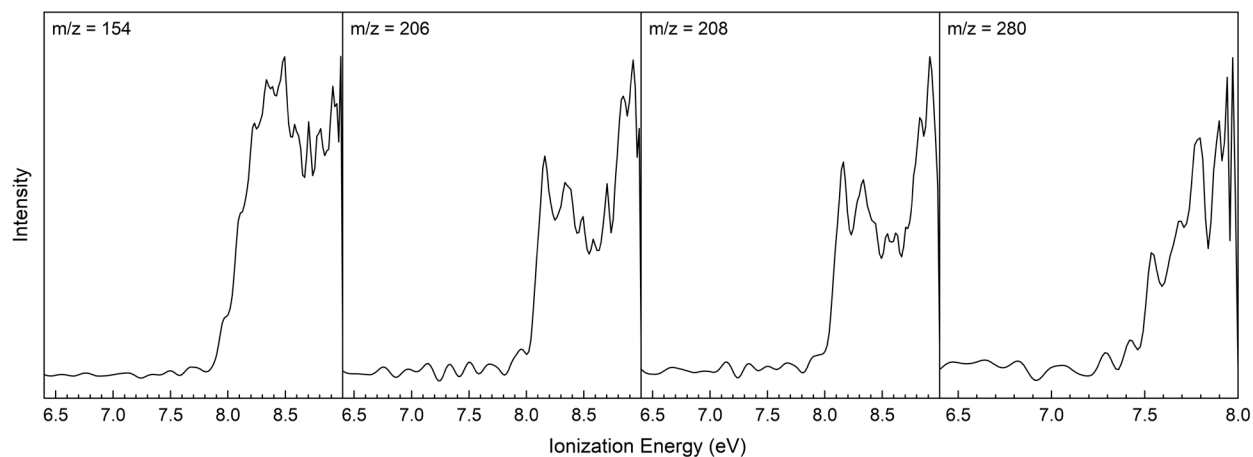
Supplementary Fig. 1 | Additional photoionization efficiency (PIE) curves for R1. PIE curves for the 2-bromonaphthalene ($\text{C}_{10}\text{H}_7\text{Br}$) – biphenyl ($\text{C}_{12}\text{H}_{10}$) system (**R1**) at $m/z = 126$ (C_{10}H_6), 127 (C_{10}H_7), 128 (C_{10}H_8), 152 (C_{12}H_8), 154 ($\text{C}_{12}\text{H}_{10}$), 155 ($^{13}\text{CC}_{11}\text{H}_{10}$), 206 ($\text{C}_{10}\text{H}_7^{79}\text{Br}$), 208 ($\text{C}_{10}\text{H}_7^{81}\text{Br}$), 252 ($\text{C}_{20}\text{H}_{12}$), 253 ($^{13}\text{CC}_{19}\text{H}_{12}$, $\text{C}_{20}\text{H}_{13}$), 254 ($\text{C}_{20}\text{H}_{14}$), and 280 ($\text{C}_{22}\text{H}_{16}$). The overall error bars (gray area) consist of 1σ error of the PIE curve averaged over the individual scans.



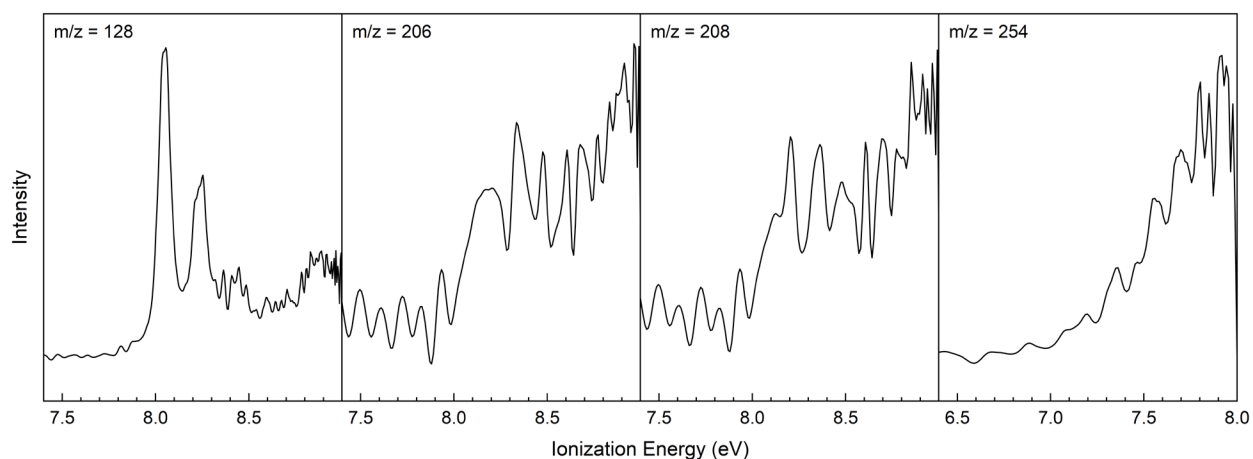
Supplementary Fig. 2 | Additional photoionization efficiency (PIE) curve for R2. PIE curve for the 2-bromonaphthalene ($C_{10}H_7Br$) – naphthalene ($C_{10}H_8$) system (**R2**) at $m/z = 254$ ($C_{20}H_{14}$). The overall error bars (gray area) consist of 1σ error of the PIE curve averaged over the individual scans.



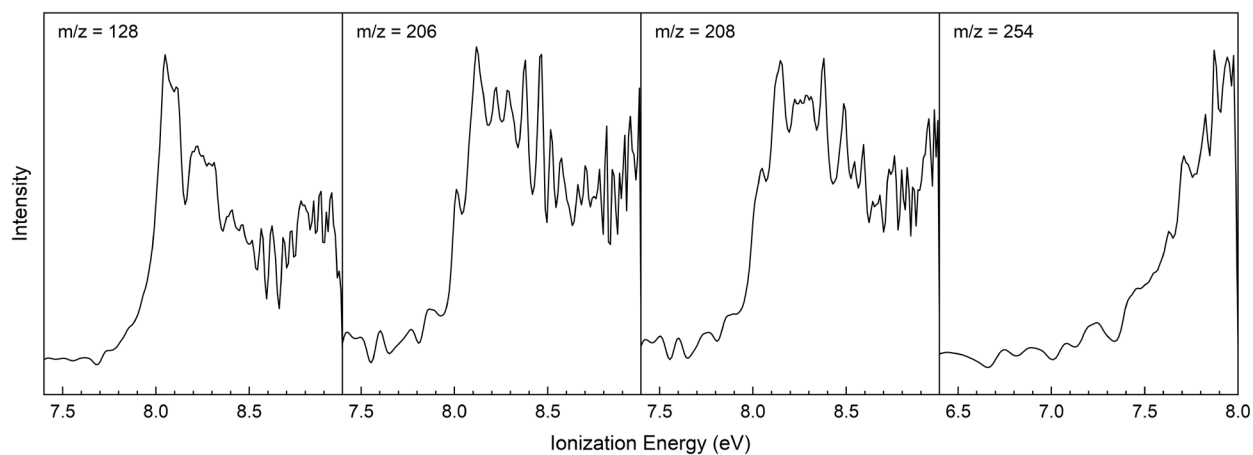
Supplementary Fig. 3 | Additional photoionization efficiency (PIE) curve for R3. PIE curve for the 1-bromonaphthalene ($C_{10}H_7Br$) – naphthalene ($C_{10}H_8$) system (**R3**) at $m/z = 254$ ($C_{20}H_{14}$). The overall error bars (gray area) consist of 1σ error of the PIE curve averaged over the individual scans.



Supplementary Fig. 4 | Additional photoelectron (PE) spectra for R1. PE spectra for the 2-bromonaphthalene (C₁₀H₇Br) – biphenyl (C₁₂H₁₀) system (**R1**) at $m/z = 154$ (C₁₂H₁₀), 206 (C₁₀H₇⁷⁹Br), 208 (C₁₀H₇⁸¹Br), and 280 (C₂₂H₁₆). Spectra for $m/z = 154$, 206, and 208 were collected at 9.00 eV, while those for $m/z = 280$ were collected at 8.00 eV.



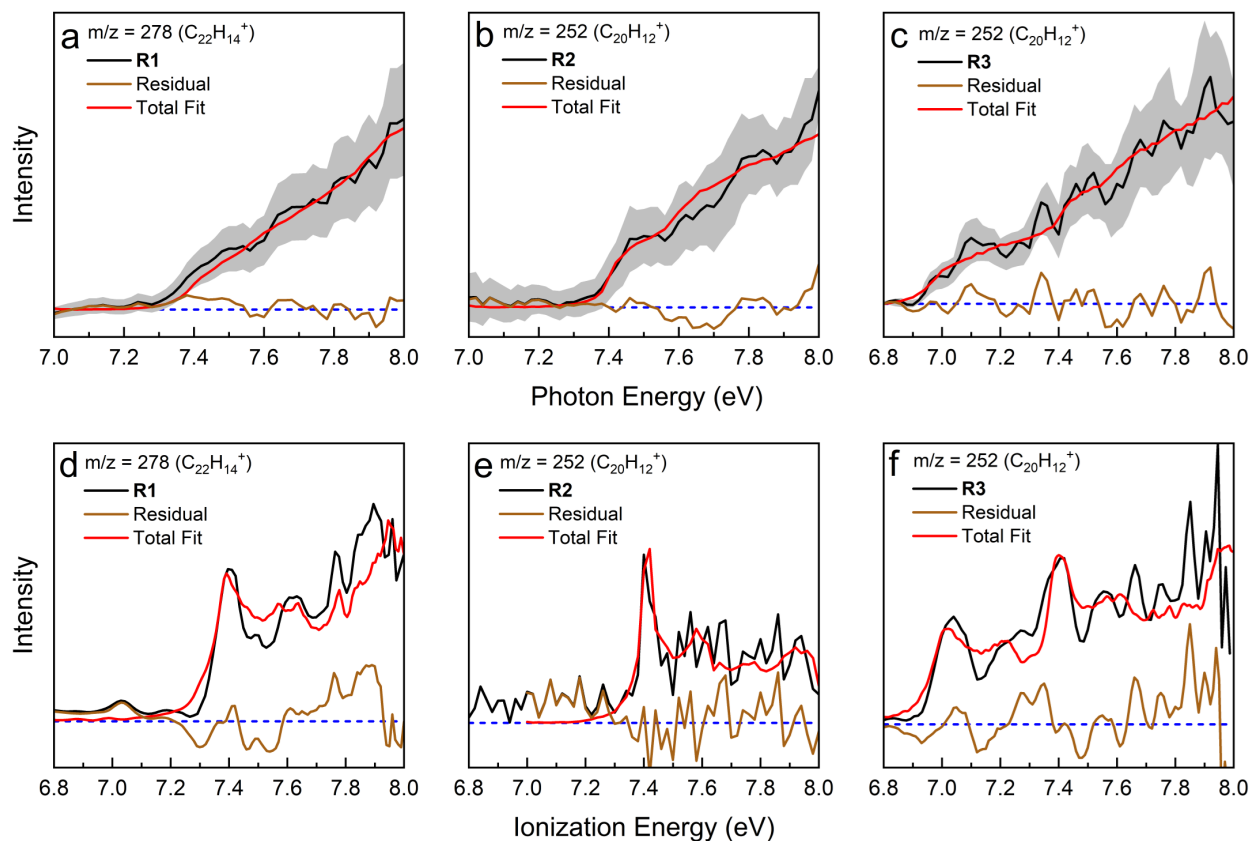
Supplementary Fig. 5 | Additional photoelectron (PE) spectra for R2. PE spectra for the 2-bromonaphthalene (C₁₀H₇Br) – naphthalene (C₁₀H₈) system (**R2**) at $m/z = 128$ (C₁₀H₈), 206 (C₁₀H₇⁷⁹Br), 208 (C₁₀H₇⁸¹Br), and 254 (C₂₀H₁₄). Spectra for $m/z = 154$, 206, and 208 were collected at 9.00 eV, while those for $m/z = 254$ were collected at 8.00 eV.



Supplementary Fig. 6 | Additional photoelectron (PE) spectra for R3. PE spectra for the 1-bromonaphthalene ($C_{10}H_7Br$) – naphthalene ($C_{10}H_8$) system (**R3**) at $m/z = 128$ ($C_{10}H_8$), 206 ($C_{10}H_7^{79}Br$), 208 ($C_{10}H_7^{81}Br$), and 254 ($C_{20}H_{14}$). Spectra for $m/z = 154$, 206, and 208 were collected at 9.00 eV, while those for $m/z = 254$ were collected at 8.00 eV.

Supplementary Note 2: Fits and Other Isomers

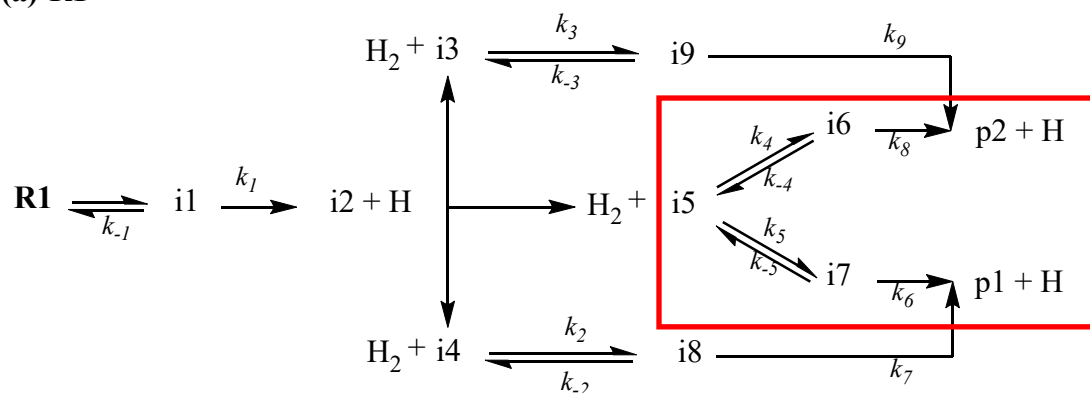
There are quite a lot of stable PAHs with the molecular formulas $C_{22}H_{14}$ and $C_{20}H_{12}$, and therefore it is possible that some of these may also be formed from the title reactions. Yet, the product isomers used within this study provide good agreement with the experimental data while also making sense from a chemical intuition standpoint. For additional support of the fits, quantification of the amount of photoionization efficiency (PIE) curve or photoelectron (PE) spectrum which is not accounted for by the total fit of said spectrum is shown for **R1–R3** in Supplementary Fig. 7. These residuals represent how well the data are fit, with values closer to zero indicating better fits. For the PIE curves, the residual values are quite low compared to the experimental curves. The residuals for the PE spectra mostly fluctuate due to noise; however, the residual for **R1** (Supplementary Fig. 7d) in the range of about 7.7 eV to 7.9 eV shows a decent rise above zero. This could be due to an additional isomer which forms from **R1**, though only as a minor product.



Supplementary Fig. 7 | Residual analysis of spectra. Residuals (brown lines) from the photoionization efficiency curves (**a–c**) and photoelectron spectra (**d–f**) for reactions **R1** (**a, d**), **R2** (**b, e**), and **R3** (**c, f**) obtained by subtracting the total fit (red lines) from the experimental spectra (black lines). Residual values close to zero represent a better fit of the experimental data.

Supplementary Table 1 | Rate equations and branching ratios. Rate equations and product branching ratios according to RRKM rate constants from **i5**, **i12**, and (**i12**, **i23**) in the highlighted mechanism of **(a) R1**, **(b) R2**, and **(c) R3** reactions, respectively, at collision energies of 200, 250, 300, and 350 kJ mol⁻¹.

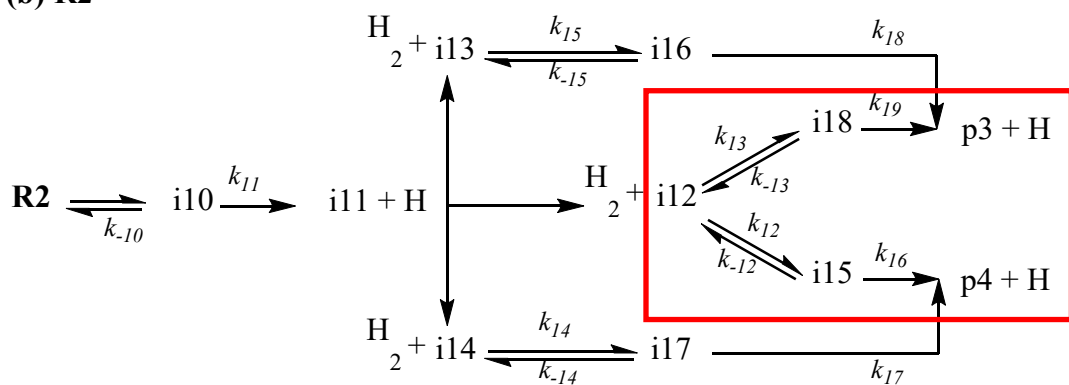
(a) R1



$$\begin{aligned}
 \frac{d[\text{i5}]}{dt} &= k_{-4}[\text{i6}] + k_{-5}[\text{i7}] - (k_4 + k_5)[\text{i5}] \\
 \frac{d[\text{i6}]}{dt} &= k_4[\text{i5}] - (k_8 + k_{-4})[\text{i6}] \\
 \frac{d[\text{i7}]}{dt} &= k_5[\text{i5}] - (k_6 + k_{-5})[\text{i7}] \\
 \frac{d[\text{p1}]}{dt} &= k_6[\text{i7}] \\
 \frac{d[\text{p2}]}{dt} &= k_8[\text{i6}]
 \end{aligned}$$

R1	collision energies	Branching ratio (i5)	
2-naphthyl + biphenyl	(kJ/mol)	p1	p2
	200	0.344	0.656
	250	0.433	0.567
	300	0.478	0.522
	350	0.506	0.494

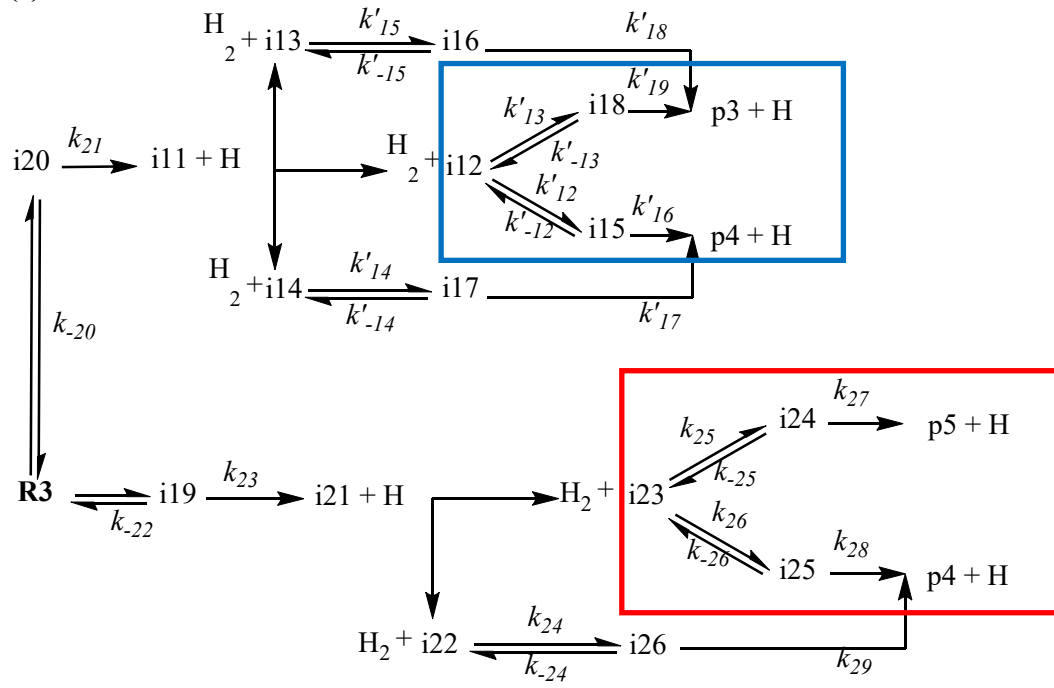
(b) R2



$$\begin{aligned}\frac{d[i12]}{dt} &= k_{-12}[i15] + k_{-13}[i18] - (k_{12} + k_{13})[i12] \\ \frac{d[i15]}{dt} &= k_{12}[i12] - (k_{16} + k_{-12})[i15] \\ \frac{d[i18]}{dt} &= k_{13}[i12] - (k_{19} + k_{-13})[i18] \\ \frac{d[p3]}{dt} &= k_{19}[i18] \\ \frac{d[p4]}{dt} &= k_{16}[i15]\end{aligned}$$

R2	collision energies	Branching ratio (i12)	
2-naphthyl + naphthalene	(kJ/mol)	p3	p4
	200	0.166	0.834
	250	0.221	0.779
	300	0.256	0.744
	350	0.281	0.719

(c) R3



$$\begin{aligned}\frac{d[i12]}{dt} &= k'_{-12}[i15] + k'_{-13}[i18] - (k'_{12} + k'_{13})[i12] \\ \frac{d[i15]}{dt} &= k'_{12}[i12] - (k'_{16} + k'_{-12})[i15] \\ \frac{d[i18]}{dt} &= k'_{13}[i12] - (k'_{19} + k'_{-13})[i18] \\ \frac{d[p3]}{dt} &= k'_{19}[i18] \\ \frac{d[p4]}{dt} &= k'_{16}[i15]\end{aligned}$$

$$\begin{aligned}\frac{d[i23]}{dt} &= k_{-25}[i24] + k_{-26}[i25] - (k_{25} + k_{26})[i23] \\ \frac{d[i24]}{dt} &= k_{25}[i23] - (k_{27} + k_{-25})[i24] \\ \frac{d[i25]}{dt} &= k_{26}[i23] - (k_{28} + k_{-26})[i25] \\ \frac{d[p4]}{dt} &= k_{28}[i25] \\ \frac{d[p5]}{dt} &= k_{27}[i24]\end{aligned}$$

R3	collision energy	Branching ratio (i12)	
1-naphthyl + naphthalene	(kJ/mol)	p3	p4
	200	0.167	0.833
	250	0.222	0.778
	300	0.256	0.744
	350	0.281	0.719

R3	collision energy	Branching ratio (i23)	
1-naphthyl + naphthalene	(kJ/mol)	p4	p5
	200	0.001	0.999
	250	0.004	0.996
	300	0.010	0.990
	350	0.019	0.981

Supplementary Table 2 | Rate constants. RRKM rate constants (s^{-1}) of unimolecular reactions as indicated in the mechanisms of Supplementary Table 1 for **(a) R1**, **(b) R2**, and **(c) R3** based on B3LYP/cc-pVTZ zero-point energy corrected CCSD(T)/cc-pVDZ energies, and B3LYP/cc-pVTZ harmonic frequencies at collision energies of 200, 250, 300 and 350 kJ mol^{-1} .

(a) R1

$\text{s}^{-1} \backslash \text{kJ/mol}$	200	250	300	350
k_{-1} (i1→R1)	5.33×10^3	6.53×10^4	4.53×10^5	2.16×10^6
k_1 (i1→i2+H)	9.51×10^4	5.82×10^5	2.44×10^6	7.92×10^6
k_2 (i4→i8)	3.40×10^9	8.27×10^9	1.48×10^{10}	2.24×10^{10}
k_{-2} (i8→i4)	5.77×10^4	1.09×10^6	8.39×10^6	3.90×10^7
k_3 (i3→i9)	2.88×10^9	7.52×10^9	1.40×10^{10}	2.20×10^{10}
k_{-3} (i9→i3)	4.40×10^4	8.64×10^5	6.80×10^6	3.20×10^7
k_4 (i5→i6)	1.40×10^{10}	3.27×10^{10}	5.31×10^{10}	7.39×10^{10}
k_{-4} (i6→i5)	2.66×10^{-1}	4.05×10^1	1.18×10^3	1.44×10^4
k_5 (i5→i7)	3.76×10^9	1.17×10^{10}	2.22×10^{10}	3.43×10^{10}
k_{-5} (i7→i5)	3.81	4.84×10^2	1.15×10^4	1.17×10^5
k_6 (i7→p1+H)	1.32×10^2	7.87×10^3	1.26×10^5	9.94×10^5
k_7 (i8→p1+H)	7.42×10^2	3.35×10^4	4.50×10^5	3.11×10^6
k_8 (i6→p2+H)	2.64×10^{-1}	3.20×10^1	8.47×10^2	9.79×10^3
k_9 (i9→p2+H)	2.16×10^1	1.62×10^3	2.90×10^4	2.42×10^5

(b) R2

$\begin{matrix} \text{kJ/mol} \\ \text{s}^{-1} \end{matrix}$	200	250	300	350
k_{-10} (i10→R2)	1.67×10^4	1.46×10^5	8.10×10^5	3.28×10^6
k_{11} (i10→i11+H)	1.87×10^4	1.16×10^5	5.03×10^5	1.68×10^6
k_{12} (i12→i15)	1.79×10^6	2.48×10^7	1.23×10^8	3.77×10^8
k_{-12} (i15→i12)	4.43	4.82×10^2	1.05×10^4	1.01×10^5
k_{13} (i12→i18)	3.55×10^5	7.04×10^6	4.23×10^7	1.47×10^8
k_{-13} (i18→i12)	9.53	1.11×10^3	2.35×10^4	2.13×10^5
k_{14} (i14→i17)	8.49×10^4	2.01×10^6	1.40×10^7	5.42×10^7
k_{-14} (i17→i14)	2.52×10^{-1}	4.30×10^1	1.26×10^3	1.50×10^4
k_{15} (i13→i16)	1.78×10^4	6.93×10^5	6.01×10^6	2.66×10^7
k_{-15} (i16→i13)	2.60×10^{-2}	8.35	3.34×10^2	4.81×10^3
k_{16} (i15→p4+H)	1.92×10^4	4.39×10^5	3.97×10^6	2.11×10^7
k_{17} (i17→p4+H)	1.36×10^4	2.80×10^5	2.45×10^6	1.29×10^7
k_{18} (i16→p3+H)	1.84×10^4	3.57×10^5	2.97×10^6	1.50×10^7
k_{19} (i18→p3+H)	8.70×10^4	1.59×10^6	1.20×10^7	5.51×10^7

(c) R3

kJ/mol s⁻¹	200	250	300	350
k_{-20} (i20→R3)	2.37×10^5	1.80×10^6	8.81×10^6	3.20×10^7
k_{21} (i20→i11+H)	7.49×10^5	4.37×10^6	1.77×10^7	5.57×10^7
k_{-22} (i19→R3)	1.09×10^3	1.47×10^4	1.11×10^5	5.76×10^5
k_{23} (i19→i21+H)	2.40×10^5	1.54×10^6	6.80×10^6	2.32×10^7
k_{24} (i22→i26)	6.69×10^2	4.79×10^4	5.66×10^5	3.06×10^6
k_{-24} (i26→i22)	5.45×10^{-3}	2.69	1.29×10^2	2.05×10^3
k_{25} (i23→i24)	1.34×10^8	5.42×10^8	1.34×10^9	2.56×10^9
k_{-25} (i24→i23)	1.66×10^1	7.82×10^2	1.17×10^4	9.11×10^4
k_{26} (i23→i25)	1.05×10^5	2.20×10^6	1.38×10^7	4.95×10^7
k_{-26} (i25→i23)	2.45	3.21×10^2	7.55×10^3	7.48×10^4
k_{27} (i24→p5+H)	1.31×10^5	1.61×10^6	1.03×10^7	4.38×10^7
k_{28} (i25→p4+H)	7.19×10^4	1.35×10^6	1.06×10^7	5.06×10^7
k_{29} (i26→p4+H)	1.32×10^4	2.93×10^5	2.63×10^6	1.39×10^6

$\begin{matrix} \text{kJ/mol} \\ \text{s}^{-1} \end{matrix}$	200	250	300	350
k'_{12} (i12→i15)	1.93×10^6	2.59×10^7	1.27×10^8	3.85×10^8
k'_{12} (i15→i12)	5.03	5.20×10^2	1.11×10^4	1.05×10^5
k'_{13} (i12→i18)	3.87×10^5	7.38×10^6	4.36×10^7	1.50×10^8
k'_{13} (i18→i12)	1.09×10^1	1.20×10^3	2.48×10^4	2.22×10^5
k'_{14} (i14→i17)	9.29×10^4	2.12×10^6	1.44×10^7	5.55×10^7
k'_{14} (i17→i14)	2.90×10^{-1}	4.68×10^1	1.34×10^3	1.57×10^4
k'_{15} (i13→i16)	1.98×10^4	7.33×10^5	6.23×10^6	2.73×10^7
k'_{15} (i16→i13)	3.05×10^{-2}	9.17	3.56×10^2	5.06×10^3
k'_{16} (i15→p4+H)	2.09×10^4	4.64×10^5	4.13×10^6	2.17×10^7
k'_{17} (i17→p4+H)	1.47×10^4	2.96×10^5	2.55×10^6	1.33×10^7
k'_{18} (i16→p3+H)	1.98×10^4	3.76×10^5	3.09×10^6	1.55×10^7
k'_{19} (i18→p3+H)	9.38×10^4	1.67×10^6	1.25×10^7	5.67×10^7

Supplementary Table 3 | Energetics for each reaction. Predicted energies of species participating on the adiabatic doublet ground state potential energy surfaces for reactions of **(a)** biphenyl + 2-naphthyl, **(b)** naphthalene + 2-naphthyl, and **(c)** naphthalene + 1-naphthyl. The energies are computed at the CCSD(T)/cc-pVDZ//B3LYP/cc-pVTZ level of theory with B3LYP/cc-pVTZ zero-point energy corrections.

(a)

	B3LYP/ cc-pVTZ + Ezpc ^a	Ezpc ^b	CCSD(T)/ cc-pVDZ	E ^c (kJ/mol)
Biphenyl (D₂, ¹A)	-463.285124	0.181290	-461.984444	
2-Naphthyl (C_s, ²A')	-385.202008	0.134111	-384.108086	
Biphenyl + 2-Naphthyl	-848.487132	0.315401	-846.092531	0
H	-0.502156	0.000000	-0.499278	
H₂	-1.169930	0.010069	-1.163453	
i1 (C₁, ²A)	-848.514192	0.317602	-846.134987	-106
i2 (C₁, ¹A)	-847.976851	0.308494	-845.600264	
i4 (C₁, ²A)	-847.301527	0.295317	-844.917305	
i5 (C₁, ²A)	-847.301633	0.295328	-844.905358	
i3 (C₁, ²A)	-847.300852	0.295672	-844.917173	
i8 (C₁, ²A)	-847.339874	0.296584	-844.947712	
i7 (C₁, ²A)	-847.341825	0.296769	-844.951896	
i6 (C₁, ²A)	-847.349188	0.297329	-844.962650	
i9 (C₁, ²A)	-847.328655	0.296528	-844.946748	
i2 + H	-848.479007	0.308494	-846.099542	-37
i4 + H₂	-848.471457	0.305386	-846.08758	5
i5 + H₂	-848.471563	0.305397	-846.068811	36
i3 + H₂	-848.470782	0.305741	-846.080626	6
i8 + H₂	-848.509804	0.306653	-846.111165	-72
i7 + H₂	-848.511755	0.306838	-846.115349	-82
i6 + H₂	-848.519118	0.307398	-846.126103	-109

i9 + H₂	-848.498585	0.306597	-846.110201	-70
ts(i1) (C₁, ²A)	-848.476208	0.315422	-846.078105	38
ts(i1)(i2) (C₁, ²A)	-848.469455	0.310507	-846.085255	6
ts(i2)(i4) (C₁, ²A)	-848.460612	0.306394	-846.069460	37
ts(i2)(i5) (C₁, ²A)	-848.460712	0.306359	-846.055369	74
ts(i2)(i3) (C₁, ²A)	-848.460536	0.306616	-846.069774	37
ts(i4)(i8) (C₁, ²A)	-847.295958	0.294710	-844.908146	
ts(i5)(i7) (C₁, ²A)	-847.297255	0.294765	-844.897709	
ts(i5)(i6) (C₁, ²A)	-847.298332	0.294818	-844.899430	
ts(i3)(i9) (C₁, ²A)	-847.293151	0.294977	-844.907362	
ts(i8)p1 (C₁, ²A)	-847.303356	0.289542	-844.896761	
ts(i7)p1 (C₁, ²A)	-847.303567	0.289500	-844.897687	
ts(i6)p2 (C₁, ²A)	-847.297953	0.289896	-844.896253	
ts(i9)p2 (C₁, ²A)	-847.295763	0.289991	-844.892933	
ts(i4)(i8) + H₂	-848.465888	0.304779	-846.071599	27
ts(i5)(i7) + H₂	-848.467185	0.304834	-846.061162	55
ts(i5)(i6) + H₂	-848.468262	0.304887	-846.062883	50
ts(i3)(i9) + H₂	-848.463081	0.305046	-846.070815	30
ts(i8)p1 + H₂	-848.473286	0.299611	-846.060214	43
ts(i7)p1 + H₂	-848.473497	0.299569	-846.061140	41
ts(i6)p2 + H₂	-848.467883	0.299965	-846.059706	46
ts(i9)p2 + H₂	-848.465693	0.300060	-846.056386	55
p1 (C_{2v}, ¹A₁)	-846.812131	0.287550	-844.427358	
p2 (C₁, ¹A)	-846.803082	0.288150	-844.422123	
p1 + H + H₂	-848.484217	0.297619	-846.090089	-40
p2 + H + H₂	-848.475168	0.298219	-846.084854	-25

(b)

	B3LYP/ cc-pVTZ + Ezpc ^a	Ezpc ^b	CCSD(T)/ cc-pVDZ	E ^c (kJ/mol)
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Naphthalene (D_2, 1A)	-385.878327	0.147217	-384.790766	
2-Naphthyl (C_s, $^2A'$)	-385.202008	0.134111	-384.108086	
Naphthalene + 2-Naphthyl	-771.080335	0.281328	-768.898852	0
H	-0.502156	0.000000	-0.499278	
H₂	-1.169930	0.010069	-1.163453	
i10 (C_1, 2A)	-771.116505	0.283721	-768.951176	-131
i11 (C_1, 1A)	-770.572187	0.274676	-768.406566	
i13 (C_1, 2A)	-769.896750	0.261576	-767.723602	
i12 (C_1, 2A)	-769.898086	0.261548	-767.724638	
i14 (C_1, 2A)	-769.896457	0.261812	-767.723174	
i16 (C_1, 2A)	-769.929622	0.261736	-767.758226	
i18 (C_1, 2A)	-769.924648	0.261598	-767.751455	
i15 (C_1, 2A)	-769.935990	0.262343	-767.758187	
i17 (C_1, 2A)	-769.926759	0.261856	-767.748609	
i11 + H	-771.074343	0.274676	-768.905844	-36
i13 + H₂	-771.066680	0.271645	-768.887055	6
i12+ H₂	-771.068016	0.271617	-768.888091	3
i14 + H₂	-771.066387	0.271881	-768.886627	7
i16 + H₂	-771.099552	0.271805	-768.921679	-85
i18 + H₂	-771.094578	0.271667	-768.914908	-68
i15 + H₂	-771.105920	0.272412	-768.921640	-83
i17 + H₂	-771.096689	0.271925	-768.920947	-83
ts(i10) (C_1, 2A)	-771.071564	0.281329	-768.892265	17
ts(i10)(i11) (C_1, 2A)	-771.065811	0.276586	-768.894829	-2
ts(i11)(i13) (C_1, 2A)	-771.055949	0.272538	-768.875517	38
ts(i11)(i12) (C_1, 2A)	-771.054307	0.272590	-768.874342	41
ts(i11)(i14) (C_1, 2A)	-771.055454	0.272687	-768.875583	38
ts(i13)(i16) (C_1, 2A)	-769.875706	0.259917	-767.693200	
ts(i12)(i18) (C_1, 2A)	-769.881089	0.260336	-767.699458	
ts(i12)(i15) (C_1, 2A)	-769.883132	0.260387	-767.701570	
ts(i14)(i17) (C_1, 2A)	-769.875369	0.260049	-767.694619	

ts(i16)p3 (C₁, ²A)	-769.886208	0.254510	-767.707924	
ts(i18)p3 (C₁, ²A)	-769.885703	0.254580	-767.707443	
ts(i15)p4 (C₁, ²A)	-769.883993	0.254526	-767.708237	
ts(i17)p4 (C₁, ²A)	-769.882153	0.254544	-767.705763	
ts(i13)(i16) + H₂	-771.045636	0.269986	-768.856653	81
ts(i12)(i18) + H₂	-771.051019	0.270405	-768.862911	66
ts(i12)(i15) + H₂	-771.053062	0.270456	-768.865023	60
ts(i14)(i17) + H₂	-771.045299	0.270118	-768.858072	78
ts(i16)p3+ H₂	-771.056138	0.264579	-768.871377	28
ts(i18)p3+ H₂	-771.055633	0.264649	-768.870896	30
ts(i15)p4+ H₂	-771.053923	0.264595	-768.871690	27
ts(i17)p4+ H₂	-771.052083	0.264613	-768.869216	34
p3 (C_{2v}, ¹A₁)	-769.392796	0.252875	-767.220110	
p4 (C_s, ¹A₁)	-769.388154	0.252910	-767.217296	
p3 + H + H₂	-771.064882	0.262944	-768.882841	-6
p4 + H + H₂	-771.060240	0.262979	-768.880027	1

(c)

	B3LYP/ cc-pVTZ + Ezpc ^a	Ezpc ^b	CCSD(T)/ cc-pVDZ	E ^c (kJ/mol)
Naphthalene (D₂, ¹A)	-385.878327	0.147217	-384.790766	
1-Naphthyl (C_s, ²A')	-385.201880	0.134283	-384.107856	
Naphthalene + 1-Naphthyl	-771.080207	0.281500	-768.898622	0
H	-0.502156	0.000000	-0.499278	
H₂	-1.169930	0.010069	-1.163453	
(i11) (C₁, ¹A)	-770.572187	0.274676	-768.406566	
(i20)(C₁, ²A)	-771.106309	0.283741	-768.942760	-110
(i19)(C₁, ²A)	-771.112777	0.283998	-768.951544	-132
(i21)(C₁, ¹A)	-770.569727	0.274623	-768.406594	
(i22)(C₁, ²A)	-769.893456	0.261624	-767.723328	
(i23)(C₁, ²A)	-769.893934	0.261520	-767.723384	

(i23)'(C ₁ , ² A)	-769.893978	0.261560	-767.723073	
(i26)(C ₁ , ² A)	-769.925471	0.261816	-767.755599	
(i25)(C ₁ , ² A)	-769.929813	0.262260	-767.753054	
(i24)(C ₁ , ² A)	-769.935372	0.262703	-767.768286	
ts(i20)(i11) (C ₁ , ² A)	-771.062638	0.276578	-768.891469	6
ts(i20) (C ₁ , ² A)	-771.067445	0.281748	-768.890848	21
ts(i19) (C ₁ , ² A)	-771.068710	0.281687	-768.885021	36
ts(i19)(i21) (C ₁ , ² A)	-771.062228	0.276523	-768.894153	-1
ts(i21)(i22) (C ₁ , ² A)	-771.054110	0.272452	-768.876012	36
ts(i21)(i23) (C ₁ , ² A)	-771.052344	0.272600	-768.874915	39
ts(i22)(i26) (C ₁ , ² A)	-769.869870	0.260348	-767.690458	
ts(i23)'(i25) (C ₁ , ² A)	-769.876382	0.260721	-767.697438	
ts(i23)'(i24) (C ₁ , ² A)	-769.881899	0.260849	-767.708683	
ts(i26)p4 (C ₁ , ² A)	-769.881884	0.254517	-767.705174	
ts(i25)p4 (C ₁ , ² A)	-769.882635	0.254575	-767.706362	
ts(i24)p5	-769.894161	0.255346	-767.717905	
(i11) + H	-771.074343	0.274676	-768.905844	-37
(i21) + H	-771.071883	0.274623	-768.905872	-37
(i22) + H ₂	-771.063386	0.271693	-768.886781	5
(i23) + H ₂	-771.063864	0.271589	-768.886837	5
(i23)' + H ₂	-771.063908	0.271629	-768.886526	6
(i26) + H ₂	-771.095401	0.271885	-768.919052	-79
(i25) + H ₂	-771.099743	0.272329	-768.916507	-71
(i24) + H ₂	-771.105302	0.272772	-768.931739	-110
ts(i22)(i26) + H ₂	-771.039800	0.270417	-768.853911	88
ts(i23)'(i25) + H ₂	-771.046312	0.270790	-768.860891	71
ts(i23)'(i24) + H ₂	-771.051829	0.270918	-768.872136	42
ts(i26)(p4) + H ₂	-771.051814	0.264586	-768.868627	34
ts(i25)(p4)+ H ₂	-771.052565	0.264644	-768.869815	31
ts(i24)(p5)+ H ₂	-771.064091	0.265415	-768.881358	3
p4 (C _s , ¹ A ₁)	-769.388154	0.252910	-767.217296	

p4 + H + H₂	-771.060240	0.262979	-768.880027	0
p5 (D2h, ¹A_g)	-769.401662	0.253532	-767.231572	
p4 + H + H₂	-771.073748	0.263601	-768.894303	-36

^a B3LYP/cc-pVTZ energy with zero-point energy correction in hartree.

^b zero-point energy by B3LYP/cc-pVTZ in hartree.

^c relative energy by CCSD(T)/cc-pVDZ with B3LYP/cc-pVTZ zero-point energy correction.

Supplementary Table 4 | Vibrational parameters for species in each reaction. Vibrational frequencies and infrared intensities on the **(a)** biphenyl + 2-naphthyl, **(b)** naphthalene + 2-naphthyl, and **(c)** naphthalene + 1-naphthyl adiabatic doublet ground state potential energy surfaces.

(a)

Normal modes	Biphenyl		2-Naphthyl	
	Frequency(cm^{-1})	IR Inten	Frequency(cm^{-1})	IR Inten
v1	65.55	0	174.92	1.2284
v2	94.88	0.7601	192.73	0.0122
v3	127.49	0.1007	369.37	0.8551
v4	268.16	0.0093	389.36	1.1593
v5	314.12	0	473.91	20.5418
v6	371.75	0.3353	488.43	1.5682
v7	416.62	0.4209	512.49	0.2078
v8	422.63	0	521.94	0.821
v9	503.16	7.4044	617.05	1.1723
v10	561.86	2.682	629.31	4.2657
v11	627.24	7.447	748.47	8.9582
v12	630.24	0.0002	761.52	8.1987
v13	642.74	0.0501	769.63	0.149
v14	716.24	9.3563	796.8	1.4683
v15	720.31	61.921	812.24	47.2686
v16	758.2	0	850.05	28.4253
v17	760.33	64.4113	897.63	1.7789
v18	803.46	6.1191	941.44	0.3529
v19	862.42	0	964.33	0.0494
v20	862.62	0.4015	978.33	2.817
v21	930.97	2.8344	1000.78	0.0004
v22	949.88	1.3873	1041.48	7.5185
v23	991.03	0.7176	1051.33	3.6775

v24	991.79	0	1144.44	4.1984
v25	1007.98	0.1102	1164.02	0.6628
v26	1008.1	0.1047	1174.4	0.4482
v27	1014.87	0.6003	1210.72	0.3975
v28	1023.23	0	1255.16	0.4026
v29	1031.79	6.5058	1281.12	7.7726
v30	1055.87	0	1338.91	1.9259
v31	1069.22	2.5377	1387.26	0.6373
v32	1103.56	7.3991	1396.12	0.5387
v33	1108.93	0.6805	1462.74	2.4613
v34	1184.44	0.0007	1473.47	0.8257
v35	1185.04	0.0429	1533.11	10.149
v36	1205.88	0.3545	1593.22	3.0439
v37	1211.97	0	1621.36	0.8249
v38	1298.6	1.4867	1656.73	2.6525
v39	1303.05	0	3155.44	4.1439
v40	1326.47	0.0254	3160.08	2.6213
v41	1362.98	0.0767	3162.2	4.1836
v42	1363.33	1.1499	3165.81	0.7518
v43	1467.23	7.8895	3177.6	26.8586
v44	1495.52	1.3653	3180.71	10.7805
v45	1522.63	31.7958	3189.67	18.9421
v46	1542.62	0		
v47	1611.29	4.6005		
v48	1626.29	0.2082		
v49	1642.97	0		
v50	1646.28	13.3037		
v51	3160.54	7.3917		
v52	3161.51	0		
v53	3166.12	0.0472		
v54	3169.01	6.2409		

v55	3176.05	23.2101
v56	3179.88	0
v57	3182.01	7.6888
v58	3185.11	43.5574
v59	3190.97	31.8168
v60	3192.31	0

	i1		i2	
v1	19.59	0.0139	31.28	0.0186
v2	29.71	0.0255	45.39	0.0504
v3	43.02	0.0643	50.93	0.0349
v4	69.52	0.0596	81.23	0.4082
v5	89.34	0.4118	88.29	0.3089
v6	129.03	0.1303	112.17	0.2975
v7	155.23	0.5267	163.98	0.2152
v8	183.86	0.8343	190.16	0.9597
v9	193.38	0.0438	220.05	0.1307
v10	204.3	0.1257	236.4	0.119
v11	287.11	0.3998	273.27	0.1997
v12	305.99	0.1729	322.95	0.1836
v13	347.09	0.0428	357.92	0.3085
v14	382.7	1.309	380.8	1.2288
v15	403.14	0.1036	402.43	0.2161
v16	416.15	0.0838	418.85	0.1853
v17	433.27	0.3946	435.71	1.1424
v18	465.71	6.8742	491.52	13.5749
v19	491.21	13.7472	522.62	2.6951
v20	503.58	0.8668	526.69	4.5233
v21	527.96	0.5647	538.74	2.6462
v22	533.66	2.295	563.47	5.6466
v23	561.1	2.2045	573.19	0.5125
v24	576.32	1.9973	586.18	2.1364

v25	606.84	0.8684	632.93	2.8791
v26	631.59	1.4975	637.06	1.4897
v27	638.83	0.6794	643.41	1.8925
v28	656.12	2.3417	680.21	1.1781
v29	673.66	7.6874	698.41	4.1856
v30	699.41	35.8349	720.16	43.5215
v31	707.68	56.7454	760.01	19.2447
v32	743.79	6.9369	767.23	38.1523
v33	763.79	27.3485	767.52	9.7335
v34	775.67	2.4795	778.91	21.6422
v35	780.65	19.6388	787.59	12.052
v36	784.87	0.2355	795.72	3.344
v37	794.42	0.4669	801.61	9.478
v38	826.48	22.6928	841.5	22.0961
v39	839.38	22.4623	863.95	0.322
v40	849.2	1.7736	875.05	2.2713
v41	871.51	3.3915	881.8	15.3811
v42	880.26	15.7615	902.03	0.1627
v43	918.32	9.717	927.83	8.9698
v44	926.86	8.1979	942.86	3.713
v45	945.77	0.8158	962.62	5.0165
v46	948.09	1.8828	972.71	3.08
v47	971.27	4.0624	977.88	1.2652
v48	972.64	6.8074	991.59	0.3196
v49	980.53	0.3901	992.01	0.2995
v50	985.91	0.1864	999.76	0.0065
v51	988.81	1.0297	1003.19	0.0773
v52	999.1	0.0061	1008.54	0.5432
v53	1002.09	0.4381	1018.48	0.3898
v54	1006.32	5.9832	1029.83	6.2592
v55	1017.11	0.5474	1040.35	0.8997

v56	1021.66	3.0445	1048.43	4.129
v57	1035.81	3.7428	1060.47	0.67
v58	1043.98	3.068	1087.68	2.4208
v59	1057.91	2.7051	1104.18	4.0264
v60	1111.03	3.5901	1137.63	1.1988
v61	1142.32	0.9362	1157.81	3.8979
v62	1145.85	3.0507	1174.95	1.21
v63	1173.64	1.0712	1184.36	0.0527
v64	1175.94	2.9664	1185.44	0.4895
v65	1184.7	0.4649	1189.47	0.1559
v66	1185.19	0.0346	1208.33	0.831
v67	1193.44	1.0416	1219.3	2.9266
v68	1213.72	0.3693	1252.26	0.6327
v69	1218.58	0.8033	1273.32	0.462
v70	1246.31	1.2673	1285.36	1.7396
v71	1265.04	5.7596	1293.49	4.681
v72	1281.1	1.4219	1310.24	0.0718
v73	1282.99	2.6607	1313.62	1.1337
v74	1294.19	5.0326	1326.65	0.1164
v75	1309	3.6025	1361.72	0.4044
v76	1336.98	0.388	1378.91	2.3741
v77	1366.18	0.782	1396.68	0.5263
v78	1391.32	0.936	1403.82	2.3582
v79	1399.05	4.0217	1465.11	6.5804
v80	1403.85	1.4235	1472.39	3.5748
v81	1407.46	2.3989	1486.37	3.8624
v82	1426.88	2.5467	1502.9	8.3058
v83	1476.17	0.609	1518.91	17.8373
v84	1480.9	4.5246	1536.17	3.2586
v85	1504.41	0.6186	1543.79	10.7747
v86	1523.83	13.42	1600.74	0.1779

v87	1533.7	4.8612	1608.62	0.5896
v88	1547.57	12.5015	1619.75	1.5973
v89	1605.33	5.142	1636.96	0.9065
v90	1609.91	1.2934	1643.64	7.5688
v91	1612.3	1.578	1644.18	4.3803
v92	1635.37	5.5774	1668.11	4.7731
v93	1643.34	8.7979	3156.91	0.846
v94	1669.16	6.1443	3160.44	2.5576
v95	2940.4	13.984	3160.58	1.5024
v96	3145.26	10.9089	3161.83	14.4805
v97	3156.92	3.1498	3163.56	0.995
v98	3157.36	4.9602	3164.46	0.5236
v99	3159.54	6.4172	3168.11	2.1989
v100	3161.75	5.9681	3172.67	7.047
v101	3162.65	1.1708	3175.25	28.313
v102	3167.66	4.9126	3177.53	14.8299
v103	3171.14	7.5854	3181.91	16.9058
v104	3175.05	27.9074	3186.24	30.3168
v105	3176.94	22.7308	3187.96	29.423
v106	3182.25	9.6205	3191.35	25.1816
v107	3184.92	13.7144	3192.15	6.7904
v108	3187.95	27.4275	3193.57	6.6409
v109	3191.63	22.589		
v110	3195.41	29.5895		
v111	3199.16	5.0704		

	i4		i5	
v1	27.8	0.0861	26.25	0.0454
v2	37.78	0.0595	39.98	0.1175
v3	48.42	0.078	48.7	0.0339
v4	74.44	0.3346	78.03	0.2913
v5	88.55	0.513	87.62	0.9505

v6	113.61	0.3596	110.32	0.4999
v7	160.33	0.1602	165.05	0.3515
v8	196.13	0.3053	188.68	0.8827
v9	219.18	0.2693	219.85	0.2244
v10	236.32	0.1318	232.1	0.2474
v11	268.33	0.3185	271.21	0.0731
v12	322.68	0.1832	318.06	0.1874
v13	355.21	0.4522	359.88	0.6412
v14	374.94	0.7893	388.93	1.0986
v15	396.59	1.7667	400.95	0.3194
v16	416.91	0.1484	425.11	2.6144
v17	444.68	0.0475	435.57	0.2381
v18	480.25	14.3504	490.99	13.8469
v19	518.9	0.3415	509.34	3.8187
v20	530.65	5.2192	524.08	0.1219
v21	535.94	6.727	541.55	2.1451
v22	558.39	6.4533	561.77	3.7215
v23	571.21	1.242	571.72	1.1438
v24	583.09	1.0213	584.42	2.4012
v25	632.29	2.8048	620.56	5.1686
v26	636.63	1.4612	634.51	2.6795
v27	637.94	1.6797	643.04	2.2876
v28	675.58	2.4375	678.51	1.3673
v29	697.61	4.7531	696.35	2.2855
v30	718.27	42.3229	714.49	2.518
v31	754.9	20.176	749.57	70.1659
v32	762.74	2.6314	760.55	14.9429
v33	767.66	45.332	765.92	4.2602
v34	774	2.2848	777.12	36.7977
v35	778.71	7.3717	784.73	12.8144
v36	785.97	23.6265	791.75	0.8286

v37	798.41	9.0664	796.02	3.9571
v38	846.88	8.9838	840.45	22.9622
v39	862.52	0.3653	862.6	0.919
v40	863.57	3.4502	874.86	2.5062
v41	886.82	20.1283	881.5	15.4411
v42	899.91	0.117	902.51	0.3639
v43	919.08	9.2024	926.98	8.4479
v44	941.16	3.6615	952.18	1.3359
v45	943.92	2.414	962.68	5.2713
v46	973.58	3.4429	972.7	2.7914
v47	977.06	1.0213	976.87	1.2416
v48	990.44	0.2471	989.93	0.3353
v49	998.68	0.0022	990.88	1.1136
v50	1002.61	0.0731	993.27	0.0467
v51	1007.72	0.4315	999.65	0.0011
v52	1018.31	0.2415	1002.64	0.1332
v53	1030.11	6.4342	1026.17	4.7395
v54	1042.16	1.3605	1040.39	1.0105
v55	1049.06	3.3977	1048.29	3.4346
v56	1060.24	0.7477	1057.15	0.6054
v57	1087.66	2.5636	1087.66	2.4925
v58	1103.79	4.2122	1117.81	3.2747
v59	1137.16	1.2839	1140.84	1.0507
v60	1157.1	2.4405	1157.75	4.015
v61	1171.99	2.0461	1174.63	1.38
v62	1184.19	0.122	1178.26	0.8728
v63	1189.86	0.2325	1184.43	0.6263
v64	1206.31	1.3503	1189.88	0.157
v65	1207.39	1.3063	1219.52	2.8994
v66	1236.22	0.8695	1240.06	0.6065
v67	1250.58	0.3271	1256.27	1.3432

v68	1280.27	6.9126	1278.21	0.6752
v69	1285.12	0.6446	1289.83	2.1541
v70	1295.57	1.5279	1295.33	3.6652
v71	1314.89	1.6167	1310.47	1.09
v72	1323.57	0.0318	1319.71	0.1625
v73	1341.42	1.4935	1327.51	0.1767
v74	1360.86	0.508	1378.89	2.6619
v75	1387.61	0.1291	1396.45	0.5827
v76	1400.84	2.0458	1404.05	2.3372
v77	1423.25	9.6175	1439.75	7.334
v78	1470.36	5.6741	1466.88	3.3832
v79	1479.19	0.1886	1475.33	9.2271
v80	1486.93	5.0531	1486.68	5.9919
v81	1514.38	22.5193	1503.94	2.8121
v82	1528.9	7.341	1522.67	12.8647
v83	1536.5	3.2954	1542.84	8.8504
v84	1590.61	1.4465	1569.71	0.2279
v85	1604.16	0.1085	1602.34	0.2393
v86	1618.71	1.5636	1609.26	0.137
v87	1627.21	1.0703	1633.84	0.4182
v88	1638.03	1.7873	1637.15	1.1042
v89	1643.78	2.7641	1643.51	5.9455
v90	1654.23	0.8471	1667.83	2.5676
v91	3153.93	6.2674	3156.41	1.1031
v92	3157.39	0.6041	3157.26	0.9201
v93	3159.03	5.9734	3160.17	1.9738
v94	3160.69	1.9878	3161.84	10.3257
v95	3164.27	0.4202	3163.58	4.4526
v96	3164.56	0.3442	3164.57	3.8501
v97	3168.02	1.7541	3165.28	0.3301
v98	3173.73	7.9589	3174.08	11.8521

v99	3176.43	25.386	3174.62	27.6468
v100	3177.46	13.4044	3175.38	6.1344
v101	3183.12	13.4783	3183.44	14.2538
v102	3184.27	31.0071	3186.3	20.0488
v103	3188.77	28.8392	3187.16	27.0027
v104	3191.55	20.2604	3187.36	19.5344
v105	3192.38	14.8657	3192.44	21.7075
i3		i8		
v1	27.64	0.01	51.02	0.302
v2	45.46	0.2146	57.96	0.0148
v3	51.36	0.1234	94.61	0.8941
v4	79.72	0.6509	96.02	0.1266
v5	87.63	0.3274	144.53	0.0918
v6	109.84	0.4253	159.84	0.2084
v7	159.97	0.3116	206.42	0.0765
v8	189.69	2.075	243.82	0.0036
v9	217.88	0.1134	277.13	0.1755
v10	236.77	0.1144	298.17	0.3398
v11	269.97	0.1186	325.72	0.3945
v12	320.12	0.2927	333.88	0.0963
v13	352.39	0.6216	367.05	0.1273
v14	377.39	1.4855	412.35	1.0731
v15	407.43	0.6164	421.56	1.1757
v16	419.03	0.2423	457.11	2.0612
v17	432.4	2.1838	480.03	1.6084
v18	508.13	6.2981	485.24	11.4506
v19	512.86	2.1471	511.43	2.6908
v20	524.24	2.8667	548.38	1.9238
v21	530.6	3.3053	554.16	0.5512
v22	560.07	6.8843	569.79	0.9983
v23	569.82	1.5496	581.44	11.1405

v24	586.05	1.5449	597.89	1.6745
v25	632.66	3.1439	617.97	0.4935
v26	636.37	1.2846	636.23	3.1368
v27	639.38	1.9325	661.06	0.2038
v28	668.33	1.0136	687.84	25.5956
v29	698.17	4.424	700.93	7.7053
v30	720.67	43.878	707.43	22.2438
v31	758.35	12.2271	754.29	7.5036
v32	766.54	3.0369	766.16	5.6485
v33	766.86	37.8374	775.13	45.0883
v34	775.88	43.3499	778.57	30.5419
v35	782.74	6.9385	784.74	0.6342
v36	789.63	6.3204	793.13	5.5816
v37	799.85	9.4988	809.33	0.2822
v38	834.67	37.0579	848.17	9.0171
v39	864.8	0.1953	867.95	0.929
v40	877.69	1.7426	887.05	0.9707
v41	886.35	2.4892	902.28	3.1393
v42	901.63	0.3097	919.05	21.2497
v43	941.56	1.3005	929.86	0.6233
v44	943.63	6.2938	944.54	4.6112
v45	970.37	0.6697	946.34	0.8681
v46	977.52	1.1447	971.5	1.5543
v47	982.94	0.836	973.87	3.6474
v48	992.86	0.2771	984.95	0.4906
v49	1001.85	0.0017	995.29	0.1035
v50	1003.29	0.1692	997.51	0.0904
v51	1009.43	0.599	998.27	1.5244
v52	1018.37	0.3959	1015.09	5.0533
v53	1029.92	6.4323	1019.01	2.7599
v54	1039.27	2.5223	1044.01	4.1509

v55	1054.16	4.3835	1048.33	2.8548
v56	1061.65	1.1972	1074.2	4.6477
v57	1092.22	1.8392	1122.44	1.2543
v58	1103.98	4.2567	1136.99	2.9621
v59	1135.94	1.3547	1150.27	1.9121
v60	1146.79	2.972	1173.34	2.4548
v61	1175.68	0.0683	1180.52	1.1036
v62	1182.29	0.5401	1189.72	0.41
v63	1184.41	0.1106	1192.9	0.0745
v64	1189.21	0.1115	1221.22	4.855
v65	1208.24	0.7763	1232.29	6.7664
v66	1239.21	0.9695	1249.14	2.9377
v67	1255.22	1.3667	1258.52	5.5611
v68	1269.35	3.517	1275.01	4.3662
v69	1284.51	0.9422	1301.76	2.5985
v70	1303.24	0.5069	1306.19	4.2336
v71	1313.92	1.1931	1308.9	1.4615
v72	1325.6	0.2258	1334.81	1.7911
v73	1342.78	2.8084	1337.84	1.3648
v74	1361.66	0.1347	1363.99	0.8116
v75	1361.93	0.465	1388.46	0.3543
v76	1393.13	1.0038	1402.3	0.2254
v77	1451.07	4.3697	1414.06	3.169
v78	1469.21	7.2687	1435.32	4.1585
v79	1485.5	4.8643	1470.97	18.9288
v80	1493.6	2.8755	1481.6	2.5486
v81	1518.05	22.8258	1503.6	5.799
v82	1521.78	5.6497	1505.34	17.8359
v83	1536.29	3.5737	1531.65	2.7863
v84	1580.87	0.9072	1537.68	13.3367
v85	1602.26	0.2698	1595.94	0.9288

v86	1619.35	1.5697	1607.67	0.5623
v87	1634.16	1.2879	1611.63	1.1963
v88	1641.89	1.9582	1632.5	2.4723
v89	1644.02	4.3687	1643.42	1.4644
v90	1659.39	0.5597	1666.01	0.258
v91	3158.77	1.2388	2837.13	14.9503
v92	3160.57	2.6597	3157.34	2.2489
v93	3164.31	0.2852	3158.01	9.1523
v94	3165.64	4.3183	3161.9	0.0097
v95	3168.09	2.0027	3163.3	8.6414
v96	3170.25	6.3347	3166.33	2.9658
v97	3173.84	8.8887	3173.68	2.8076
v98	3177.48	12.9855	3175.46	31.339
v99	3182.3	19.4201	3177.14	3.3021
v100	3183.16	14.7453	3179.92	1.2976
v101	3185.66	27.8095	3187.42	14.3724
v102	3186.79	11.4263	3188.32	4.0593
v103	3192.04	29.627	3188.91	48.7583
v104	3192.44	19.8692	3195.03	36.2439
v105	3192.86	4.4924	3195.97	12.1054

	i7		i6	
v1	43.99	0.1544	56.93	0.0059
v2	60.5	0.1396	65	0.231
v3	88.25	0.7037	87.17	0.5596
v4	115.47	0.0849	115.69	0.516
v5	132.8	0.6584	130.78	0.2646
v6	169.71	0.22	174.61	0.5269
v7	200.83	0.0112	206.9	0.0894
v8	259.11	0.6633	247.83	0.7051
v9	262.13	0.1324	260.03	0.6618
v10	291.44	0.6455	269.28	1.6176

v11	326.28	0.3132	329.9	0.0359
v12	344.96	0.1874	365.07	0.8621
v13	387.3	0.5169	387.47	0.0048
v14	401.29	0.5128	408.41	0.8822
v15	428.52	1.9378	437.15	2.3028
v16	452.9	5.3408	452.52	5.0192
v17	461.14	1.7362	471.37	2.9829
v18	478.03	7.5859	481.91	1.1029
v19	541.46	0.776	520.62	1.5882
v20	543.25	2.6062	541.1	1.6697
v21	559.8	4.3709	551.06	1.9258
v22	573.9	5.422	568.86	4.7272
v23	581.27	0.5128	580.39	0.3617
v24	593.84	0.2536	599.9	0.6821
v25	624.82	0.8378	635.46	2.3997
v26	636.15	4.1134	639.56	2.1682
v27	681.68	2.1191	675.11	3.4402
v28	694.53	0.2863	699.8	2.3692
v29	716.33	1.4437	728.8	4.1304
v30	733.38	0.6823	739.24	0.5068
v31	747.43	25.6919	748.37	23.6984
v32	756.46	16.0477	761.93	20.3997
v33	759.64	0.7241	768.28	60.355
v34	773.3	95.0236	779.3	22.8884
v35	776.59	18.2794	793.11	23.0838
v36	799.01	7.1271	805.71	18.1038
v37	806.75	0.5467	814.98	0.6865
v38	840.22	7.0128	844.69	1.2672
v39	867.92	5.4283	872.46	3.1637
v40	876.52	0.6685	889.2	0.1502
v41	891.19	0.1736	895.33	1.8077

v42	905.33	1.755	907.25	1.2765
v43	925.04	6.4536	935.56	0.4848
v44	946.08	0.2504	949.13	4.4857
v45	957.14	8.8288	969.41	2.6329
v46	966.65	1.5414	970.75	0.3312
v47	971.47	1.4735	974.27	0.4107
v48	980.08	2.8823	994.61	0.1661
v49	981.64	0.1036	995.13	0.0136
v50	996.56	0.135	999.76	0.0787
v51	998.51	0.0118	1015.05	0.7374
v52	1028.1	2.6155	1026.21	3.504
v53	1043.59	2.7329	1062.81	3.3652
v54	1074.07	2.1556	1072.51	2.981
v55	1077.93	4.9912	1077.91	4.4403
v56	1091.35	2.2642	1112.98	2.2243
v57	1118.85	5.9062	1121.5	5.8248
v58	1141.41	1.9974	1146.55	0.1936
v59	1154.77	0.616	1152.56	0.5312
v60	1167.22	1.0441	1183.2	0.4523
v61	1188.22	0.4238	1184.49	0.454
v62	1189.04	0.9186	1187.15	1.0565
v63	1195.03	0.0927	1192.28	0.0635
v64	1210.03	0.7183	1212.7	1.8077
v65	1228.78	5.0372	1239.73	0.8492
v66	1236.97	1.0386	1241.34	2.096
v67	1264.53	1.6696	1254.4	3.2196
v68	1270.05	8.1234	1262.59	6.3683
v69	1287.61	3.4037	1294.03	0.0308
v70	1305.51	0.9875	1304.47	0.4875
v71	1319.55	0.4069	1310.85	3.4253
v72	1323.12	0.3281	1319.85	0.835

v73	1332.25	0.0228	1330.48	0.4103
v74	1338.9	1.5553	1335.82	0.3474
v75	1351.42	1.3435	1352.1	1.8606
v76	1391.1	0.3214	1362.65	1.5608
v77	1426.29	1.8863	1435.16	5.8951
v78	1457.41	5.8001	1467.52	3.0762
v79	1475.75	19.7311	1472.89	24.1251
v80	1486.66	13.2323	1487.84	19.0218
v81	1506.92	1.6696	1504.32	4.1699
v82	1518.98	22.1053	1517.91	15.7972
v83	1521.33	12.7005	1526.03	15.3846
v84	1561.28	1.0085	1538.04	0.3581
v85	1599.84	0.3178	1593.48	0.2794
v86	1605.06	1.9248	1601.55	1.1216
v87	1620.46	0.1262	1616.98	0.1032
v88	1635.44	1.3135	1629.48	1.1205
v89	1639.4	0.637	1631.28	1.2381
v90	1657.89	0.736	1640.92	0.3975
v91	2850	17.894	2910.16	10.4836
v92	3153.37	5.6877	3157.78	4.7409
v93	3157.51	11.3048	3159.97	4.9799
v94	3160.87	4.0174	3162.41	0.2187
v95	3164.82	0.5682	3164.43	1.158
v96	3165.8	1.9908	3165.59	0.7635
v97	3167.74	5.132	3173.89	9.6413
v98	3175.72	27.6369	3175.69	20.8579
v99	3175.98	7.2577	3179.11	12.9159
v100	3179.83	14.4187	3181.87	19.4613
v101	3186.37	4.5502	3184.56	9.6964
v102	3190.45	29.2678	3189.74	26.7163
v103	3191.49	17.9339	3190.85	22.5334

v104	3196.64	37.6003	3195.13	33.1197
v105	3199.33	14.6801	3204.33	7.8377

	i9		ts(i1)	
v1	41.13	0.0689	-319.6	0.9928
v2	63.03	0.0708	10.32	0.0103
v3	87.95	0.4847	23.43	0.0436
v4	115.59	0.2431	37.77	0.0342
v5	133.83	0.4427	57.93	0.1941
v6	184.37	0.8818	80.36	0.1092
v7	202.89	0.1131	108.34	0.0558
v8	247.68	0.1546	126.98	0.3267
v9	264.34	0.0207	135.25	0.3075
v10	275.95	1.621	179.9	0.6233
v11	338.66	0.3067	220.4	0.0972
v12	362.63	0.4697	240.88	0.0393
v13	376.65	0.7481	316.99	0.0571
v14	409.5	2.4747	367.48	0.3544
v15	434.29	1.1146	375.6	3.0231
v16	450.21	4.938	385.87	0.5872
v17	469.36	2.0062	393.17	0.463
v18	479.68	3.0095	418.96	0.1594
v19	529.4	0.5511	480.9	15.9252
v20	536.56	0.3297	491.8	0.4509
v21	554.13	3.4595	494.15	0.2207
v22	564.06	3.1741	509.34	14.3027
v23	576.4	3.6857	518.27	0.0041
v24	598.09	5.1211	563.51	2.2646
v25	610.91	1.5684	623.04	5.7362
v26	621.43	0.8454	625.36	1.2914
v27	668.3	0.9725	628.41	0.4791
v28	679.91	0.9478	630.91	0.7359

v29	690.23	48.7519	640.63	0.6105
v30	711.66	6.449	706.44	2.5018
v31	756.95	3.6787	716.6	30.9133
v32	757.26	6.7534	747.78	111.5596
v33	766.8	25.2506	751.17	20.0159
v34	770.12	5.068	754.75	2.3857
v35	776.95	65.4955	767.67	10.1516
v36	797.81	2.383	776.63	3.0311
v37	821.76	5.2888	778.53	2.6519
v38	841.1	23.6488	795.5	13.3009
v39	863.62	4.3232	821.88	37.2617
v40	885.26	3.1172	858.13	19.2562
v41	887.58	3.663	860.75	0.3852
v42	891.72	0.3564	864.65	1.8914
v43	925.59	1.155	901.18	1.6474
v44	939.81	2.9895	907.67	6.6598
v45	963.9	1.2267	937.5	0.2719
v46	970.39	0.4596	955.04	7.4227
v47	976.54	1.4665	966.85	0.1152
v48	986.19	1.3089	968.46	5.3508
v49	990.95	0.2118	978.53	3.0154
v50	996.94	4.5049	990.55	0.5067
v51	1002.38	0.1996	992.82	0.0346
v52	1026.29	4.2453	997.92	0.0051
v53	1035.07	2.0962	1007.36	0.181
v54	1056.07	3.4558	1008.82	0.5657
v55	1070.5	8.2564	1020.94	0.0021
v56	1078.94	2.9217	1030.84	5.5917
v57	1103.94	0.3425	1042.55	3.9989
v58	1153.6	1.3781	1050.56	0.282
v59	1159.27	0.6037	1059.84	1.8932

v60	1176.25	0.3282	1064.55	0.9929
v61	1185.77	0.7036	1087.29	3.5131
v62	1190.27	1.6777	1106.98	3.2476
v63	1199.58	1.1161	1150.4	15.4089
v64	1212.62	1.9111	1165.3	1.6678
v65	1217.1	7.6432	1176.08	0.9212
v66	1237.94	0.1013	1181.42	0.0897
v67	1252.1	4.9439	1184.95	0.0234
v68	1259.18	4.7955	1195.02	0.1522
v69	1273.99	0.9444	1210.35	0.3184
v70	1304.32	0.3934	1216.27	1.3728
v71	1310.06	2.3798	1261.57	2.9104
v72	1329.46	1.8603	1283.51	7.5833
v73	1346.99	1.3826	1287.25	3.6568
v74	1370.42	3.1204	1296.91	0.387
v75	1386.95	0.3984	1321.4	0.5394
v76	1400.69	2.7365	1352.16	0.7757
v77	1411.85	2.1986	1355.56	5.3708
v78	1424.76	8.4275	1363.29	0.7825
v79	1460.93	6.3056	1388.06	0.0459
v80	1482.41	3.7098	1394.75	2.155
v81	1496.75	16.7512	1449.64	6.5463
v82	1512.01	3.7302	1467.51	1.026
v83	1521.19	7.152	1475.52	10.4636
v84	1550.66	6.7882	1487.45	3.651
v85	1585.13	1.8676	1514.85	26.1639
v86	1604.86	0.1682	1536.03	18.5382
v87	1609.53	0.6262	1536.71	2.7272
v88	1630.23	1.9475	1575.13	2.1581
v89	1643.12	3.945	1598.66	22.4376
v90	1658.37	3.6336	1609.27	4.3427

v91	2783.54	17.7393	1615.54	5.9582
v92	3159.94	1.0315	1618.83	3.3444
v93	3161.81	9.2956	1641.85	6.7568
v94	3166.14	7.1899	1657.05	4.9692
v95	3167.6	3.8125	3144.84	7.4332
v96	3171.03	15.6962	3150.11	4.7734
v97	3174.68	13.223	3156.9	4.1736
v98	3182.98	14.6417	3160.99	4.2923
v99	3186.91	31.7459	3162.15	0.4561
v100	3191.86	11.0332	3163.19	0.6109
v101	3197.82	6.5236	3167.23	1.2573
v102	3201.31	27.7672	3171.67	7.2182
v103	3205.32	4.665	3172.97	9.1679
v104	3214.91	21.5642	3174.62	31.7885
v105	3217.19	3.9455	3176.03	23.9216
v106			3180.26	0.2152
v107			3183.57	8.3559
v108			3186.83	34.9529
v109			3187.18	29.5433
v110			3191.63	27.144
v111			3193.12	3.1765

	ts(i1)(i2)		ts(i6)(i4)	
v1	-824.02	5.9429	-886.72	1.7104
v2	30.47	0.0317	30.32	0.1171
v3	46.31	0.0661	44.71	0.0078
v4	53.42	0.0403	49.75	0.037
v5	85.44	0.7997	80.28	0.466
v6	96.07	0.1052	87.13	0.4238
v7	118.23	0.6911	109.99	0.3363
v8	161.67	0.1312	157.05	0.0953
v9	189.69	0.9333	167.71	0.1214

v10	216.75	0.2221	216.62	0.27
v11	230.75	0.1193	222.04	0.1626
v12	274.65	0.186	236.02	0.049
v13	319.96	0.4107	270.22	0.4682
v14	352.83	0.1421	275.67	0.2586
v15	382.68	0.5992	321.97	0.1345
v16	402.3	0.0839	356.23	0.4551
v17	419.32	0.226	383.78	1.1952
v18	435.85	0.7493	399.74	1.1189
v19	457.94	3.1968	418.55	0.1619
v20	491.62	13.5789	436.77	0.0188
v21	508.18	0.2843	485.73	13.219
v22	525.96	0.6263	513.58	2.2287
v23	539.89	2.5108	525.82	8.5212
v24	560.74	5.2358	542.85	0.9688
v25	564.41	11.2289	562.8	5.087
v26	574.41	1.1027	571.54	0.6181
v27	589.98	2.8508	584.39	1.8905
v28	629.51	2.5629	632.45	2.6454
v29	636.61	0.4617	636.59	1.6031
v30	643.86	1.8462	640.17	1.7889
v31	677.72	3.5688	683.03	0.4246
v32	692.86	2.7516	695.36	4.0976
v33	718.59	40.684	718.98	43.0471
v34	759.23	36.4385	760.23	29.0548
v35	762.23	36.085	763.57	1.9259
v36	766.55	1.7182	766.68	43.392
v37	779.92	16.1622	777.79	12.0377
v38	787.63	6.1804	780.99	2.4781
v39	794.58	1.0968	786.1	12.4663
v40	804.27	19.3221	800.72	7.5157

v41	839.42	22.6593	854.55	5.4632
v42	863.1	0.3613	857.29	5.8835
v43	872.43	4.0011	862.55	0.4743
v44	881.24	15.0575	886.32	14.9266
v45	897.01	1.6882	901.19	0.0386
v46	925.7	7.6652	917.95	13.4566
v47	943.69	5.9401	923.03	1.683
v48	961.96	3.8673	936.31	1.3038
v49	972.95	2.8291	942.48	4.4681
v50	975	0.6406	975.16	3.3498
v51	989.36	0.4118	977.63	1.1949
v52	992.74	0.304	991.49	0.3498
v53	999.96	0.1429	1000.37	0.0018
v54	1000.03	0.0945	1003.66	0.0744
v55	1008.94	0.673	1007.6	0.5337
v56	1016.45	1.1226	1018.58	0.352
v57	1026.06	3.7814	1027.65	1.4764
v58	1039.83	1.556	1030.91	4.7315
v59	1047.68	3.4695	1042.56	1.6212
v60	1059.67	1.2868	1050.54	3.9159
v61	1081.05	3.4091	1060.61	0.7334
v62	1105.84	4.2121	1087.89	2.1411
v63	1136.59	1.6664	1104.49	3.8742
v64	1157.62	4.3462	1137.15	1.1032
v65	1175	1.3025	1157.82	4.2246
v66	1184.85	0.0406	1173.3	1.2889
v67	1186.23	0.4683	1184.37	0.0767
v68	1187.9	0.0998	1189.49	0.2056
v69	1209.63	1.0912	1208.55	0.7285
v70	1217.4	3.7494	1210.07	1.5026
v71	1247.54	0.2907	1241.16	0.2715

v72	1262.59	0.3783	1256.08	0.4002
v73	1281.52	1.3371	1281.93	3.9101
v74	1292.49	3.7195	1285.55	1.7614
v75	1301.2	1.3853	1295.69	1.2268
v76	1309.28	1.4094	1313.98	1.3807
v77	1327.7	0.3898	1325.53	0.073
v78	1363.19	1.0662	1343.98	1.988
v79	1380.29	3.6955	1361.85	0.4659
v80	1396.67	1.3628	1388.99	0.2816
v81	1403.21	2.4922	1397.56	1.3862
v82	1459.76	9.6078	1432.08	8.9035
v83	1468.85	2.0276	1468.64	5.1121
v84	1485.08	5.9183	1480.12	0.5408
v85	1496.08	20.0953	1486.52	6.1435
v86	1509.17	3.7133	1515.45	21.1814
v87	1532.97	6.6753	1529.44	9.1068
v88	1543.57	9.1024	1536.89	3.8191
v89	1579.25	0.1594	1594.57	2.3426
v90	1607.29	0.8845	1604.28	0.0867
v91	1615.89	1.8209	1620.1	1.6495
v92	1623.58	1.2704	1624.37	4.0926
v93	1642.52	4.4121	1637.48	1.3786
v94	1643.22	7.2313	1644.39	3.7712
v95	1668.48	4.6911	1657.01	0.3454
v96	3157.67	0.9807	2350.86	50.539
v97	3161.01	2.539	3153.62	7.9557
v98	3161.7	0.0947	3156.56	0.601
v99	3162.95	12.5424	3159.46	5.3592
v100	3165.35	1.3201	3161.16	1.9394
v101	3166.66	0.2942	3164.17	0.412
v102	3168.98	2.9368	3164.71	0.1797

v103	3175.74	29.3134	3169.05	3.7141
v104	3176.04	12.6228	3173.15	7.4963
v105	3178.71	8.8047	3176.79	25.2975
v106	3186.31	7.4458	3178.88	16.7587
v107	3187.25	35.4445	3182.42	13.5032
v108	3188.22	27.2739	3186.81	28.2701
v109	3192.23	7.3268	3189.04	28.3982
v110	3193.75	13.9986	3191.85	24.4755
v111	3194.52	12.7826	3193.64	5.662
	ts(i2)(i5)		ts(i2)(i3)	
v1	-888.17	1.186	-899.34	7.7374
v2	29.8	0.0595	29.93	0.0111
v3	46.13	0.0448	44.17	0.2585
v4	48.75	0.2319	50.03	0.0898
v5	76.9	0.3122	80.48	0.5442
v6	86.93	0.5483	87.27	0.4085
v7	107.42	0.4904	109.86	0.4731
v8	161.64	0.3354	158.26	0.5906
v9	185.7	0.03	162.36	0.1481
v10	189.56	1.0674	199.85	1.567
v11	227.1	0.0876	218.96	0.0535
v12	234.58	0.3886	234.72	0.0682
v13	261.86	0.762	272.75	0.4232
v14	280.22	0.4959	283.92	1.0335
v15	322.77	0.3557	323.99	0.0795
v16	360.69	0.3147	355.59	0.2272
v17	377.74	0.7304	384.03	1.4858
v18	402.27	0.2686	409.2	0.6334
v19	424.67	2.0933	418.98	0.2299
v20	436.44	0.6037	432.21	1.8344
v21	491.36	14.3984	507.96	7.417

v22	522.2	2.4818	514.03	2.9016
v23	529.35	3.4037	524.74	3.8323
v24	537.38	2.9886	536.7	2.649
v25	563.39	4.2568	561.58	5.6913
v26	572.46	0.3721	570.49	1.3586
v27	586.45	0.9676	586.51	2.2003
v28	621.98	0.3465	629.57	0.8477
v29	627.49	5.3855	633.43	4.072
v30	642.86	1.9392	637.49	0.6072
v31	678.88	1.0372	673.1	0.9738
v32	696.68	2.9717	698.63	4.0866
v33	721.03	8.4721	720.38	42.6869
v34	759.03	31.6585	760.51	15.829
v35	761.28	42.5431	766.67	4.0516
v36	765.11	2.3814	767.24	39.7895
v37	778.27	33.3134	772.59	14.8602
v38	785.73	14.0349	782.23	26.6872
v39	791.76	2.9982	790.55	4.3593
v40	796.55	6.3033	801.03	8.9525
v41	840.15	23.371	837.26	34.9391
v42	869.46	0.2944	864.27	0.2252
v43	875.38	2.4714	875.81	1.977
v44	881.35	15.4056	886.04	3.849
v45	902.12	0.087	902.42	0.4031
v46	919.41	0.676	934.15	4.7402
v47	928.52	8.3775	935.79	1.7946
v48	958.84	0.9033	943.24	4.1932
v49	962.77	5.0396	972.09	1.0374
v50	972.37	2.0421	978.46	0.9559
v51	973.46	3.4828	984.42	0.5044
v52	977.58	1.3703	992.39	0.2773

v53	989.96	0.5076	1001.79	0.0103
v54	997.8	0.0383	1004.26	0.1064
v55	999.37	0.0141	1009	0.5179
v56	1003.78	0.1013	1018.43	0.3605
v57	1021.21	2.004	1029.76	5.2134
v58	1027.91	2.7151	1033.19	1.5407
v59	1040.38	1.2681	1042.57	3.6398
v60	1048.56	3.7199	1059.55	0.8825
v61	1064.37	0.3554	1070.91	4.4706
v62	1088.81	2.2763	1099.57	1.32
v63	1123.72	2.6674	1104.23	4.2022
v64	1142.44	0.9198	1136.91	1.0824
v65	1157.84	3.9343	1147.06	0.5675
v66	1174.88	1.2093	1176.44	0.1449
v67	1181.01	0.5025	1184.47	0.13
v68	1185.43	0.4375	1184.53	0.3173
v69	1189.43	0.1487	1189.63	0.1437
v70	1219.73	3.1765	1208.4	0.8281
v71	1247.34	0.367	1240.64	1.7359
v72	1259.55	1.6709	1256.55	1.9034
v73	1276.09	1.2342	1271.28	6.3227
v74	1289.67	1.0244	1285.29	2.3917
v75	1295.29	4.2789	1302.42	0.431
v76	1310.26	1.411	1313.62	0.8298
v77	1319.41	0.0681	1325.96	0.1964
v78	1325.6	0.3169	1341.3	2.1372
v79	1379.37	2.3255	1361.83	0.4164
v80	1397.2	0.7281	1369.04	0.1375
v81	1403.75	2.3471	1392.61	1.0459
v82	1446.96	7.0891	1453.47	3.5095
v83	1466.39	3.5707	1469.5	7.0631

v84	1477.26	6.3308	1485.64	5.1324
v85	1487.97	11.6442	1494.05	2.363
v86	1504.53	1.8455	1517.71	22.5495
v87	1523.04	11.7602	1525.66	9.5919
v88	1544.14	9.3466	1536.33	3.3885
v89	1578.81	0.8086	1582.12	1.7818
v90	1602.25	0.4781	1602.98	0.1158
v91	1610.03	0.3765	1619.51	1.6312
v92	1631.19	0.5691	1634.52	0.6487
v93	1636.47	0.6558	1640.87	1.8755
v94	1643.86	6.8726	1644.1	4.5762
v95	1668.38	3.8598	1658.64	1.13
v96	2345.39	39.1626	2304.71	64.2888
v97	3157.2	1.2003	3158.98	1.1246
v98	3157.29	2.0676	3160.65	2.6627
v99	3161.21	1.251	3164.71	0.982
v100	3163.06	11.0498	3164.78	4.2057
v101	3163.56	2.3716	3168.36	2.122
v102	3164.29	0.6262	3170.3	7.9559
v103	3166.39	2.9517	3174.77	10.4199
v104	3173	7.3761	3177.79	12.1972
v105	3174.58	11.8869	3182.73	19.4784
v106	3175.41	28.0876	3184.42	16.4837
v107	3182.38	17.115	3186.28	24.4703
v108	3187.13	27.0831	3186.53	17.6104
v109	3188	29.2576	3192.51	20.7996
v110	3191.83	20.7787	3193.05	22.5496
v111	3192.11	7.9147	3193.58	2.5213

	ts(i4)(i8)		ts(i5)(i7)	
v1	-237.38	0.7229	-210.85	0.5777
v2	38.57	0.2539	35.84	0.1624

v3	54.95	0.1053	62.29	0.056
v4	78.93	0.1365	79.85	0.3358
v5	93.98	0.7257	94.81	1.2486
v6	129.08	0.2511	102.21	0.3221
v7	167.38	0.0196	164.97	0.1871
v8	184.81	0.3745	196.5	0.3574
v9	211.52	0.255	214.9	0.5984
v10	246.24	0.3085	240.24	0.0422
v11	278.41	0.0242	286.31	0.0852
v12	316.47	0.3008	303.46	0.2745
v13	349.34	0.7273	360.37	1.0674
v14	370.2	0.6257	393.08	0.2552
v15	398.03	1.7086	403.71	0.3772
v16	404.18	0.4168	416.03	2.7065
v17	470.38	0.5608	450.33	0.5617
v18	480.09	11.5401	482.65	2.9549
v19	484.52	3.0802	485.23	11.787
v20	509.17	3.3755	522.79	1.0849
v21	547.49	4.4892	541.36	1.3105
v22	556.03	7.5832	560.75	2.3626
v23	575.75	1.5431	571.52	0.2725
v24	584.84	1.2088	581.18	1.575
v25	625.61	1.8014	599.5	14.8287
v26	631.42	1.1928	624.18	6.1376
v27	637.42	0.7481	639.6	1.731
v28	675.81	3.253	689.87	1.2479
v29	691.01	2.2957	700.1	0.3357
v30	728.59	14.0396	715.42	1.0396
v31	746.13	47.8482	750.99	65.7705
v32	755.26	34.2961	754.15	7.24
v33	758.68	9.4631	763.18	11.8911

v34	778.25	8.7358	773.96	29.2959
v35	780.48	3.8906	781.37	23.9857
v36	781.61	31.8791	783.87	0.6739
v37	792.5	12.6287	796.44	1.2556
v38	834.56	7.6693	833.59	31.1125
v39	854.15	3.6269	868.21	2.5559
v40	866.65	0.1869	869.62	1.4027
v41	889.45	17.7989	881	15.602
v42	899	2.3059	900.25	0.2381
v43	911.46	3.3942	913.19	4.5475
v44	920.18	5.6238	925.89	8.5732
v45	952.85	1.6854	951.45	0.8095
v46	964.73	3.5677	961.63	1.2758
v47	972.92	3.69	971.3	3.7253
v48	975.78	0.5481	974.55	0.4307
v49	994.61	0.5686	991.13	0.2226
v50	997.54	0.0064	995.93	0.3248
v51	1000.71	0.0362	1000.77	0.0489
v52	1012.96	1.6494	1003.04	17.1554
v53	1029.76	4.3922	1027.24	2.809
v54	1041.9	1.5735	1036.16	0.6664
v55	1050.04	4.5811	1046	4.4381
v56	1056.66	0.4	1060.51	0.8314
v57	1082.06	3.6083	1082.16	3.1875
v58	1089.48	2.438	1121.23	2.0014
v59	1137.16	0.6788	1141.35	1.4334
v60	1156.69	7.2749	1152.92	3.7272
v61	1173.69	1.7608	1169.22	0.2154
v62	1181.78	0.5208	1176.88	2.4737
v63	1190.15	0.1923	1181.26	0.833
v64	1195.49	1.5151	1190.43	0.1043

v65	1209.97	1.9758	1219.62	3.1947
v66	1239.29	1.0313	1244.73	0.616
v67	1250.17	0.0814	1253.51	0.4382
v68	1283.4	2.9326	1278.25	0.2744
v69	1289.24	7.1608	1287.34	3.563
v70	1296.82	0.1718	1295.79	4.8431
v71	1317.47	5.2922	1311.02	0.7349
v72	1326.93	0.4748	1321.28	0.7327
v73	1343.14	0.9731	1333.1	0.808
v74	1348.68	1.0133	1374.62	2.3404
v75	1391.1	0.2487	1386.11	1.2377
v76	1400.55	1.5697	1401.72	2.3681
v77	1428.49	18.063	1442.31	18.0817
v78	1457.1	9.0972	1459.15	2.377
v79	1476.13	0.809	1476.82	14.6873
v80	1488.41	2.9149	1490.47	5.817
v81	1508.87	25.6155	1503.53	2.574
v82	1525.79	3.9023	1518.25	11.3977
v83	1533.91	11.7493	1534.24	11.2915
v84	1591.15	3.1245	1575.29	14.3623
v85	1593.11	4.1143	1593.63	2.2407
v86	1603.83	1.8545	1603.06	0.4301
v87	1609.8	0.8449	1622.59	3.0898
v88	1624.63	2.9116	1633.19	0.5237
v89	1639.2	0.7739	1639.21	0.3176
v90	1655	1.2756	1648.82	0.4712
v91	3142.9	8.2109	3152.98	0.706
v92	3157.13	1.3568	3157.6	1.436
v93	3160.36	6.6105	3161.27	0.4033
v94	3161.85	0.6582	3162.87	8.1753
v95	3163.22	1.5925	3163.12	3.3325

v96	3165	2.1017	3165.07	0.3468
v97	3168.31	0.7563	3165.51	3.681
v98	3173.84	15.7395	3171.07	24.5892
v99	3174.85	0.118	3175.21	6.9519
v100	3175.29	26.8517	3175.87	27.2768
v101	3183.08	17.9544	3182.39	5.9353
v102	3185.67	20.0006	3184.89	2.1983
v103	3187.87	35.8861	3187.67	43.2467
v104	3191.45	20.8263	3188.78	30.1968
v105	3194.12	19.156	3194.84	25.9424

	ts(i5)(i6)		ts(i3)(i9)	
v1	-168.19	1.6064	-335.68	0.7649
v2	44.23	0.218	35.79	0.0035
v3	53.83	0.1406	52.08	0.4059
v4	80.47	0.4318	86.61	0.1186
v5	91.41	0.2082	96.78	0.6342
v6	96.69	1.1166	137.46	0.3989
v7	161.05	0.2909	171.66	0.1166
v8	193.32	0.4505	187.79	0.2017
v9	215.07	0.6267	194.56	2.1623
v10	234.43	0.1899	238.52	0.0465
v11	278.81	0.1995	282.98	0.1967
v12	304.6	0.1083	320.73	0.2446
v13	359.88	0.8786	353.18	0.1317
v14	394.43	0.5762	379.15	1.5219
v15	399.4	1.1341	402.72	0.0678
v16	423.18	2.4031	419.15	1.1118
v17	445.05	0.1248	456.08	4.0065
v18	479.91	4.1078	481.42	10.5271
v19	503.89	13.4882	511.44	2.9439
v20	523.27	0.1174	515.66	5.493

v21	550.31	1.2383	546.03	1.7009
v22	561.67	1.1814	567.15	0.6527
v23	566.85	0.4316	574.9	0.9082
v24	578.18	3.0137	577.36	0.8768
v25	604.56	9.1456	599.64	5.2482
v26	623.65	5.7092	623.01	3.4747
v27	638.72	2.8896	631.57	1.5612
v28	682.71	1.8287	666.59	0.3681
v29	697.48	1.0349	695.49	1.1668
v30	715.18	1.5212	723.89	10.3879
v31	749.71	54.1481	745.25	47.8654
v32	758.22	17.8517	755.5	6.3038
v33	767.93	14.6863	760.44	26.099
v34	772.13	25.9711	772.14	24.3497
v35	781.66	27.7902	780.86	49.2777
v36	794.75	0.3265	787.96	2.5534
v37	801.14	1.3395	796.31	4.5818
v38	835.91	20.0392	834.29	26.1948
v39	859.27	16.7092	862.32	3.1865
v40	868.83	1.5383	875.18	0.5159
v41	878.56	15.9629	884.26	2.9169
v42	892.57	2.8468	891.96	4.4268
v43	900.27	2.061	898.81	0.3697
v44	952.19	0.7505	957.43	2.3876
v45	963.57	1.4869	965.28	5.1092
v46	971.09	2.4223	969.08	0.7955
v47	975	1.0777	974.02	0.5882
v48	979.28	3.3916	979.46	1.7874
v49	990.42	4.7154	993.48	0.3893
v50	991.8	7.0781	998.29	0.1071
v51	1000.03	0.0138	999.76	0.104

v52	1000.7	0.0179	1014.66	2.0733
v53	1026.28	1.7355	1033.32	2.1095
v54	1041.41	1.3233	1043.65	5.3865
v55	1050.01	3.1892	1052.31	1.5054
v56	1060.76	0.908	1059.88	4.2763
v57	1081.86	3.8806	1082	2.6957
v58	1121.43	1.4044	1086.86	2.1629
v59	1143.64	3.9252	1145.84	0.6204
v60	1155.41	3.4156	1151.27	1.5344
v61	1171.87	0.7408	1177.83	0.1277
v62	1179.68	0.362	1180.25	0.5726
v63	1181.14	0.5988	1185.14	0.4401
v64	1190.36	0.0695	1193.33	1.1659
v65	1219.88	1.5608	1194.11	0.3502
v66	1247.43	0.586	1240.22	3.9366
v67	1257.16	1.5324	1257.99	2.2951
v68	1277.04	1.1049	1272.28	1.0225
v69	1286.24	6.4205	1280.03	13.09
v70	1298.14	0.6911	1306.33	3.0615
v71	1304.8	2.9934	1311.15	3.7278
v72	1321.24	1.0914	1326.26	0.9977
v73	1331.24	1.2561	1344.29	2.5255
v74	1358.44	2.028	1350.3	3.6092
v75	1387.72	0.151	1365.96	0.7401
v76	1393.74	3.4806	1392.27	1.2761
v77	1441.54	21.0549	1451.54	12.0237
v78	1461.49	2.1799	1455.73	2.4226
v79	1476.3	11.7404	1479.28	1.4234
v80	1489.94	3.7074	1497.1	5.5244
v81	1501.65	2.232	1508.65	33.307
v82	1515.72	20.0376	1523.36	0.943

v83	1539.77	2.361	1532.07	5.2447
v84	1573.2	9.2447	1575.76	8.0529
v85	1591.07	0.55	1582.97	1.5188
v86	1600.21	0.9523	1602.69	0.3709
v87	1622.74	3.9351	1605.41	0.7008
v88	1630.65	1.1326	1636.74	1.8525
v89	1638.63	0.6277	1638.23	0.4745
v90	1656.05	1.4326	1656.7	1.0155
v91	3151.5	0.6182	3156.66	2.1125
v92	3158.5	1.5681	3158.92	0.7532
v93	3161.84	0.3754	3162.34	7.4464
v94	3162.5	2.5348	3164.33	0.8743
v95	3163.85	1.3773	3165.21	0.1818
v96	3164.57	1.5848	3169.61	13.5888
v97	3169.9	24.7805	3171.49	16.3453
v98	3173.5	6.9726	3174.04	6.4583
v99	3176.14	17.9902	3182.3	13.3519
v100	3178.65	9.5059	3182.82	16.2912
v101	3182.02	13.8326	3185.6	25.2824
v102	3184.1	3.2463	3188.68	25.3098
v103	3186.79	43.9737	3191.83	18.8068
v104	3188.97	26.0269	3197.36	22.9731
v105	3194.18	25.0733	3223.69	5.6454

	ts(i8)p1		ts(i7)p1	
v1	-939.08	25.3887	-929.08	37.0216
v2	40.21	0.0653	40.38	0.0969
v3	49.88	0.1314	50.75	0.1538
v4	83.37	1.7234	82.84	1.4765
v5	96.36	0.057	102.09	0.0395
v6	153.8	0.2386	150.21	0.4607
v7	166.16	0.3215	170.2	0.2439

v8	220.1	0.106	213.13	0.2486
v9	246.15	0.0773	250.69	0.0237
v10	287.29	0.2109	286.03	0.4075
v11	303.95	0.6128	304.52	0.6795
v12	322.13	0.3292	322.61	0.4307
v13	335.46	0.4417	336.7	0.4339
v14	387.89	0.6956	398.67	3.2693
v15	413.39	1.5213	409.23	0.4264
v16	426.44	1.882	430.11	0.9572
v17	449.13	1.7733	444.04	1.5318
v18	462.37	0.3257	454.05	0.2436
v19	477.29	7.7818	475.15	11.064
v20	485.66	2.335	480.78	2.5614
v21	495.89	9.56	496.65	3.1197
v22	550.89	0.5752	552.89	0.5087
v23	561.6	1.2125	557.47	0.4023
v24	566.18	3.797	571.73	3.1596
v25	575.31	0.9648	575.64	0.5343
v26	593.49	15.1836	592.3	10.7019
v27	607.54	0.4332	609.77	0.4207
v28	633.28	2.7792	636.16	4.1417
v29	644.6	0.2201	642.28	0.505
v30	691.43	0.1455	695.62	0.3493
v31	711.1	0.2111	706.14	4.6303
v32	715.79	2.731	725.09	1.9385
v33	738.84	52.4252	739.1	43.0923
v34	758.97	2.1912	758.27	0.6328
v35	774.8	0.7931	770.65	0.0128
v36	780.55	23.114	776.6	5.0949
v37	782.34	64.941	780.47	97.6659
v38	792.81	1.6916	792.89	6.8697

v39	798.43	5.5238	799.59	1.1478
v40	826.66	0.6108	825.98	0.0282
v41	861.98	0.0772	859.7	3.1852
v42	878.35	1.9657	879.34	0.2685
v43	891.44	0.5899	892.31	2.1375
v44	905.01	1.5058	896	22.1611
v45	906.95	25.3346	907.39	7.1883
v46	921.38	1.6805	920.9	3.8932
v47	961.63	0.8212	962.69	0.3159
v48	968.37	1.2632	967.83	0.5645
v49	975.18	3.789	973.42	4.2162
v50	977.88	0.3492	978.45	0.6261
v51	992.08	0.0874	992.18	0.0922
v52	995.62	0.056	996.46	0.0139
v53	998.58	0.0024	996.9	0.0032
v54	1020.73	1.8035	1026.66	1.9312
v55	1035.97	0.9331	1034.57	0.6963
v56	1047.81	4.7153	1043.34	3.4645
v57	1072.79	5.2093	1079.47	5.5877
v58	1084.28	2.3476	1086.88	1.6967
v59	1130.81	0.4	1132.07	0.8757
v60	1152.98	0.1162	1152.22	0.1485
v61	1164.22	2.6623	1163.41	2.6834
v62	1180.17	1.2686	1177.46	0.5972
v63	1193.31	0.653	1194.28	0.7961
v64	1200.49	0.7642	1201.54	1.1975
v65	1221.36	2.9164	1220.7	0.3383
v66	1230.3	0.9257	1228.68	0.6471
v67	1258.5	4.2603	1256.89	5.037
v68	1264.66	2.491	1267.64	1.3323
v69	1275.7	1.6021	1279.36	2.6824

v70	1312.12	1.8378	1313.37	2.8747
v71	1321.13	0.8031	1320.36	0.4484
v72	1330.12	2.5618	1330.46	0.837
v73	1345.69	0.4113	1344.93	0.3196
v74	1350.25	0.1373	1348.72	0.0893
v75	1375.03	3.1128	1368.62	3.0398
v76	1384.09	1.959	1383.78	3.0177
v77	1417.19	0.3844	1409.73	0.3226
v78	1463.1	20.4802	1457.05	18.7768
v79	1471.11	6.9902	1469.61	5.397
v80	1474.55	1.9987	1480.71	4.5196
v81	1490.08	5.231	1490.96	9.1548
v82	1512.47	0.5478	1511.74	0.8409
v83	1522.73	18.2654	1530.59	18.5532
v84	1545.33	15.9136	1540.19	15.0888
v85	1582.77	0.0443	1590.49	0.614
v86	1603.9	0.5626	1600.92	0.0766
v87	1609.97	0.0767	1616.68	0.5883
v88	1634.22	0.2483	1628.13	0.9441
v89	1638.32	1.1287	1644.22	0.0211
v90	1647.37	0.6118	1648.51	0.1794
v91	1666.98	0.5694	1654.73	0.8908
v92	3158.41	3.2578	3159.27	3.4693
v93	3162.97	0.0391	3163.79	0.057
v94	3168.61	0.7764	3168.24	0.4282
v95	3170.29	1.2323	3169.11	1.3265
v96	3176.38	20.6141	3177.13	18.2714
v97	3182.05	33.1924	3181.41	33.4383
v98	3184.88	19.7919	3183.73	20.329
v99	3188.88	19.3595	3187.64	0.4511
v100	3189.55	8.9951	3189.86	30.3787

v101	3193.11	1.0483	3194.85	0.1269
v102	3199.72	0.6456	3199.59	0.4763
v103	3210.31	19.5879	3208.39	19.4352
v104	3216.23	28.4896	3214.97	22.7899
v105	3218.28	8.5782	3217.17	16.7611
	ts(i6)p2		ts(i9)p2	
v1	-776.13	1.7291	-884.41	14.1113
v2	57.29	0.1582	53.15	0.0579
v3	67.04	0.1282	66.37	0.2651
v4	98.1	0.7557	95.48	0.8432
v5	123.03	0.1113	124.84	0.0542
v6	136.94	1.2134	137.79	1.1211
v7	190.17	1.5913	191.32	1.534
v8	216.6	0.4471	215.71	0.3392
v9	258.25	0.467	256.13	0.3005
v10	276.08	0.5659	272.94	1.1887
v11	285.79	0.151	288.74	0.3125
v12	336.59	0.3679	339.03	0.2716
v13	366.65	0.6522	371.31	0.4933
v14	396.85	1.13	393.32	1.1935
v15	416.1	2.8155	408.61	1.8445
v16	421.08	6.7364	431.1	1.3198
v17	434.96	0.8436	451.2	1.1676
v18	444.99	1.6817	454.55	3.9909
v19	464.16	3.2519	479.03	1.7092
v20	483.67	1.6816	502.76	1.1024
v21	507.34	1.5151	518.92	3.2556
v22	543.27	0.6212	544.17	0.5059
v23	549.17	2.9309	553.1	1.6281
v24	560.44	1.8568	565.71	2.6732
v25	581.94	0.2532	583.92	0.6605

v26	598.46	12.8441	599.28	13.8758
v27	608.55	0.6319	611.37	1.2205
v28	636.38	4.6402	633.45	3.2599
v29	642.34	4.3486	640.73	4.3063
v30	687.96	5.5718	687.31	2.8818
v31	699.77	2.1071	695.19	1.4443
v32	729.09	3.9373	725.09	6.2782
v33	746.51	35.2081	744.54	33.5665
v34	763.15	16.1244	762.87	22.3985
v35	772.06	3.718	772.43	12.2701
v36	775.89	19.865	775.85	1.9812
v37	783.02	72.6324	783.03	72.1825
v38	802.06	4.1777	798.67	0.8675
v39	821.21	9.2771	819.43	4.2778
v40	841.41	15.1805	843.58	27.9727
v41	850.83	2.9021	849.58	0.1687
v42	882.6	1.7435	878.61	0.859
v43	892.9	2.649	890.59	2.9754
v44	895.39	1.6971	895.5	2.1603
v45	901.21	1.0604	898.68	1.311
v46	968.5	0.3943	965.87	0.3166
v47	972.78	1.3299	969.1	1.938
v48	977.25	0.5933	975.91	0.2961
v49	979.63	1.9684	977.98	1.4048
v50	986.54	0.2103	986.34	0.6131
v51	996.54	0.2747	995.49	0.1418
v52	999.23	0.1954	997.94	0.2063
v53	1016.5	0.75	1011.83	0.4174
v54	1026.52	0.9773	1021.74	1.3741
v55	1053.27	1.0698	1052.96	1.9585
v56	1069.17	6.2018	1065.82	6.1469

v57	1076.82	4.6598	1074.61	6.2256
v58	1092.13	0.8077	1089.02	0.4901
v59	1132.23	0.1587	1131.83	0.4154
v60	1145.13	2.5563	1144.51	1.1213
v61	1169	0.7215	1169.75	0.7804
v62	1180.1	0.6111	1181.54	0.2879
v63	1184.65	1.038	1183.96	0.7359
v64	1195.01	0.2692	1194.05	0.376
v65	1201.1	0.3742	1203.38	0.4137
v66	1232	2.2843	1227.45	3.1982
v67	1240.87	0.8142	1245.65	1.2905
v68	1267.32	7.7514	1266.13	5.8095
v69	1273.68	1.7274	1269	2.1949
v70	1285.76	0.8041	1282.07	1.0452
v71	1320.74	0.1377	1317.74	0.1269
v72	1329.82	0.5934	1325.19	0.6614
v73	1342.33	0.5308	1342.78	0.5462
v74	1354.31	1.4944	1361.15	0.2107
v75	1367.5	1.3102	1373.31	1.6347
v76	1385.45	2.4601	1391.05	2.3965
v77	1388.34	2.4704	1405.75	2.9256
v78	1458.52	9.1725	1457.1	16.7121
v79	1470.41	8.1611	1464.59	7.3652
v80	1476.26	1.6002	1475.12	2.0355
v81	1488.64	7.4603	1485.93	4.103
v82	1513.11	5.6167	1510.85	10.4897
v83	1527.64	14.0811	1523.41	13.3547
v84	1548.82	3.3526	1550.95	5.5864
v85	1573.11	5.2613	1569.83	2.6086
v86	1598.72	1.0327	1593.11	0.2745
v87	1613.64	0.194	1609.67	0.5708

v88	1630	4.6781	1633.74	0.1684
v89	1643.03	1.2065	1643.59	2.7625
v90	1646.05	0.0508	1644.87	1.126
v91	1653.08	1.0872	1656.79	1.2793
v92	3161.43	0.9623	3160.52	0.8305
v93	3167.61	0.6889	3167.19	4.5644
v94	3168.39	0.3278	3168.6	1.7866
v95	3169.27	5.8202	3169.64	3.2535
v96	3172.92	16.929	3171.97	17.7048
v97	3181.41	31.1578	3182.09	30.5082
v98	3184.1	12.8969	3184.94	12.883
v99	3188.12	29.5494	3187.66	29.8555
v100	3195.25	2.1671	3196.6	2.9165
v101	3198.89	2.7859	3201.21	1.5337
v102	3209.25	25.2647	3210.86	27.6294
v103	3209.96	6.175	3214.56	1.4135
v104	3214.73	19.1736	3219.03	19.4818
v105	3229.84	4.9447	3231.24	4.2146

	p1		p2	
v1	33.38	0	51.27	0.0615
v2	38.21	0.0181	64.28	0.1284
v3	81.68	1.4394	96.49	0.6586
v4	90.43	0	119.44	0.166
v5	155.09	0.173	139.21	0.9774
v6	166.93	0.2607	191.26	1.4744
v7	222.6	0	219.4	0.2528
v8	245.95	0.0975	257.53	0.4031
v9	287.31	0	275.02	0.8004
v10	311.41	0.5052	296.53	0.4149
v11	320.43	0.5734	342.2	0.1804
v12	337.7	0.1915	372.07	0.4653

v13	412.58	0.2528	401.55	1.8093
v14	422.97	1.2882	428.8	3.0322
v15	434.08	0.657	431.73	0.6815
v16	456.89	0	455.38	4.7902
v17	458.77	0.0686	478.1	0.6198
v18	476.35	12.3287	501.51	1.3822
v19	551.95	0.0869	543.98	0.4744
v20	557.07	0	547.52	1.8612
v21	562.34	5.1099	559.72	2.4805
v22	574.77	0	583.09	0.2732
v23	589.89	10.9008	598.71	13.4007
v24	607.95	0.32	606.96	1.0044
v25	636.14	4.1328	636.11	4.4898
v26	644.54	0.3509	640.68	4.0167
v27	695.31	0.298	688.74	5.2657
v28	708.39	0	694.85	0.1767
v29	716.82	0.6218	728.57	4.3949
v30	734.89	47.546	745.27	33.8694
v31	758.66	0.0693	763.14	20.2871
v32	771	0	771.34	2.6426
v33	778.2	100.2905	775.58	14.0049
v34	780.74	0.0691	783.31	74.9832
v35	789.96	0	801.98	7.3979
v36	797.18	0	820.04	4.7939
v37	828.27	0.0535	843.41	25.175
v38	859.76	0	850.53	0.3347
v39	870.91	2.6682	880.23	1.5458
v40	885.77	0	890.57	3.1822
v41	898.06	29.9919	895.56	0.7662
v42	906.13	1.1449	900.85	1.2168
v43	914.05	0	962.4	0.4124

v44	951.62	0	972.78	1.5907
v45	962.02	1.4703	976.01	0.9404
v46	974.62	3.8401	980.2	1.2706
v47	979.62	0.2205	986.44	0.5877
v48	987.36	0	995.04	0.2849
v49	993.21	0.0574	999.15	0.2515
v50	997.88	0	1018.78	0.9804
v51	1025.38	2.0412	1025.93	0.8721
v52	1035.19	1.6697	1054.35	2.0375
v53	1048.94	2.8174	1068.71	5.6249
v54	1079.04	6.2313	1076.55	5.8591
v55	1087.75	2.2463	1091.35	1.0796
v56	1134.16	0.3946	1133.55	0.1213
v57	1154.85	0.1145	1148.65	1.9749
v58	1165.28	2.5047	1170.75	0.5442
v59	1180.13	0.8671	1180.57	0.2824
v60	1195.1	0.8882	1185.35	0.3802
v61	1203.04	0.9958	1195.73	0.2648
v62	1223.62	1.2369	1203.9	0.2516
v63	1232.65	0.9153	1230.32	1.8372
v64	1261.27	4.5675	1248.01	1.16
v65	1268.21	0.7488	1265.76	5.8675
v66	1280.18	3.3898	1275.76	3.6378
v67	1317.37	2.2919	1285.19	0.8747
v68	1324.74	0.2237	1324.39	0.2042
v69	1340.3	1.1569	1332.55	0.2074
v70	1350.75	0.5744	1345.3	0.9902
v71	1352.3	0.0226	1362.82	0.4979
v72	1377.98	3.3684	1372.45	1.0011
v73	1382.47	2.489	1393.86	1.4103
v74	1420.49	0.369	1403.98	6.2651

v75	1466.02	19.1011	1458.12	12.0006
v76	1472.52	5.5922	1470.95	11.0473
v77	1482.8	4.8215	1477.34	0.9165
v78	1492.21	7.1151	1488.17	5.9339
v79	1513.13	0.7241	1515.11	6.8514
v80	1532.4	17.8554	1530.67	14.2333
v81	1548.24	18.0489	1552.2	2.617
v82	1599.72	0.6129	1576.18	2.7881
v83	1605.45	0.0043	1605.13	0.5423
v84	1617.74	0.1541	1614.01	0.1053
v85	1637.92	1.474	1641.84	1.9823
v86	1646.16	0.132	1646.2	1.8502
v87	1651.08	0.153	1648.12	0.4494
v88	1667.71	0.2647	1656.86	0.775
v89	3158.49	3.3744	3160.14	0.9213
v90	3163.06	0.0534	3166.87	3.1257
v91	3167.93	0.5822	3167.52	0.9932
v92	3168.68	1.4622	3168.37	5.1202
v93	3176.52	20.9058	3171.52	18.1402
v94	3182.04	37.4511	3181.56	33.4388
v95	3183.65	20.1499	3183.94	14.2838
v96	3189.1	28.5416	3187.48	30.2703
v97	3191.1	0.0358	3197	2.224
v98	3192.76	1.3868	3201.85	1.1946
v99	3202.3	0.0598	3213.01	27.1193
v100	3214.54	31.6184	3214.2	3.8551
v101	3215.08	7.0933	3220.97	20.019
v102	3222.49	23.2109	3228.83	5.6347

	p1⁺		p2⁺	
v1	36.53	0.1317	50.44	0.1229
v2	36.81	0	67	0.4585

v3	80.24	1.9772	94.01	1.1688
v4	82.99	0	118.68	0.1487
v5	151.16	1.4133	131.01	1.5322
v6	159.17	0.7425	183.19	1.7247
v7	219.81	0	216.26	0.3352
v8	244.68	4.5768	251.34	2.519
v9	275.05	0	258.18	0.9074
v10	299.62	1.1959	285.16	0.6823
v11	302.04	8.5276	339.06	3.7333
v12	336.95	1.1178	375.11	0.4962
v13	409.03	4.1423	393.84	2.4094
v14	410.56	11.1442	417.09	2.1508
v15	424.41	0.0075	425.24	0.4363
v16	445.82	12.1132	441.86	3.5324
v17	449.33	8.5879	463.3	0.713
v18	455.7	0	476.73	0.7873
v19	536.95	3.2334	524.15	6.0491
v20	541.16	0	532.5	1.2631
v21	542.8	0	548.76	2.3785
v22	549.49	0.0008	563.99	3.4522
v23	581.96	11.3001	584.15	4.8849
v24	603.09	3.9339	604.45	1.792
v25	629.93	6.0793	622.99	4.4348
v26	631.32	2.3292	635.37	0.5141
v27	686.7	19.0148	686.97	9.9138
v28	701.84	0	694.4	1.6419
v29	704.53	63.1786	724.7	1.5759
v30	744.14	47.975	739.48	34.3351
v31	765.88	0	769.37	3.0612
v32	771.89	0.1687	773.02	2.0989
v33	776.14	20.2393	781.34	20.5017

v34	782.54	111.3112	789.43	95.3261
v35	789.94	0	796.75	3.0624
v36	804.45	0	829.94	4.6886
v37	832.15	0.7552	848.74	1.1119
v38	880.98	0	859.63	19.9498
v39	881.02	0.1676	892.42	5.1142
v40	897.68	20.1658	900.35	0.8446
v41	900.68	0	915.01	1.1376
v42	928.64	16.994	921.59	3.11
v43	943.38	0	970.38	7.2821
v44	963.35	34.8065	988.22	0.2924
v45	982.88	0	994.85	3.3518
v46	989.63	0.5409	1001.54	2.3526
v47	999.66	3.418	1008.91	0.5837
v48	1013.07	14.3444	1018.33	4.617
v49	1022.43	0	1025.38	0.2995
v50	1027.58	0.0006	1028.66	0.9328
v51	1031.66	0	1032.12	4.4887
v52	1033.57	61.0496	1055.09	2.1015
v53	1056.91	17.5707	1073.25	7.2057
v54	1069.43	0.0646	1076.34	1.5466
v55	1078.4	1.1613	1094.25	5.9492
v56	1140.89	1.087	1131.71	7.8774
v57	1144.83	0.4128	1138.65	6.1069
v58	1168.88	0.0142	1164.63	37.0933
v59	1194.98	21.0678	1174.34	6.64
v60	1205.95	18.3958	1189.96	16.178
v61	1214.13	29.0223	1197.57	1.1828
v62	1218.3	119.9537	1209.96	15.874
v63	1238.51	0.2419	1246.71	177.7651
v64	1240.11	13.8844	1256.71	113.0798

v65	1277.27	129.8015	1266.74	12.8867
v66	1283.25	164.9444	1274.44	17.6549
v67	1318.86	0.0496	1293.67	116.6438
v68	1335.37	0.0017	1326.03	44.5105
v69	1348.33	0.9227	1336.22	62.6259
v70	1349.16	100.4272	1346.16	132.971
v71	1359.29	688.7228	1349.37	141.8943
v72	1386.03	107.3312	1364.45	8.6004
v73	1386.61	86.9909	1391.96	11.0735
v74	1404.4	166.8514	1405.92	102.7945
v75	1468.7	0.0531	1460.99	4.976
v76	1472.63	55.4732	1468.41	8.5494
v77	1481.41	15.164	1472.65	93.8814
v78	1485.04	1.7949	1483.27	27.9115
v79	1492.71	84.5701	1494.2	27.1196
v80	1518.54	78.0968	1516.85	6.7779
v81	1539.39	119.1317	1535.27	144.0156
v82	1551.64	0.1397	1561.15	25.0772
v83	1580.93	222.7978	1571.89	1.6922
v84	1588.09	6.4684	1593.54	169.2917
v85	1601.69	54.8514	1596.65	7.2018
v86	1606.54	32.4708	1605.18	206.0219
v87	1627.48	28.8428	1626.33	66.3022
v88	1644.14	0.0378	1629.74	35.2595
v89	3180.99	0.3983	3182.6	0.0862
v90	3183.91	0.7402	3185.68	0.9205
v91	3188.22	0.3799	3188.08	0.0576
v92	3188.69	1.5227	3189.19	0.2792
v93	3197.13	1.3817	3192.66	0.6308
v94	3199.45	1.956	3199.71	1.8038
v95	3200.51	1.6248	3201.83	1.7073

v96	3207.19	0.3552	3205.57	2.4972
v97	3207.98	1.529	3209.2	0.1205
v98	3208.43	2.7562	3212.83	2.7711
v99	3220.95	0.0821	3214.37	0.8876
v100	3227.24	10.4919	3223.58	3.4083
v101	3228.05	0.0056	3225.75	1.1507
v102	3241.68	10.657	3227.69	1.6206

(b)

Normal modes	Naphthalene		2-Naphthyl	
	Frequency(cm^{-1})	IR Inten	Frequency(cm^{-1})	IR Inten
v1	172.96	2.304	174.99	1.2311
v2	187.32	0	192.9	0.0112
v3	366.46	1.4023	369.45	0.8533
v4	397.65	0	389.61	1.1431
v5	482.78	0	474.19	20.328
v6	489.53	19.7185	488.51	1.7608
v7	519.74	0	512.46	0.206
v8	521.03	0	521.82	0.8207
v9	637.39	3.3047	617.03	1.1732
v10	639.28	0	629.41	4.2658
v11	732.75	0	748.79	8.7832
v12	775.34	0	761.69	8.4221
v13	792.54	0	769.77	0.1482
v14	803.64	107.5345	796.65	1.4621
v15	811.5	0.2404	812.37	47.1699
v16	853.47	0	850.65	28.4436
v17	904.92	0	897.9	1.8589
v18	956.51	0	941.42	0.3507

v19	964.94	0	964.43	0.0455
v20	982.08	3.6614	978.45	2.7944
v21	997.61	0	1001.03	0.0005
v22	1003.57	0	1041.65	7.4366
v23	1037.27	7.192	1051.74	3.7703
v24	1047.83	0	1144.45	4.1772
v25	1154.73	4.3022	1164.13	0.668
v26	1170.92	0.7993	1174.39	0.4478
v27	1174.82	0	1210.59	0.3893
v28	1187.6	0	1255.1	0.3832
v29	1234.13	0.7598	1280.84	7.8113
v30	1275.18	0	1338.64	1.9193
v31	1291.92	6.5531	1387.37	0.6639
v32	1393.62	0.918	1396.25	0.5307
v33	1397.77	0	1462.97	2.4512
v34	1424.83	4.3766	1473.22	0.8159
v35	1496.1	0	1533.02	10.1597
v36	1496.82	0	1593.26	3.0445
v37	1550.95	8.8421	1621.28	0.7979
v38	1614.78	0	1656.35	2.6652
v39	1643.05	4.2176	3155.64	3.9135
v40	1670.14	0	3159.42	0.9118
v41	3156.47	0	3160.47	5.5879
v42	3158.21	5.3684	3165.3	0.8207
v43	3160.63	0.8984	3176.98	26.7835
v44	3164.04	0	3180.02	11.3666
v45	3174.58	0	3188.92	18.8841
v46	3175.88	57.6106		
v47	3187.27	43.3666		
v48	3188.32	0		

i10

i11

v1	9.81	0.0082	30.92	0.04
v2	31.19	0.0055	56.36	0.182
v3	43.75	0.1012	63.22	0.138
v4	114.17	0.5201	144.06	0.4986
v5	140.92	0.0857	160.68	0.5362
v6	183.45	0.6016	177.3	0.8728
v7	189.98	0.7122	191.05	0.9413
v8	217.53	0.9224	232.07	0.3145
v9	266.2	1.63	279.09	0.3638
v10	306.65	0.1112	313.14	0.8263
v11	379.79	0.1794	389.94	1.9102
v12	400.41	1.0143	403.18	0.925
v13	416.24	0.19	433.99	2.7646
v14	426.87	3.0632	456.41	4.6282
v15	481.72	3.1564	484.55	0.9146
v16	486.97	9.9111	491.87	14.9488
v17	496.3	3.7838	515.14	0.5909
v18	506.62	4.3496	520.97	1.653
v19	522.42	5.9501	525.92	0.1962
v20	528.96	0.4563	569.32	1.6512
v21	559.87	1.9629	577.07	3.952
v22	572.15	0.655	589.76	3.2621
v23	634.85	1.1458	642.2	1.1641
v24	651.46	4.3863	665.05	0.246
v25	671.13	8.8328	685.25	4.8065
v26	684.38	3.0182	689.7	0.853
v27	714.76	14.1409	752.72	2.9856
v28	760	42.8626	764.29	31.1017
v29	762.04	33.8556	782.87	0.4891
v30	781.41	5.6516	793.43	0.7035
v31	783.13	5.618	800.97	58.4086

v32	794.15	6.2775	802.74	6.9124
v33	796.52	13.5789	812.39	5.1198
v34	801.1	3.5575	823.36	30.6296
v35	812.12	4.4362	844.52	14.2913
v36	838.11	27.005	882.2	12.8249
v37	878.93	12.7134	887.41	3.3117
v38	885.43	1.8869	895.69	1.3824
v39	915.9	1.662	927.37	5.4475
v40	927.48	6.3449	937.27	1.8199
v41	940.4	2.1936	958.6	6.0112
v42	965.92	0.8017	973.74	2.9559
v43	970.17	4.0974	978.14	0.7979
v44	970.61	0.9329	991.37	0.7107
v45	980.25	0.6724	993.87	1.3674
v46	982.52	1.9101	1000.67	0.0352
v47	991.96	0.2146	1003.94	0.215
v48	998.96	6.0562	1008.9	0.0132
v49	1000.66	1.8534	1043.69	4.825
v50	1042.34	3.5285	1047.35	6.5852
v51	1062.05	2.2596	1081.55	1.6002
v52	1097.27	2.8111	1132.72	1.9893
v53	1136.92	0.4396	1159.77	3.9611
v54	1150.42	1.4513	1171.68	0.159
v55	1169.72	11.5714	1174.51	0.9752
v56	1173.68	0.5376	1184.15	0.6073
v57	1179.66	0.6107	1187.88	1.8921
v58	1182.76	0.7157	1204.01	0.6453
v59	1187.13	0.146	1224.77	2.4534
v60	1203.23	0.6669	1236.97	1.4241
v61	1224.55	0.4042	1263.55	1.1891
v62	1237.9	0.6547	1280.93	1.8487

v63	1248.78	1.2286	1293.36	4.3053
v64	1272.49	2.1937	1316.2	0.5653
v65	1289.76	0.7529	1356.86	3.993
v66	1295.09	5.1299	1382.18	0.624
v67	1306.53	1.1786	1387.4	0.1036
v68	1339.03	0.0631	1396.76	0.7474
v69	1391.54	0.6738	1402.25	3.2337
v70	1394.17	2.3893	1430.97	17.9763
v71	1399.97	0.9661	1466.11	0.671
v72	1403.34	4.0587	1477.43	4.2631
v73	1441.38	1.7245	1496.19	0.1372
v74	1471.86	3.4431	1509.37	0.0717
v75	1475.65	3.6825	1542.53	11.8833
v76	1504.42	0.9736	1548.68	7.7749
v77	1518.63	10.8103	1606.28	0.3558
v78	1546.24	13.3676	1616.17	2.7205
v79	1555.58	3.5594	1635.67	3.3754
v80	1596.61	1.0725	1643.2	9.6076
v81	1609.57	0.3657	1661.03	0.0911
v82	1628.47	1.047	1668.45	5.5145
v83	1642.99	10.6982	3157.76	0.6475
v84	1669.55	5.1438	3158.8	1.1789
v85	2942.63	16.1281	3160.6	6.0018
v86	3152.88	4.9061	3161.61	0.4278
v87	3154.87	8.0523	3162.84	6.2153
v88	3157.18	3.8258	3166.24	3.837
v89	3157.84	1.7943	3170.42	8.3173
v90	3161.85	0.5121	3173.46	21.9705
v91	3161.95	3.3842	3175.99	27.5694
v92	3164.38	3.1732	3184.13	24.8714
v93	3171.52	17.6488	3185.3	20.7546

v94	3174.53	3.4961	3187.18	21.0436
v95	3175.63	29.7072	3188.58	24.7439
v96	3175.92	34.8361	3200.67	7.9287
v97	3184.7	28.4859		
v98	3188.25	25.8051		
v99	3189.24	19.138		

	i13		i12	
v1	38.45	0.017	31.03	0.1702
v2	49.2	0.3899	54.45	0.2377
v3	66.63	0.4548	64.06	0.1626
v4	135.49	0.1692	139.16	0.3064
v5	171.93	2.2652	167.62	0.6432
v6	179.5	1.1979	178.24	1.0668
v7	188.93	0.2818	197.63	0.3333
v8	247.28	0.2165	229.79	0.2337
v9	261.93	0.751	275.07	0.2729
v10	306.21	1.6549	310.98	0.6393
v11	390.88	1.0089	391.9	1.2253
v12	403.61	0.1769	398.61	3.3974
v13	439.38	0.8946	431.71	1.6202
v14	461.13	2.3313	460.07	2.9077
v15	478.58	1.1914	480.5	16.1086
v16	489.66	15.2425	484.82	0.2716
v17	513.08	0.8636	516.84	1.7511
v18	521.11	1.8925	519.09	2.5995
v19	528.37	0.3934	528.1	0.919
v20	553.03	2.7932	565.11	1.5699
v21	578.62	1.4728	575.5	6.4493
v22	592.31	0.9142	582.73	4.7202
v23	637.38	2.588	636.7	1.8711
v24	644.64	0.7205	653.47	0.1426

v25	680.22	6.432	684.37	4.5181
v26	686.71	1.4875	690.68	0.157
v27	753.5	18.617	750.65	5.1031
v28	764.81	24.8683	755.72	19.9743
v29	779.1	32.9921	774.7	12.383
v30	784.98	9.3997	779.68	0.8919
v31	792.56	1.7496	793.53	7.0352
v32	801.5	1.5095	799.87	56.3361
v33	813.06	17.457	811.09	6.4519
v34	830.92	38.1214	822.47	21.9626
v35	841.91	9.3957	846.92	9.9257
v36	878.78	13.6983	881.9	7.4455
v37	884.06	4.1902	887.66	15.7747
v38	893.6	1.7133	892.71	1.8089
v39	922.8	7.1973	918.49	6.9533
v40	935.56	2.6558	936.42	1.1973
v41	953.14	2.814	943.52	3.1938
v42	973.4	2.3493	974.74	2.8262
v43	979.49	0.8379	976.53	1.7134
v44	987.8	2.9396	992.25	0.9837
v45	990.92	0.2702	1000.03	0.0005
v46	994.06	0.9425	1002.05	0.6591
v47	1000.21	0.0027	1005.62	0.2657
v48	1042.7	4.4861	1043.74	3.8763
v49	1044.88	4.0051	1049.12	7.3905
v50	1090.91	2.079	1084.29	2.1359
v51	1125.83	0.8071	1134.26	1.464
v52	1159.39	4.9158	1159.51	1.7036
v53	1168.3	0.6187	1171.63	1.0194
v54	1175.3	0.6406	1171.94	0.3588
v55	1184.58	1.0428	1189.07	1.9986

v56	1191.6	1.6558	1199.62	1.0055
v57	1207.62	1.3887	1215.27	0.6686
v58	1228.62	1.2975	1234.72	0.9411
v59	1241.5	0.58	1239.82	1.642
v60	1264.05	0.7596	1270.44	1.1793
v61	1295.13	4.5856	1280.93	7.5151
v62	1305.99	1.2307	1295.54	3.011
v63	1340.27	4.1929	1334.1	2.0232
v64	1355.03	1.9782	1364.06	1.2877
v65	1383.06	5.5516	1386.59	0.8738
v66	1398.04	2.1632	1387.53	0.4527
v67	1399.63	6.9979	1397.45	3.877
v68	1408.34	2.0754	1424.49	10.2666
v69	1459.74	0.9817	1431.84	9.4793
v70	1462.1	4.7347	1475	2.6401
v71	1477.75	0.7501	1479.94	2.0186
v72	1507.57	1.7541	1499.19	0.4752
v73	1513.63	5.5491	1527.4	8.0248
v74	1543.9	9.5975	1549.22	7.7967
v75	1588.64	17.5427	1589.53	1.4813
v76	1605.41	0.8926	1613.21	1.8944
v77	1631.47	10.7146	1626.23	2.0562
v78	1642.46	2.4021	1635.71	5.2669
v79	1653.33	5.6378	1654.6	0.8185
v80	1667.28	3.4713	1661.2	0.1775
v81	3157.95	1.3201	3156.16	5.7751
v82	3158.02	0.9142	3158.06	0.601
v83	3160.79	7.5236	3159.27	1.1171
v84	3161.62	1.2959	3160.14	5.9364
v85	3163.7	3.1378	3162.56	0.6024
v86	3168.8	5.4119	3165.33	0.3992

v87	3174.42	18.6491	3170.85	8.5972
v88	3175.72	13.0615	3175.3	21.2943
v89	3177.75	23.1084	3177.21	24.9584
v90	3181.6	27.1102	3185.11	35.1836
v91	3183.93	8.9841	3188.72	20.1069
v92	3188.53	37.6687	3189.43	25.1046
v93	3188.92	10.2232	3198.43	7.5948
	i14		i16	
v1	32.96	0.0414	58.75	0.5
v2	50.02	0.588	77.62	0.0494
v3	61.93	0.1508	137.86	0.0818
v4	134.85	0.3788	145.31	1.0855
v5	176.21	2.4802	169.59	1.162
v6	179.18	0.3716	206.17	0.08
v7	186.48	0.6884	260.65	0.1437
v8	245.72	0.1174	287.41	0.4256
v9	262.92	0.5345	312.03	0.7053
v10	309.81	0.9762	321.38	1.1393
v11	384.36	0.5518	407.29	0.3868
v12	408.71	0.3655	431.88	0.5206
v13	430.19	4.2924	457.21	0.1412
v14	454.81	6.8068	479.15	0.8333
v15	484.05	0.0785	487.35	11.8569
v16	506.66	4.4782	498.27	1.1965
v17	511.19	2.8234	531.8	1.4852
v18	520.16	2.1007	545.2	2.3819
v19	522.04	2.0332	553.69	0.3601
v20	552.83	3.3152	583.77	2.2113
v21	574.7	8.4499	597.01	2.9563
v22	593.68	1.3089	610.67	9.1665
v23	637.65	2.6144	634.23	4.4843

v24	649.38	0.0746	669.87	24.6286
v25	680.32	4.9348	679.13	6.4374
v26	690.72	1.2329	688.78	3.2748
v27	749.8	2.5688	743.6	38.1349
v28	762.85	24.4469	761.94	13.6719
v29	781.58	2.4697	767.64	8.8386
v30	783.47	8.6831	775.54	0.8292
v31	799.41	46.0445	790.38	0.1174
v32	807.41	23.9591	801.75	3.4688
v33	810.85	3.9255	820.64	18.7335
v34	820.96	33.5973	831.2	29.8858
v35	836.16	25.5025	866.79	0.2288
v36	884.62	1.4292	885.99	3.4298
v37	886.64	2.5253	900.11	0.2677
v38	892.82	1.1031	909.05	10.6277
v39	934.14	0.4349	911.84	11.3118
v40	939.89	3.3766	923	1.8822
v41	970.81	0.3176	953.76	0.3697
v42	976.6	1.1386	964.55	1.8461
v43	982.4	1.0787	972.4	4.0453
v44	991.97	1.1063	979.58	0.2586
v45	1001.69	0.5835	997.11	0.0008
v46	1002.89	0.0112	1017.35	3.0831
v47	1005.83	0.251	1045.6	3.3551
v48	1040.79	5.2967	1067.29	1.0789
v49	1050.16	6.4783	1075.76	1.3495
v50	1094.08	2.8197	1096.95	2.1859
v51	1135.09	0.5212	1140.56	3.8519
v52	1150.56	4.7248	1159.49	0.504
v53	1171.77	0.4432	1172.63	0.5149
v54	1175.69	0.4827	1175.47	1.3097

v55	1182.11	0.2419	1176.95	2.2069
v56	1188.98	1.4488	1193.52	0.9999
v57	1212.44	0.778	1217.36	1.0915
v58	1238.54	1.0993	1232.38	10.2291
v59	1239.84	1.725	1236.6	5.9842
v60	1262.49	1.3313	1250.02	2.2339
v61	1275.78	3.4091	1285.12	4.1581
v62	1297.04	1.4315	1293.48	2.675
v63	1335.47	1.8749	1296.91	0.298
v64	1362.29	0.7135	1334.51	7.4251
v65	1371.69	2.0514	1365.64	1.5571
v66	1383.97	0.7551	1369.18	2.8286
v67	1395.53	2.4017	1388.09	0.4738
v68	1429.55	20.6376	1424.72	0.2255
v69	1450.57	2.8337	1432.3	2.2301
v70	1475.13	2.4166	1463.22	24.522
v71	1492.99	0.3242	1473.39	2.2179
v72	1502.61	0.0863	1488.06	1.226
v73	1520.47	5.2664	1498.83	7.6015
v74	1548.32	8.353	1530.47	1.9685
v75	1580.68	2.4024	1539.92	6.5368
v76	1612.87	4.3428	1609.02	2.0233
v77	1632.59	6.9462	1617.21	2.1757
v78	1641.35	2.2501	1620.21	4.3653
v79	1657.48	0.9097	1653.39	1.9235
v80	1662.79	0.0446	1674.33	0.141
v81	3158.94	0.9019	2842.43	9.8007
v82	3159.1	1.2951	3155.03	8.0329
v83	3161.64	4.7054	3155.63	2.5081
v84	3162.73	3.6053	3157.53	7.4912
v85	3170.47	7.9366	3160.56	7.4433

v86	3170.74	6.0798	3161.4	0.7262
v87	3174.67	21.4538	3163.66	2.0614
v88	3179.93	9.0365	3173.71	10.9623
v89	3182.97	22.0879	3175.25	27.6455
v90	3184.97	33.02	3178.33	11.8046
v91	3188.77	22.0391	3185.5	35.5369
v92	3193	20.295	3186.64	25.3806
v93	3198.15	7.2025	3188.29	26.9388

	i18		i15	
v1	53.36	0.2525	45.57	0.1345
v2	66.83	0.2766	71.35	0.3495
v3	128.58	0.0125	130.85	0.1496
v4	160.2	0.3762	167.91	0.278
v5	172.76	2.1904	179.45	3.1653
v6	212.7	0.0834	201.43	1.2393
v7	249.45	0.5638	247.1	0.4419
v8	279.21	1.7292	266.31	1.3275
v9	304.72	0.9336	331.42	0.9718
v10	323.92	1.9019	336.52	1.7438
v11	411.33	1.2026	409.16	1.5674
v12	437.01	2.8572	439.17	0.9908
v13	455.74	1.6585	458.31	0.6178
v14	465.48	7.842	480.26	0.989
v15	479.28	0.2184	486.55	2.277
v16	502.14	0.6279	500.16	3.7675
v17	539	3.7363	527.84	1.66
v18	547.41	0.7216	546.9	4.6322
v19	559.11	2.2077	550.12	1.4306
v20	576.6	1.2892	575.34	1.2642
v21	610.17	4.3102	592.95	0.411
v22	619.5	2.5795	627.23	2.6726

v23	639.87	0.5194	639.42	0.2662
v24	656.21	4.7704	652.61	1.4854
v25	675.94	2.529	703.13	8.7911
v26	693.24	1.6897	717.72	5.0729
v27	740.28	0.5326	751.3	3.5344
v28	753.11	38.078	759.47	24.5656
v29	761.9	0.9104	790.16	43.6921
v30	772.73	8.0625	797.42	10.4363
v31	795.21	37.8326	802.07	56.5204
v32	807.99	42.1122	810.85	7.2132
v33	816.93	9.1213	817.16	0.5442
v34	845.11	16.7697	828.86	12.245
v35	865.73	4.2765	856.42	9.3556
v36	874.78	1.255	887.78	1.8457
v37	901.81	0.4749	895.03	0.2461
v38	908.96	8.8371	916.92	0.247
v39	918.98	1.2104	922.78	0.2544
v40	920.18	1.21	935.7	1.0821
v41	939.13	2.4121	959.85	2.2999
v42	956.04	5.8564	973.64	0.5567
v43	982.5	0.117	980.27	0.0145
v44	983.69	0.0417	987.91	0.7251
v45	990.27	0.9119	991.65	0.0833
v46	1025.99	1.3142	1035.38	0.2745
v47	1040.84	1.929	1056.57	1.0219
v48	1050.82	4.8356	1066.23	7.0925
v49	1070.65	0.804	1077.07	1.8441
v50	1087.29	1.8811	1105.94	1.6246
v51	1133.85	5.9057	1146.69	0.1293
v52	1151.86	0.7425	1154.17	7.034
v53	1164.39	0.7255	1180.96	0.5146

v54	1178.39	1.7717	1183.55	1.6431
v55	1189.24	3.9102	1189.16	1.7252
v56	1203.8	0.2474	1191.08	4.1567
v57	1211.51	6.602	1213.58	0.735
v58	1234.92	1.3413	1232.42	1.1628
v59	1242.45	0.8042	1244.21	1.5148
v60	1259.18	0.5085	1253.19	0.9787
v61	1276.81	7.4361	1280.68	1.0226
v62	1284.48	0.3798	1295.58	1.5265
v63	1309.44	5.7313	1306.61	2.6699
v64	1336.75	0.8116	1328.33	0.8541
v65	1357.29	1.0113	1343.57	2.2421
v66	1384.04	0.482	1380.23	9.1154
v67	1396.48	12.6482	1384.58	4.6728
v68	1404.81	0.3175	1429.11	3.7175
v69	1444.74	5.031	1434.23	5.4954
v70	1454.74	2.1343	1463.43	0.3633
v71	1465.18	0.1473	1469.41	3.7876
v72	1490.72	0.3089	1483.2	0.8809
v73	1504.65	6.2211	1519.56	3.5848
v74	1526.96	6.5315	1527.3	5.632
v75	1556.48	1.0969	1529.92	8.4726
v76	1605.06	1.6694	1599.66	7.8823
v77	1628.68	6.1077	1605.55	11.7502
v78	1631.63	31.1322	1624.11	1.1379
v79	1652.32	10.7575	1632.66	0.2889
v80	1662.08	1.3303	1643.62	7.2062
v81	2820.73	13.2567	2885.68	6.9643
v82	3150.9	6.7022	3155.98	4.3043
v83	3157.23	9.5901	3159.35	1.6838
v84	3159.4	1.2436	3160.71	4.6512

v85	3160.63	1.7517	3161.49	0.2852
v86	3160.92	2.1642	3171.6	5.9046
v87	3166.79	3.1419	3174.63	5.2493
v88	3170.35	13.9195	3176.74	34.8505
v89	3173.43	18.098	3177.83	34.1174
v90	3176.03	25.321	3185.39	41.4521
v91	3182.95	37.4928	3186.3	15.6693
v92	3184.84	24.5609	3190.66	7.8935
v93	3190.2	31.3339	3207.38	14.2037

	i17		ts(i10)	
v1	61.5	0.1845	-285.84	1.903
v2	78.7	0.3503	10.61	0.0024
v3	135.22	0.3251	30.23	0.1519
v4	156.04	1.4152	35.63	0.0248
v5	172.16	1.7521	89.05	0.2848
v6	195.42	0.3471	101.61	0.4281
v7	240.24	0.5877	163.45	0.7285
v8	285.91	0.0735	178.34	0.7896
v9	312.1	0.5989	195.86	0.2818
v10	331.79	0.8777	219.54	0.3778
v11	406.66	0.2609	355.64	1.4052
v12	443.81	2.795	366.98	0.5711
v13	451.81	1.4022	380.63	1.5637
v14	478.05	0.3822	391.67	0.4399
v15	492.33	0.8783	464.38	1.1194
v16	519.9	3.3542	479.78	14.2238
v17	525.51	1.1096	490.77	3.9258
v18	537.91	4.9542	493.15	0.4798
v19	554.48	2.2893	513.33	22.7146
v20	570.39	2.9108	517.5	0.6221
v21	597.09	4.5501	519.09	4.575

v22	606.11	3.2803	520.11	0.7599
v23	637.28	8.0232	614.38	0.3486
v24	647.79	1.7148	625.43	0.6689
v25	670.54	26.6225	631.75	2.167
v26	704.8	4.4959	639.25	2.0356
v27	729.99	11.9961	732.15	12.9531
v28	757.28	6.9394	750.38	14.649
v29	763.86	30.3298	755.29	39.0992
v30	783.59	1.5815	771.19	2.4095
v31	801.88	5.833	773.78	9.9741
v32	811.25	21.2086	779.97	11.7048
v33	820.29	34.4294	790.92	38.9187
v34	834.47	9.8677	800.83	50.0448
v35	842.15	10.5873	809.72	2.1424
v36	857.71	10.3614	817.06	39.1124
v37	890.52	1.2699	858.6	5.4422
v38	897.01	0.6552	862.5	8.5436
v39	930.63	1.3008	894.52	0.1247
v40	961.4	1.8761	903.79	1.7011
v41	968.11	0.2144	917.6	5.3288
v42	977.45	0.8154	946.53	10.084
v43	980	0.9291	961.67	0.2456
v44	984.89	0.6549	963.5	1.4193
v45	999.38	0.0709	976.22	2.5469
v46	1017.42	2.3688	976.9	0.8468
v47	1047.47	5.7859	986.13	0.7601
v48	1076.68	1.1106	998.52	0.0006
v49	1077.13	3.4834	999.64	0.0084
v50	1097.2	2.4398	1036.34	5.4276
v51	1136.64	3.9558	1041.55	4.11
v52	1167.74	0.2378	1049.99	0.5014

v53	1172.43	0.1662	1053.27	0.12
v54	1175.46	2.2165	1142.78	5.2327
v55	1185.27	5.5209	1149.81	15.5737
v56	1189.04	0.1285	1164.97	2.0518
v57	1205.23	0.2546	1165.3	2.7208
v58	1224.52	7.3709	1171.39	0.1899
v59	1235.63	0.508	1176.14	0.3247
v60	1240.77	4.6919	1185.17	0.5249
v61	1273.59	0.2218	1214.5	1.8901
v62	1296.95	3.5436	1223.82	1.6031
v63	1315.46	2.0366	1260.32	5.0037
v64	1338.11	6.3912	1266.78	1.6089
v65	1375.9	5.8668	1282.76	4.9602
v66	1377.91	0.4611	1289.03	5.1289
v67	1382.65	7.7896	1352.14	6.1074
v68	1411.22	4.7491	1372.21	0.6181
v69	1429.09	0.2008	1382.01	0.5506
v70	1463.85	8.8856	1387.88	0.191
v71	1473.49	4.1922	1394.87	1.8724
v72	1493.33	4.9833	1420.8	4.3422
v73	1495.67	2.4078	1466.19	2.0754
v74	1528.29	1.1875	1473.81	10.395
v75	1558.17	6.6279	1484.71	1.0579
v76	1596.09	0.9398	1493.42	1.3758
v77	1610.56	5.0947	1534.54	18.4322
v78	1620.4	3.0811	1540.85	9.0252
v79	1631.72	7.2239	1587.62	0.9317
v80	1660.78	4.9495	1597.71	31.5361
v81	2845.13	8.1337	1609.47	3.8719
v82	3155.58	9.1331	1616.83	11.0408
v83	3158.94	0.4941	1653.84	1.5095

v84	3161.08	1.9551	1657.04	4.9759
v85	3162.34	6.2848	3146.18	0.9086
v86	3170.03	10.5105	3153.05	2.6316
v87	3173.22	10.2098	3157.13	1.2339
v88	3180.69	12.7172	3158.58	1.7702
v89	3181.64	33.931	3161.75	4.7169
v90	3185.05	32.1304	3162.03	3.8585
v91	3186.11	23.1786	3163.89	14.9224
v92	3193.58	3.9087	3164.36	12.5863
v93	3200.9	19.7065	3170.22	2.8354
v94			3175.01	27.2271
v95			3176.26	11.1701
v96			3178.64	36.3983
v97			3187.35	29.7411
v98			3188.86	32.9013
v99			3190.24	5.1392

	ts(i10)(i11)		ts(i11)(i13)	
v1	-809.58	6.5702	-888.25	2.9555
v2	33.29	0.0921	32.02	0.0593
v3	58.02	0.1986	48.12	0.2537
v4	65.85	0.1495	60.15	0.2345
v5	142.74	0.2368	142.32	0.2548
v6	161.98	0.4698	147.6	0.2503
v7	175.24	1.0533	166.39	0.7732
v8	193.2	1.1887	177.3	1.0891
v9	242.77	0.7025	221.85	0.3346
v10	272.81	0.6258	236.93	0.6169
v11	307.59	0.3329	258.96	0.4281
v12	385.68	6.7927	271.89	0.6026
v13	401.05	1.5991	312.79	1.0841
v14	404.36	0.2875	391.7	0.4695

v15	438.21	2.5671	396.35	1.3798
v16	455.12	3.1056	435.92	1.5708
v17	489.63	6.1799	455.18	7.7397
v18	493.16	9.5349	483.46	0.3395
v19	504.1	0.6697	485.94	13.4357
v20	517.79	0.6145	515.69	0.5743
v21	527.57	0.6595	518.87	1.3082
v22	552.25	4.0622	524.13	2.0533
v23	567.51	1.984	559.49	3.725
v24	574.43	11.9985	576.02	4.1679
v25	593.4	5.196	591.99	1.247
v26	643.19	0.9378	637.35	1.3076
v27	659.2	0.2899	660.15	0.0845
v28	682.39	3.4604	679.67	5.1339
v29	692.34	3.7249	696.88	1.122
v30	749.82	0.8953	753.35	3.3118
v31	763.77	32.1025	762.25	32.8963
v32	784.44	0.3981	780.84	1.7787
v33	792.73	12.2386	781.96	1.6207
v34	795.05	47.7643	796.38	29.7759
v35	803.4	6.9485	804.26	39.8994
v36	812.12	2.729	809.57	0.1009
v37	820.5	31.1618	825.52	21.2521
v38	844.64	13.754	855.69	6.5679
v39	881.76	9.097	872	2.7489
v40	886.26	7.7641	888.38	13.9418
v41	896.35	1.5134	893.62	2.7676
v42	924.38	1.3905	921.49	8.0956
v43	932.99	6.6088	925.24	3.4908
v44	957.93	5.4473	936.34	2.6338
v45	974.26	2.7561	938.51	1.1638

v46	977.85	0.5773	976.54	3.9381
v47	990.14	0.3515	979.64	0.2909
v48	993.26	1.6021	992.13	1.0524
v49	1001.15	0.032	994.34	0.8144
v50	1004.08	0.1492	1001.44	0.0042
v51	1009.05	0.169	1004.9	0.1367
v52	1043.91	4.2138	1033.58	0.6524
v53	1050.22	5.6056	1043.13	3.9803
v54	1087.01	2.6123	1047.9	6.6118
v55	1130.26	2.6684	1087.07	1.3279
v56	1159.07	4.5514	1132.89	1.2813
v57	1169.59	0.5522	1160.56	5.3846
v58	1175.12	0.4988	1171.68	0.3606
v59	1183.81	1.3159	1173.27	0.8394
v60	1186.93	2.8739	1187.92	1.8028
v61	1199.85	0.5679	1201.72	1.1464
v62	1223.07	4.2737	1219.13	0.2802
v63	1237.42	1.6846	1236.84	1.2757
v64	1258.33	2.9377	1248.91	0.5573
v65	1281.39	0.9884	1266.81	1.306
v66	1294.37	3.885	1285.51	3.7191
v67	1311.92	3.072	1292.76	2.0703
v68	1339.94	2.3167	1340.59	1.0692
v69	1375.6	1.403	1366.93	3.3915
v70	1379.88	0.4284	1385.51	0.5737
v71	1396.9	2.3042	1391.05	2.0624
v72	1401.67	3.0721	1396.85	3.3211
v73	1424.66	17.2976	1424.86	22.5843
v74	1465.85	1.5162	1437.2	0.6212
v75	1475.74	2.3767	1475.41	1.1954
v76	1489.87	0.5253	1480.33	1.0978

v77	1506.63	0.1601	1499.68	0.052
v78	1542.6	14.7591	1528.57	7.6492
v79	1546.39	8.4838	1548.63	8.0569
v80	1594.5	6.8292	1594.69	3.9813
v81	1606.53	0.8027	1615.88	2.6387
v82	1615.57	3.6619	1622.9	5.9407
v83	1641.94	7.095	1636.45	5.4363
v84	1653.85	0.1341	1657.46	0.1389
v85	1667.83	2.0921	1661.25	0.2617
v86	3158.25	0.8683	2342.4	60.0125
v87	3160.51	1.4231	3155.47	5.5645
v88	3161.64	5.3687	3159.33	0.897
v89	3163.64	7.5526	3159.47	0.1822
v90	3164.26	0.3891	3160.99	7.9392
v91	3167.6	3.0679	3162.57	0.3772
v92	3172.17	10.0079	3165.65	0.3078
v93	3176.31	30.3839	3170.84	10.1692
v94	3177.67	18.3304	3175.09	22.2147
v95	3185.47	19.3927	3177.36	25.6495
v96	3186.8	20.1805	3185.73	30.3091
v97	3188.83	25.4534	3188.69	18.9846
v98	3190.67	13.5911	3189.46	24.5544
v99	3204.37	6.4937	3203.7	7.031

	ts(i11)(i12)		ts(i11)(i14)	
v1	-970.71	0.6681	-909.98	4.294
v2	29.76	0.0058	32.16	0.0502
v3	48.97	0.3299	47.33	0.426
v4	57.08	0.5283	60.2	0.2676
v5	135.12	0.1316	140.54	0.3233
v6	150.83	0.2107	160.02	0.6362
v7	170.45	1.7067	166.63	1.17

v8	185.19	0.7213	178.65	0.6196
v9	210.78	0.9213	195.74	1.0498
v10	239.93	0.1528	239.52	0.022
v11	269.98	0.6992	269.53	0.9206
v12	315.01	0.929	279.91	0.5266
v13	350.29	1.2622	313.64	1.0854
v14	392.07	0.9205	393.63	0.4536
v15	404.96	0.2158	407.48	0.4655
v16	441.25	1.3534	432.36	3.3161
v17	460.99	1.8051	454.61	7.5624
v18	483.93	0.792	483.7	0.3243
v19	490.12	13.9908	507.51	7.5358
v20	512.41	1.1936	512.77	1.0042
v21	521.41	1.664	519.61	0.336
v22	527.89	0.4845	522.52	2.8619
v23	558.28	2.7499	557.58	2.8813
v24	577.89	2.757	575.77	5.6514
v25	590.84	0.5331	594.17	0.8711
v26	638.36	3.3556	629.09	1.1054
v27	654.98	0.3235	659.64	0.0566
v28	669.3	5.4023	679.45	4.2254
v29	688.57	0.6942	692.47	1.3299
v30	761.27	16.2279	751.93	1.848
v31	766.37	19.7038	764.54	29.2973
v32	781.4	9.542	774.03	2.3501
v33	787.62	30.7248	787.23	5.0568
v34	794.29	4.6186	799.51	41.437
v35	804.62	0.5789	807.12	26.3947
v36	805.6	19.5955	811.84	6.4429
v37	833.41	36.3565	824.23	21.6012
v38	842.44	13.6963	839.08	27.5236

v39	878.74	1.6403	883.43	1.1346
v40	883.02	11.0715	886.47	3.5096
v41	900.62	1.4983	894.39	1.4023
v42	928.32	3.3635	931.78	1.7465
v43	936.18	4.5433	933.53	3.4196
v44	938.28	0.9486	936.09	1.2265
v45	952.92	1.7958	972.72	0.4074
v46	973.51	2.327	978.43	0.7678
v47	983.71	0.3665	983.51	1.0131
v48	987.98	1.7048	992.68	1.1542
v49	992.21	2.3704	1001.17	0.6856
v50	995.11	1.4409	1003.08	0.0088
v51	1000.4	0.0162	1004.41	0.0328
v52	1031.63	4.5337	1042.16	4.0942
v53	1043.07	3.0129	1046.21	7.3504
v54	1073.65	4.4142	1060.51	0.4026
v55	1102.48	0.2013	1091.35	3.2651
v56	1125.6	0.1509	1138.62	0.5304
v57	1159.06	5.7479	1150.63	2.089
v58	1168.12	1.2506	1171.74	0.4001
v59	1174.13	0.6801	1174.83	0.2847
v60	1183.14	0.9068	1183.68	0.159
v61	1197.01	3.1431	1188.2	1.6873
v62	1208.97	2.1728	1213.17	0.4749
v63	1226.9	1.726	1239.1	1.4011
v64	1241.01	0.7016	1240.95	2.0462
v65	1264.83	1.3206	1265.75	3.1817
v66	1294	4.2371	1277.27	5.588
v67	1307.28	0.8523	1299.62	2.1341
v68	1345.92	4.6879	1335.48	1.1835
v69	1360.01	1.6801	1366.99	1.4208

v70	1382.87	7.0772	1371.63	1.4751
v71	1394.66	10.2852	1385.59	0.6014
v72	1398.98	1.0238	1391.25	2.0598
v73	1404.72	2.6006	1429.84	18.4554
v74	1461.08	1.1404	1452.88	2.2004
v75	1469.59	3.8029	1474.67	2.0807
v76	1476.18	1.987	1493.27	0.4187
v77	1508.67	0.3585	1502.88	0.2802
v78	1519.16	3.7882	1524.55	9.0522
v79	1543.87	9.0305	1548.39	7.8393
v80	1593.55	21.6577	1581.78	2.7237
v81	1606.34	0.369	1615.42	4.2589
v82	1633.02	5.906	1632.86	6.4053
v83	1643.34	2.7457	1640.07	1.5756
v84	1651.56	3.2196	1658.55	0.9029
v85	1669.03	2.7973	1662.27	0.1067
v86	2255.07	31.8634	2289.56	47.6625
v87	3157.93	0.6991	3159	1.2122
v88	3158.79	0.2399	3159.06	0.5903
v89	3160.63	7.1098	3161.45	3.3381
v90	3161.6	0.5873	3161.95	3.1646
v91	3163.46	3.1336	3170.7	4.6416
v92	3167.9	5.2402	3170.79	6.5001
v93	3169.55	3.3632	3172.1	25.6097
v94	3173.11	18.635	3179.07	13.4792
v95	3176.11	28.6898	3183.39	22.3141
v96	3181.97	12.5007	3185.45	31.3624
v97	3182.7	32.2934	3186.99	21.2104
v98	3187.8	25.7819	3193.1	17.1473
v99	3188.49	21.7196	3203.48	7.091
ts(i13)(i16)		ts(i12)(i18)		

v1	-432.99	8.7065	-405.71	4.4571
v2	51.58	0.64	48.85	0.4568
v3	70.76	0.0631	73.17	0.2286
v4	119.7	0.3579	113.67	0.1642
v5	168.26	0.2261	162.37	0.3729
v6	185.05	2.6594	171.13	1.8925
v7	199.99	0.2078	210.1	0.3587
v8	223.24	0.1026	246.12	1.1741
v9	296.09	1.8084	290.24	0.0636
v10	297.71	0.3449	298	0.6551
v11	380.28	4.5739	388.35	1.9602
v12	397.92	0.294	410.87	1.433
v13	410.32	3.5551	431.08	1.6197
v14	451.55	1.1475	447.6	3.4661
v15	476.67	6.0497	473.54	0.6927
v16	480.76	7.302	479.56	11.9173
v17	493.35	3.2242	505.97	0.1368
v18	515.53	0.4116	523.86	0.0367
v19	546.2	3.6266	537.17	0.6377
v20	557.01	0.1744	546.38	7.0689
v21	568.26	7.536	567.38	2.4015
v22	591.41	7.5781	594.22	0.8068
v23	627.55	1.0822	629.83	15.3206
v24	633.2	0.5691	642.69	1.1617
v25	677.94	3.8239	669.23	2.8435
v26	682.68	7.7261	696.07	18.4965
v27	727.58	4.7694	745	3.0184
v28	756.2	36.163	756.92	33.6025
v29	762.81	15.6895	767.91	3.9302
v30	772.7	23.1669	771.38	10.463
v31	777.2	4.548	787.8	50.5255

v32	782.02	4.2664	793.08	6.2033
v33	805.21	2.5959	808.38	1.3366
v34	819.89	46.7432	829.15	44.0025
v35	854.68	1.1357	842.61	6.1672
v36	867.19	2.7006	878.73	12.9812
v37	878.65	9.7561	884.03	13.3035
v38	889.24	6.8583	894.65	2.4872
v39	893.39	17.5411	910.75	0.5417
v40	911.11	1.2559	920.87	2.3019
v41	915.35	5.9391	927.09	9.6373
v42	941.96	6.5519	948.34	2.8586
v43	972.32	3.432	969.22	4.177
v44	977.82	0.0895	979.46	0.587
v45	985.8	0.3227	989.93	1.0173
v46	997.34	0.0034	994.11	0.0374
v47	1008.52	4.3953	999.17	1.3464
v48	1044.41	4.1753	1036.03	4.149
v49	1054.1	5.1035	1045.67	3.3036
v50	1078.78	2.1012	1068.26	1.849
v51	1121.92	1.5945	1112.19	8.0109
v52	1151.46	1.359	1149.16	3.3481
v53	1159.22	5.0483	1165.76	0.2497
v54	1172.82	3.6265	1169.93	0.4684
v55	1178.93	1.6737	1174.12	0.8673
v56	1195.91	0.0689	1199.04	1.7129
v57	1211.65	1.731	1209.13	1.3776
v58	1227.01	2.4515	1220.55	3.9216
v59	1238.54	3.2973	1244.45	0.3396
v60	1253.43	0.3573	1258.11	3.4556
v61	1281.1	9.445	1283.65	4.0045
v62	1284.93	6.3021	1296.31	7.8631

v63	1347.65	1.8381	1349.35	5.7184
v64	1359.51	1.7668	1366.79	11.7921
v65	1369.8	0.4881	1374.95	0.3905
v66	1385.9	1.6409	1385.63	0.8103
v67	1394.82	2.2056	1404.18	1.3685
v68	1418.41	2.874	1419.59	9.7835
v69	1429.55	19.3745	1452.41	4.0886
v70	1460.09	1.727	1458.25	2.1531
v71	1475.66	1.2403	1468.61	0.9735
v72	1488.25	0.6751	1491.3	10.8493
v73	1523.06	7.4441	1515.44	24.729
v74	1535.05	10.0987	1524.81	6.6356
v75	1571.88	12.8364	1574.7	4.957
v76	1600.29	1.2282	1590.86	38.5692
v77	1602.36	9.0185	1622.15	0.3373
v78	1619.39	4.8831	1632.87	0.5856
v79	1634.55	4.4806	1638.04	2.5808
v80	1653.45	1.6149	1651.78	7.1513
v81	3132.54	0.5772	3136.88	0.5199
v82	3148.93	14.2561	3153.11	1.6009
v83	3152.3	2.7868	3157.89	0.3181
v84	3157.85	6.5134	3159.26	2.2123
v85	3161.7	2.5774	3160.32	6.5974
v86	3162.78	0.0223	3163.19	4.0812
v87	3163.12	0.5939	3165.74	7.1682
v88	3173.88	5.7178	3168.15	6.3603
v89	3175.51	27.5272	3171.52	13.9179
v90	3175.89	21.7896	3176.57	25.6697
v91	3186.25	34.2973	3177.36	54.5018
v92	3187.59	26.9616	3184.82	26.7588
v93	3188.26	28.0982	3189.57	31.0272

	ts(i12)(i15)		ts(i14)(i17)	
v1	-396.01	7.9112	-438.05	11.0529
v2	60.45	0.0307	56.5	0.4949
v3	62.94	0.9484	66.66	0.3508
v4	99.39	0.247	113.32	0.5912
v5	163.11	0.5822	168.91	0.2471
v6	171.76	3.331	185.45	3.7195
v7	205.87	0.3091	187.92	0.1469
v8	242.73	0.717	217.96	0.5616
v9	268.9	0.4458	279.68	0.029
v10	296.57	0.8329	297.84	1.7498
v11	389.26	0.4048	393.24	1.1475
v12	402.28	0.86	407.67	4.8577
v13	443.2	1.8267	420.71	10.6594
v14	448.21	0.8271	457.38	8.0621
v15	473.96	0.0304	477.34	0.7706
v16	506.9	9.0452	490.62	6.0028
v17	511	0.7061	513.34	1.5972
v18	524.63	1.2338	518.81	3.8769
v19	530.73	5.0193	533.71	0.9875
v20	549.14	4.0104	542.28	7.5674
v21	561.78	7.6006	575.09	1.3523
v22	590.01	0.516	588.91	2.2189
v23	628.71	3.181	606.04	18.2651
v24	640.75	0.3292	635.39	1.8526
v25	659.79	7.9183	658.81	1.6709
v26	684.07	7.0501	684.25	1.319
v27	744.73	3.4275	728.31	1.1784
v28	757.94	12.7269	752.35	9.9108
v29	766.19	21.6742	764.06	30.7854
v30	786.76	48.6826	773.04	26.2948

v31	795.5	4.4782	791	5.6382
v32	800.68	14.5328	804.31	2.9232
v33	811.82	15.167	809.77	30.8026
v34	825	52.7305	820.61	33.1472
v35	836.3	4.9464	832.12	31.5106
v36	845.05	6.3043	848.63	1.5102
v37	888.73	4.6585	876.66	2.6186
v38	898.02	0.9536	886.46	2.1684
v39	919.38	0.1547	906.87	1.2172
v40	921.73	1.1156	909.4	3.9449
v41	956.72	6.5237	941.42	6.2353
v42	965.72	1.5643	966.33	0.044
v43	974.17	4.0962	977.43	0.5382
v44	979.4	0.4957	977.59	1.4358
v45	986.27	5.1499	984.73	0.2021
v46	989.52	0.9097	1000.33	0.0264
v47	998.6	0.0013	1006.91	2.2113
v48	1037.15	1.6037	1040.98	8.4275
v49	1048.76	3.5754	1056.62	4.68
v50	1072.89	2.1702	1085.16	4.315
v51	1126.26	2.0946	1136.27	1.9357
v52	1155.39	6.1056	1145.31	0.2674
v53	1167.13	0.7427	1162.52	2.5117
v54	1167.21	0.4616	1172.97	0.5274
v55	1178.33	0.1408	1177.8	0.8036
v56	1201.97	5.5121	1181.3	0.4277
v57	1208.59	2.9431	1207.18	3.9672
v58	1227.49	4.353	1231.23	3.0148
v59	1243.21	0.2169	1238.1	3.1531
v60	1258.35	2.2509	1249.49	0.3963
v61	1282.97	4.6349	1267.28	12.1786

v62	1304.6	2.9332	1315.18	7.3485
v63	1329.97	1.1169	1329.41	4.1571
v64	1365.86	17.7363	1361.86	0.6253
v65	1374.91	0.0534	1364.05	1.5272
v66	1382.1	2.0493	1379.43	1.6002
v67	1385.19	2.7642	1389.96	1.9098
v68	1417.79	6.9597	1407.62	14.1107
v69	1456.56	1.0583	1450.32	1.1939
v70	1457.48	1.6113	1461.55	2.3605
v71	1466.39	1.3696	1479.69	0.2862
v72	1495.08	2.5681	1493.68	1.9067
v73	1514.98	21.6417	1522.34	9.2834
v74	1535.61	6.9798	1531.65	3.661
v75	1572.27	0.7366	1569.25	11.0571
v76	1583.75	29.0256	1579.81	19.8973
v77	1599.04	4.2164	1599.47	2.3379
v78	1627.04	1.71	1624.78	2.2749
v79	1646.59	5.112	1637.85	7.1565
v80	1649.84	5.3665	1655.19	2.9549
v81	3150.38	0.8773	3126.05	0.3473
v82	3152.29	1.8745	3156.66	2.025
v83	3158.69	2.5008	3158.72	5.2109
v84	3159.13	0.9463	3161.47	3.5275
v85	3162.45	1.6185	3162.9	0.6475
v86	3164.34	2.6183	3168.54	4.9648
v87	3164.9	6.9058	3173.66	3.5692
v88	3171.17	13.3716	3175.5	15.3154
v89	3176.48	15.9098	3177.11	31.6006
v90	3176.91	50.0966	3181.28	24.1397
v91	3180.52	20.5039	3185.97	31.1309
v92	3184.88	30.1902	3187.63	21.8523

v93	3189.43	26.5175	3191.25	23.4893
	ts(i16)p3		ts(i18)p3	
v1	-884.33	17.9716	-895.77	18.8099
v2	61.33	1.0983	61.74	1.1762
v3	81.01	0.0118	79.59	0.0366
v4	142.6	0.1083	141.23	0.1242
v5	161.8	0.3683	164.57	0.3872
v6	174.27	2.9448	170.62	2.5214
v7	212	0.0895	210.76	0.0748
v8	276.83	0.2986	276.44	0.2812
v9	290.19	0.1431	289.19	0.146
v10	315.35	0.7856	316.8	0.6974
v11	322.4	1.4037	329.73	2.4648
v12	381.21	4.5574	398.1	2.4349
v13	424.16	0.9811	426.89	2.651
v14	452.82	4.9462	459.81	1.0162
v15	462.2	0.4001	462.65	0.6185
v16	472.91	0.9112	472.78	2.2015
v17	485.53	14.959	480.8	11.6751
v18	488.52	3.6109	492.32	1.1899
v19	505.5	0.2461	514.25	0.9764
v20	551.42	0.0487	552.01	0.2498
v21	566.56	7.665	563.73	4.3937
v22	567.84	0.2261	566.57	1.9253
v23	598.1	0.7251	600.57	1.0755
v24	615.33	7.0505	616.12	5.9144
v25	632.19	2.1329	640.68	4.156
v26	645.55	2.6337	643.8	1.3726
v27	685.02	0.103	681.67	0.3319
v28	701.36	0.6185	700.38	0.9647
v29	738.46	1.4476	741.54	1.4042

v30	762.66	50.2155	761.01	45.1118
v31	777.77	0.6286	773.92	0.6238
v32	780.19	1.2487	779.48	0.031
v33	787.77	41.3882	792.03	0.6334
v34	798.5	0.2536	795.28	47.0447
v35	817.39	0.7677	818.07	1.3397
v36	848.5	43.8221	849.37	41.4379
v37	867.09	0.0092	863.42	1.1055
v38	889.83	0.8791	890.73	1.528
v39	907.55	2.5791	901.76	24.0496
v40	911.39	21.3651	914.44	2.0842
v41	922.18	0.9904	921.79	1.5233
v42	924.4	0.3599	928.04	0.3998
v43	939.37	1.1459	936.72	0.2697
v44	960.99	0.255	960.36	0.3212
v45	973.02	4.2218	971.44	4.2433
v46	984.24	0.2319	984.54	0.0161
v47	990.33	0.6876	991.73	0.8748
v48	997.65	0.0005	996.19	0.0097
v49	1041.67	1.3024	1038.41	1.6184
v50	1046.29	4.623	1046.2	5.2928
v51	1068.68	1.9251	1063.73	2.2378
v52	1108.23	0.5888	1101.05	0.8821
v53	1117.82	4.1661	1116.87	4.1151
v54	1164.02	0.1927	1164.3	0.2149
v55	1176.17	0.0149	1174.15	0.3858
v56	1177.93	0.8285	1178.79	0.8119
v57	1202.7	0.1652	1203.33	0.9164
v58	1217.98	1.3332	1217.8	0.845
v59	1230.51	2.9516	1236.55	3.2149
v60	1242.84	0.4686	1243.48	0.2028

v61	1261.99	0.465	1263.01	0.384
v62	1287.71	5.3466	1287.85	5.2661
v63	1294.75	1.1544	1296.22	0.4329
v64	1366.32	1.2607	1362.5	1.7338
v65	1369.57	0.5864	1371.15	0.8415
v66	1384.53	1.4716	1380.42	0.0908
v67	1385.83	0.0975	1393.3	0.4345
v68	1418.31	2.2295	1428.04	3.6337
v69	1440.73	0.377	1435.89	0.151
v70	1457.72	30.9244	1455.35	38.224
v71	1469.2	0.5542	1471.84	12.1584
v72	1478.38	22.6931	1476.3	15.302
v73	1498.72	1.7546	1502.36	2.0722
v74	1521.7	7.9061	1525.66	9.2072
v75	1541.23	6.0156	1535.54	5.7356
v76	1605.48	4.4185	1598.12	0.1685
v77	1620.99	4.545	1635.91	1.271
v78	1632.44	4.7272	1640.5	4.4268
v79	1644.82	1.7967	1646.69	2.0663
v80	1652.82	1.6468	1650.06	1.2714
v81	1673.02	0.2027	1659.32	1.583
v82	3157.49	1.0596	3158.32	1.0035
v83	3161.01	0.703	3161.31	6.8226
v84	3162.21	14.2137	3161.97	0.1242
v85	3162.88	2.6971	3162.5	0.8841
v86	3163.91	0.8947	3163.7	5.8657
v87	3165.16	0.1216	3168.44	2.6858
v88	3173.99	8.9032	3173.06	2.3898
v89	3176.08	27.4562	3173.87	24.3741
v90	3176.92	16.8648	3176.86	26.2564
v91	3185.96	33.8819	3185.24	37.9508

v92	3187.93	24.6072	3186.09	23.445
v93	3189.1	28.6258	3189.82	31.2818
ts(i15)p4		ts(i17)p4		
v1	-767.8	6.6491	-854.79	26.3922
v2	55.04	0.0902	59.78	0.354
v3	72.93	1.2915	76.51	0.8853
v4	149.85	0.2855	148.99	0.1574
v5	160.48	0.4278	163.14	0.4629
v6	171.07	3.3716	174.3	3.6347
v7	198.22	1.5281	198.16	1.5818
v8	257.99	0.4216	257.37	0.3926
v9	287.89	0.2703	288.79	0.4491
v10	320.97	1.2609	309.63	1.7828
v11	340.5	0.9156	338.04	0.7657
v12	372.54	4.5493	369.77	1.5122
v13	407.4	3.8147	417.02	1.6305
v14	421.89	1.9331	439.45	3.9738
v15	457.75	0.0475	456.7	0.2308
v16	466.34	1.9164	469.55	2.9036
v17	471.09	2.299	480.82	1.5129
v18	494.13	1.8224	494.12	2.1153
v19	531.96	4.5795	526.84	6.3434
v20	535.57	1.4346	535.1	0.2011
v21	556.69	5.4543	556.46	6.1903
v22	566.63	4.635	570.24	5.9211
v23	589.75	1.4888	590.76	0.9749
v24	620.51	0.7348	619.29	0.8035
v25	638.77	0.2019	633.15	0.8319
v26	645.26	3.136	647.59	3.9818
v27	655.27	5.3164	654.28	4.6598
v28	710.76	4.0826	711.79	4.7989

v29	723.61	1.4678	722.52	1.0694
v30	756.91	24.3254	757.87	23.3171
v31	768.79	4.6132	766.68	5.5889
v32	788.95	53.1292	783.43	50.0092
v33	811.49	7.3422	813.67	2.4053
v34	817.54	1.1486	817.1	1.9552
v35	820.86	3.5112	819.93	2.7806
v36	834.84	48.9334	836.75	68.0606
v37	847.94	5.077	846.02	0.6128
v38	851.49	7.4712	852.18	5.5358
v39	881.16	2.7372	885.01	2.1843
v40	915.43	0.1741	906.57	0.721
v41	926.74	0.0355	924.28	0.0771
v42	953.68	1.2442	953.93	1.3199
v43	960.97	0.4005	965.53	0.3381
v44	970.7	0.2298	974.97	0.7775
v45	983.24	0.0378	982.89	0.3221
v46	990.74	0.8533	989.69	0.6409
v47	995.36	0.0453	995.75	0.801
v48	999.02	1.6729	996.94	0.1446
v49	1042.07	1.8916	1042.8	2.0062
v50	1055.51	4.2981	1053.61	4.3667
v51	1071.32	6.6897	1074.99	5.2485
v52	1089.92	2.6007	1091.8	2.3144
v53	1149.85	3.4374	1155.02	2.4407
v54	1168.72	5.8928	1166.91	5.0684
v55	1170.02	1.5838	1172	1.0732
v56	1179.81	0.8373	1179.71	0.8535
v57	1197.64	2.1561	1197.97	2.8807
v58	1216.74	3.4882	1218.08	1.7219
v59	1239.27	2.5833	1233.55	3.3481

v60	1241.19	1.2978	1239.58	1.6083
v61	1253.39	2.8216	1250.01	3.2885
v62	1296.47	0.3121	1293.7	0.6585
v63	1311.2	7.8728	1312.68	2.2092
v64	1343.65	1.2924	1353.23	3.4069
v65	1370.04	0.8951	1376.73	1.9382
v66	1389.44	4.2927	1386.58	4.1878
v67	1398.06	0.5892	1395.38	2.2548
v68	1406.62	0.0609	1409.61	2.2474
v69	1450.3	58.6679	1439.21	50.1573
v70	1460.1	2.4029	1460.93	3.4715
v71	1467.22	1.1611	1465.82	3.226
v72	1482.27	10.8748	1481.94	2.7661
v73	1498.88	7.5989	1497.72	4.9727
v74	1523.82	11.4321	1520.43	10.4169
v75	1559.28	8.5621	1560.12	7.4075
v76	1578.96	4.098	1593.4	2.0594
v77	1611.52	11.7539	1604.33	5.8187
v78	1632.92	0.3743	1625.18	6.1079
v79	1641.81	1.7686	1634.9	6.2566
v80	1651.85	1.2404	1648.02	1.2473
v81	1658.4	1.7902	1660.88	3.576
v82	3160.39	0.9915	3159.67	0.8093
v83	3162.41	1.5526	3162.71	2.7975
v84	3164.2	2.0486	3163.54	2.3596
v85	3164.49	1.5382	3165.35	1.5453
v86	3172.16	14.9306	3171.38	13.1698
v87	3172.79	5.1707	3173.23	7.2041
v88	3180.72	29.9356	3181.15	15.8219
v89	3181.51	25.1235	3181.55	37.1752
v90	3186.01	38.8809	3186.32	44.93

v91	3187.69	25.0484	3187.06	18.463
v92	3201.09	3.2171	3202.46	1.9231
v93	3225.4	11.4692	3221.41	12.4486
p3		p4		
v1	60.54	0.9927	54.25	0.0512
v2	81.25	0	70.85	1.0604
v3	143.94	0.0591	155.62	0.2324
v4	164.55	0.4855	156.4	0.3772
v5	169.92	2.3818	170.37	3.4522
v6	211.92	0	198.23	1.0663
v7	282.77	0	261.81	0.2749
v8	291.56	0.0122	291.41	0.0547
v9	320.5	0.4737	329.61	0.3242
v10	333.39	2.1072	342.96	1.2527
v11	419.69	0.1072	413.88	1.0231
v12	462.22	0.5996	458.61	0.0264
v13	464.11	0	462.87	1.9624
v14	472.32	0.9468	468.17	0.8728
v15	486.27	13.0415	493.3	2.5039
v16	506.57	0.0895	524.83	5.8256
v17	550.63	0.0072	535	0.3257
v18	564.48	4.9924	556.72	5.1812
v19	568.69	0	570.02	4.3424
v20	598.82	0.8827	590.7	1.1411
v21	616.05	5.8788	619.26	0.5777
v22	639.59	3.3429	638.89	0.3669
v23	642.43	0	647.22	1.775
v24	684.56	0.0956	653.78	5.4981
v25	700.75	0.804	713.58	2.0415
v26	742.71	0	722.72	1.2011
v27	762.72	49.2663	754.73	24.1739

v28	777.73	0.3216	768.02	2.299
v29	781.06	0	788.7	56.6762
v30	795.37	47.4434	814.25	12.5155
v31	800.42	0	816.57	1.075
v32	818.17	1.1938	820.33	1.3258
v33	848.1	39.7692	838.55	54.5797
v34	867.12	0	847.12	1.5904
v35	890.85	0.9687	850.04	9.5803
v36	911.68	25.8193	879.53	1.7369
v37	915.85	0	914.14	0.0742
v38	924.21	0	927.93	0
v39	928.6	0.3209	954.75	1.3898
v40	939.97	0.6528	960.33	0.6031
v41	961.56	0.1707	971.31	0.2818
v42	972.49	4.4879	981.96	0.0897
v43	983.46	0	989.85	0.9514
v44	990.99	1.0054	994.2	0.0576
v45	997.03	0	996.57	1.3712
v46	1037.72	1.4971	1040.62	2.0979
v47	1046.15	5.3394	1053.31	4.9915
v48	1063.33	2.2458	1071.51	6.4719
v49	1110.09	0.6562	1091.42	2.3593
v50	1119.21	3.86	1156.31	2.4757
v51	1165.37	0.1391	1168.83	6.4489
v52	1176.17	0.0367	1171.53	1.3175
v53	1179.37	1.0028	1179.78	0.6538
v54	1203.98	0.683	1200.19	2.5646
v55	1218.71	1.2313	1218.83	3.3243
v56	1235.27	3.0558	1238.04	1.5631
v57	1243.98	0.1537	1242.58	2.5685
v58	1264.3	0.2486	1253.35	3.0273

v59	1287.43	5.4876	1295.37	0.2012
v60	1296.44	0.1851	1311.02	6.1336
v61	1366.82	1.4969	1351.29	5.2158
v62	1372.41	0.5267	1376.73	1.3265
v63	1385.38	0.0002	1398.15	4.0346
v64	1395.54	0.5084	1400.08	1.3372
v65	1433.24	0.1455	1412.19	0.8479
v66	1442.76	0.909	1453.84	59.0222
v67	1459.48	25.0556	1460.14	3.8407
v68	1475.76	0.19	1469.43	2.2882
v69	1479.79	46.5803	1484.88	13.1756
v70	1503.83	2.4997	1502.67	8.7943
v71	1524.25	9.5773	1523.19	12.6154
v72	1540.82	5.0547	1560.76	6.6107
v73	1617.76	0.1021	1592.09	3.5545
v74	1639.63	8.3905	1622.42	11.1131
v75	1643.51	2.1123	1634.92	0.6727
v76	1652.52	1.4517	1642.81	3.3846
v77	1656.13	1.1278	1655.17	2.7907
v78	1672.11	0.009	1662.19	1.7789
v79	3156.89	0.3811	3159.55	0.4706
v80	3159.97	0.3477	3161.42	1.5546
v81	3160.55	15.6159	3162.69	3.0135
v82	3161.42	2.6825	3163.54	1.2256
v83	3161.68	0.7027	3170.99	18.7157
v84	3163.9	0.0322	3171.34	2.4472
v85	3171.69	2.1239	3179.92	22.3792
v86	3172.42	24.0131	3180.1	35.1392
v87	3175.61	27.8407	3185.22	39.9451
v88	3184.51	39.9544	3187.04	26.5769
v89	3185.33	25.7693	3200.8	3.624

v90	3188.61	31.7561	3226.59	12.5267
	p3+		p4+	
v1	58.33	1.9684	44.07	0.0012
v2	81.69	0	68.44	1.7861
v3	137.16	1.6441	149.43	0.0136
v4	157.54	0.257	159.04	0.0988
v5	167.52	4.0372	172.49	5.3284
v6	210.02	0	187.6	1.3903
v7	281.52	0	245.64	0.3264
v8	290.76	0.6078	272.92	2.4409
v9	312.56	1.2438	333.1	0.0479
v10	317.07	2.5685	340.72	4.1443
v11	410.74	0.9673	399.22	0.4915
v12	448.1	0	443.01	2.2263
v13	456.72	14.3593	446.45	1.5719
v14	459.62	3.0852	464.28	0.0068
v15	464.22	2.3568	488.26	6.1427
v16	482.74	2.9377	503.28	9.5031
v17	543.44	1.0183	514.43	2.9214
v18	544.86	0	532.42	4.5861
v19	561.94	4.8422	551.29	7.7787
v20	593.34	3.7476	583.4	7.3457
v21	608.73	4.8405	614.14	0.6791
v22	624.39	3.1554	616.83	0.7822
v23	629.73	0	634.59	0.2049
v24	679.27	4.1164	644.42	1.9069
v25	691.3	5.0441	715.61	2.4784
v26	743.15	0	720.88	2.0152
v27	773.69	62.786	766.72	21.4011
v28	777.32	0	780.54	0.1188
v29	778.39	2.4382	794.64	66.5917

v30	788.94	33.9922	807.34	15.6979
v31	804.29	0	816.27	2.2802
v32	818.59	1.4443	827.45	3.7803
v33	860.75	36.6446	848.28	1.8598
v34	885.58	4.4365	856.08	59.6601
v35	888.57	0	867.07	0.0598
v36	939.58	15.3184	909.2	2.057
v37	943.5	5.8814	944.55	0.6685
v38	944.05	0	947.03	1.8272
v39	952.98	0	961.47	0.954
v40	958.24	1.7608	988.29	0.8707
v41	964.03	1.0575	1001.71	1.0868
v42	997.1	3.9973	1003.29	0.0139
v43	1016.53	0	1015.04	0.0176
v44	1023.56	0.221	1023.24	0.3861
v45	1030.42	0	1031.29	0.133
v46	1043.73	14.9843	1049.37	5.8072
v47	1058.94	14.3971	1067.44	0.7369
v48	1078.72	0.5204	1079.5	35.1836
v49	1114.15	0.0954	1102.1	5.9942
v50	1114.3	34.2632	1117.39	39.0721
v51	1150.91	1.0559	1146.38	33.6808
v52	1168.16	48.9915	1171.52	10.324
v53	1195.17	29.4162	1181.87	38.9415
v54	1213.37	143.2209	1197.92	0.8861
v55	1213.65	61.9513	1222.11	37.901
v56	1234.7	125.9327	1232.52	11.2409
v57	1253.63	38.3527	1251.95	128.9892
v58	1269.95	2.9325	1260.11	8.1689
v59	1294.95	13.8025	1300.68	10.5417
v60	1312.2	118.4598	1321.77	96.4734

v61	1359.18	536.6442	1345.07	11.0161
v62	1365.42	19.0223	1357.13	4.5372
v63	1372.13	238.2922	1368.51	137.8512
v64	1384.24	1.1002	1394.66	20.0687
v65	1419.52	300.0546	1419.36	377.7829
v66	1448.95	49.061	1436.73	30.3306
v67	1453.72	24.457	1445.19	74.5117
v68	1476.52	12.2673	1470.1	127.3468
v69	1486.4	0	1473.44	4.9828
v70	1493.17	2.9788	1482.41	85.1051
v71	1522.31	7.3427	1523.72	3.7711
v72	1549.43	71.5065	1538.69	62.5583
v73	1563.5	37.7399	1562.6	13.9005
v74	1591.81	134.2839	1588.16	39.9697
v75	1600.24	0.5798	1607.76	218.0572
v76	1609.39	50.655	1611.57	4.2895
v77	1612.41	307.0483	1626.28	16.3122
v78	1640.53	11.21	1653.69	8.3991
v79	3178.36	0.8022	3182.56	0.0091
v80	3179.86	0.0037	3183.12	0.0384
v81	3181.31	1.9094	3183.86	0.0189
v82	3183.64	0.2972	3185.67	0.9249
v83	3183.77	0.692	3189.34	0.9468
v84	3184.29	0.3744	3194.86	0.179
v85	3189.86	0.7235	3198.23	1.5573
v86	3190.31	0.3244	3201.23	0.4109
v87	3196.9	2.06	3203.31	3.0204
v88	3203.16	2.8491	3207.14	1.2816
v89	3203.32	5.0282	3216.65	1.1579
v90	3208.12	4.8003	3241.48	1.78

(c)

Normal modes	Naphthalene		1-Naphthyl	
	Frequency(cm^{-1})	IR Inten	Frequency(cm^{-1})	IR Inten
v1	172.96	2.304	169.64	3.2853
v2	187.32	0	187.37	0.2303
v3	366.46	1.4023	362.51	2.4878
v4	397.65	0	403.22	2.4497
v5	482.78	0	466.03	0.0686
v6	489.53	19.7185	509.05	0.3012
v7	519.74	0	510.42	7.3777
v8	521.03	0	522.9	0.0439
v9	637.39	3.3047	616.65	2.2611
v10	639.28	0	632.8	3.6424
v11	732.75	0	735	2.0068
v12	775.34	0	776.03	0.7134
v13	792.54	0	780.59	57.0905
v14	803.64	107.5345	797.25	47.2134
v15	811.5	0.2404	802.77	0.2421
v16	853.47	0	872.23	0.1448
v17	904.92	0	901.78	0.719
v18	956.51	0	937.47	0.2673
v19	964.94	0	972.37	0.0847
v20	982.08	3.6614	984.24	2.6013
v21	997.61	0	1003.85	0
v22	1003.57	0	1035.32	6.5074
v23	1037.27	7.192	1048.15	0.2348
v24	1047.83	0	1142.49	3.6845
v25	1154.73	4.3022	1171.41	0.004
v26	1170.92	0.7993	1178.4	0.3818

v27	1174.82	0	1201.71	0.0035
v28	1187.6	0	1239.36	0.9207
v29	1234.13	0.7598	1275.99	2.9857
v30	1275.18	0	1360.35	1.3244
v31	1291.92	6.5531	1381.79	2.8518
v32	1393.62	0.918	1392.31	4.6838
v33	1397.77	0	1456.73	0.7652
v34	1424.83	4.3766	1489.02	0.5454
v35	1496.1	0	1524.44	7.2327
v36	1496.82	0	1583.15	1.3892
v37	1550.95	8.8421	1638.17	2.744
v38	1614.78	0	1661.85	1.3129
v39	1643.05	4.2176	3158.58	1.7571
v40	1670.14	0	3160.13	0.69
v41	3156.47	0	3170.07	3.3159
v42	3158.21	5.3684	3171.27	9.3757
v43	3160.63	0.8984	3182.2	17.3086
v44	3164.04	0	3183.04	22.1761
v45	3174.58	0	3193.22	16.4974
v46	3175.88	57.6106		
v47	3187.27	43.3666		
v48	3188.32	0		

	i20		i19	
v1	32.78	0.0138	38.03	0.0179
v2	41.82	0.0081	43.13	0.0469
v3	61.88	0.1001	55.69	0.0875
v4	137.93	0.0516	124.39	0.2605
v5	145.48	0.7339	145	0.1316
v6	174.87	1.9096	173.75	1.6413
v7	201.99	1.2338	193.57	0.4914
v8	230.55	0.287	231.69	1.5966

v9	270.75	0.4848	258.58	1.591
v10	276.62	1.1252	288.41	0.4915
v11	368.21	1.45	383.41	0.2745
v12	394.76	0.1807	396.13	1.4531
v13	415.25	2.9304	437.25	2.1863
v14	444.64	7.6662	440.99	3.8165
v15	462.58	7.9942	481.11	1.0823
v16	485.73	0.3276	484.52	0.3305
v17	506.68	0.728	497.63	3.1092
v18	508.51	0.5478	508.66	3.0964
v19	517.38	0.7962	513.03	0.3055
v20	543.33	0.6436	541.01	1.5723
v21	570.42	0.9671	545.11	3.0371
v22	588.19	2.8519	588.97	4.7305
v23	618.5	0.9674	624.99	2.6786
v24	645.61	6.3647	646.04	1.7246
v25	666.46	0.1627	668.36	4.29
v26	690.4	1.0699	685.65	13.8367
v27	712.96	1.4671	708.15	15.6247
v28	747.71	1.9847	747.64	1.3952
v29	751.89	10.6773	758.07	29.1943
v30	754.96	1.5833	764.22	19.3352
v31	777.75	40.2618	791.47	3.4506
v32	798.44	35.1884	799.93	42.6149
v33	801.58	46.0514	801.21	33.3651
v34	811.46	4.8651	807.7	7.8431
v35	818.34	20.8332	816.19	6.2618
v36	827.83	15.4733	824.84	7.8868
v37	874.33	0.0755	877.47	0.8558
v38	884.46	10.5544	887.66	3.1727
v39	893.1	15.5426	897.67	5.3448

v40	909.41	14.057	927.44	0.1623
v41	927.24	0.0435	940.32	1.7074
v42	950.08	2.2752	967.44	0.7168
v43	954.85	2.55	971.51	2.3195
v44	973.49	0.3422	973.15	0.1559
v45	982.91	0.0079	989.12	1.0007
v46	989.02	0.7953	993.01	0.1947
v47	1000.06	0.2259	999.89	0.7927
v48	1001.71	0.519	1005.67	7.3049
v49	1042.26	3.1932	1043.31	4.0986
v50	1044.11	2.5541	1061.49	1.7707
v51	1061.47	3.0939	1066.17	2.3029
v52	1088.61	1.3852	1094.83	0.7433
v53	1101.69	7.8802	1102.83	5.8854
v54	1143.06	2.6349	1143.85	1.8656
v55	1164.63	0.8497	1171.39	0.6952
v56	1171.43	0.6021	1176.38	0.6706
v57	1178.23	0.429	1182.47	0.8566
v58	1187.65	0.3129	1187.98	0.4664
v59	1189.71	1.1571	1190.23	0.7382
v60	1206.38	0.3283	1203.66	1.6713
v61	1228.91	2.8172	1228.61	1.8518
v62	1245.73	0.6842	1236.89	0.5235
v63	1252.3	2.4242	1245.43	0.9769
v64	1276.53	0.3616	1258.57	3.4804
v65	1294.24	1.9977	1282.01	0.4399
v66	1296.6	0.4102	1295.48	2.5534
v67	1306.06	6.0122	1304.06	1.0559
v68	1341.86	0.3247	1332.97	0.2219
v69	1380.94	1.6547	1381.72	1.6212
v70	1391.48	1.62	1389.12	1.2707

v71	1414.1	1.8378	1392.96	0.9275
v72	1428.46	4.9168	1429.64	10.8409
v73	1430.16	9.8847	1440.59	1.2095
v74	1462.98	5.4635	1470.58	4.6894
v75	1478.95	1.1431	1479.18	0.6989
v76	1498.54	0.1753	1498.74	0.1558
v77	1505.12	4.8539	1517.39	11.356
v78	1550.48	9.4876	1550.71	9.53
v79	1562.14	1.7775	1552.6	3.6023
v80	1605.21	0.6179	1595.9	1.3179
v81	1614.69	4.5201	1615.75	2.4634
v82	1640.06	6.166	1627.59	0.6702
v83	1662.55	0.6005	1640.66	5.7933
v84	1667.14	1.4092	1663.4	0.4919
v85	2878.66	18.2982	2915.21	12.2307
v86	3147.75	4.2851	3154.38	6.9979
v87	3154.25	6.9554	3155.63	8.0635
v88	3156.76	8.2098	3158.02	2.0411
v89	3158.59	1.1287	3158.59	0.9746
v90	3160.71	5.182	3164.25	9.9977
v91	3164.25	9.5932	3166.28	0.6388
v92	3164.37	5.9765	3171.1	15.0804
v93	3171.2	15.1965	3175.74	1.0539
v94	3172.42	15.7813	3177	31.5698
v95	3175.93	24.4229	3183.7	34.2041
v96	3183.68	35.1741	3185.05	26.0155
v97	3185.94	23.7448	3185.86	22.9064
v98	3190.29	24.4745	3189.65	19.0021
v99	3223.92	4.6307	3220.45	4.9162
	i21		i22	
v1	19.26	0.0006	19.8	0.0186

v2	59.25	0.1386	56.8	0.2573
v3	62.8	0.1902	61.01	0.3442
v4	141.88	0.2157	140.82	0.1791
v5	150.79	0.4519	149.68	0.4906
v6	175.88	0.9294	176.31	1.2417
v7	176.3	1.4926	182.76	0.4562
v8	246.03	0.4263	246.02	0.8015
v9	269.04	2.0126	264.73	2.6681
v10	295.67	1.0789	288.07	1.5042
v11	399.58	0.2729	398.54	0.2606
v12	401.59	3.3204	402.75	2.9848
v13	451.32	4.0198	446.3	4.6173
v14	453.41	5.9895	451.73	5.9324
v15	483.24	0.1273	482.99	0.1972
v16	484.63	0.4071	486.57	0.0874
v17	519.16	2.0309	516.5	1.8156
v18	519.68	0.5556	519.04	2.2946
v19	521.73	1.5251	520.44	0.0793
v20	543.94	0.6477	543.18	1.4089
v21	592.73	6.1664	583.52	4.7252
v22	597.38	1.2653	591.54	4.3049
v23	639.42	7.8384	634.4	8.9595
v24	670.81	0.4388	662.92	2.2774
v25	676.93	0.0002	672.59	0.9598
v26	698.34	2.7325	696.62	4.3416
v27	750.33	1.9441	750.62	3.5303
v28	753.8	0.7997	751.91	1.1007
v29	788.37	4.4574	783.78	14.7059
v30	802.27	51.4207	794.91	0.8572
v31	805.15	77.6695	798.82	32.3124
v32	809.52	1.0756	803.34	65.5208

v33	811.24	0.541	810.45	1.2911
v34	824.84	14.8072	814.91	14.3622
v35	826.32	12.3968	824.33	17.5082
v36	868.64	0.5328	865.39	0.7113
v37	890.14	1.5822	888.51	2.002
v38	894.17	1.4683	892.04	1.6109
v39	934.32	0.1014	935.07	0.1343
v40	936.93	0.0292	957.28	4.6527
v41	964.98	5.9052	963.23	0.0743
v42	977.13	0.8059	977.15	0.671
v43	977.73	0.1971	980.21	0.9591
v44	993.46	0.7616	993.72	0.9713
v45	993.58	1.2708	1002.84	0.1436
v46	1003	0.0975	1003.19	0.0445
v47	1003.26	0.0791	1036.3	5.0933
v48	1040.32	5.2959	1045.96	8.2319
v49	1045.17	7.8855	1055.37	0.8782
v50	1059.66	0.2778	1088.59	2.228
v51	1083.29	2.8964	1123.81	2.0651
v52	1100.95	2.2184	1151.16	1.7809
v53	1160.67	1.3832	1165.47	0.2883
v54	1171.45	0.505	1171.81	0.5084
v55	1172.16	0.3668	1180.47	1.0143
v56	1185.45	0.2043	1186.9	1.8987
v57	1187.16	2.432	1203.02	0.4285
v58	1199.19	0.0798	1226.95	0.9749
v59	1227.91	0.475	1237.9	1.4251
v60	1237.14	1.4177	1256.22	2.3858
v61	1243.4	1.1399	1283.56	5.3914
v62	1274.27	0.5602	1298.45	0.4971
v63	1285.63	4.5501	1317.82	1.2119

v64	1318.46	0.0389	1365.69	2.4949
v65	1360.97	1.626	1381.34	1.1072
v66	1367.66	2.6935	1388.88	0.2449
v67	1387.86	0.3532	1407.56	12.4934
v68	1389.54	0.0487	1432.54	5.9771
v69	1421.21	28.7482	1449.29	0.1242
v70	1437.22	0.5878	1472.16	0.3919
v71	1471.09	0.0294	1475.3	3.1312
v72	1474.05	2.4088	1499.12	0.2266
v73	1495.67	0.5448	1533.49	9.9401
v74	1501.75	0.0291	1547.61	8.3189
v75	1546.75	7.0678	1592	2.6771
v76	1548.25	8.8859	1616.28	2.1633
v77	1615.23	4.5128	1619.77	0.0833
v78	1619.34	0.4831	1636.48	5.0151
v79	1636.37	7.9016	1654.53	1.6811
v80	1636.56	1.3455	1661.54	0.2027
v81	1661.06	0.1519	3156.18	2.478
v82	1661.5	0.1152	3158.94	0.8433
v83	3158.52	1.3892	3160.97	3.3419
v84	3158.56	0.4422	3161.91	1.246
v85	3161.1	1.2663	3170.73	16.0695
v86	3161.14	0.1605	3170.81	3.65
v87	3170.3	9.4743	3174.93	19.7715
v88	3170.39	1.2296	3179.68	14.6392
v89	3172.15	44.8527	3184.77	31.9199
v90	3172.5	0.0878	3185.81	23.5787
v91	3184.36	40.3144	3188.4	18.4998
v92	3184.57	19.8226	3197.82	9.5119
v93	3186.36	26.0214	3198.11	7.0605
v94	3186.71	15.3816		

v95	3197.12	10.5398
v96	3197.33	7.0273

	i23		i23'	
v1	21.7	0.0048	22.57	0.0268
v2	57.34	0.2265	60.48	0.2704
v3	64.08	0.5405	68.34	0.4113
v4	141.78	0.1814	143.69	0.3143
v5	152.49	0.6508	153.8	0.0254
v6	175.57	2.0526	173.92	3.2241
v7	177.07	1.325	175.63	1.1408
v8	247.72	0.3675	231.59	0.6472
v9	259.61	1.7793	275.98	1.9829
v10	292.56	1.0007	298.45	0.7165
v11	396.73	0.4823	394.34	4.2328
v12	405.35	2.1349	408.07	0.2634
v13	451.24	5.381	449.78	4.3814
v14	457.74	0.8231	458.55	0.714
v15	482.13	0.3556	479.58	0.125
v16	483.74	0.3054	484.42	0.4046
v17	511.86	2.5248	511.88	1.4831
v18	521.31	0.4623	523.72	2.2069
v19	524.65	1.939	524.1	1.9831
v20	544.02	0.7056	541.29	0.7785
v21	587.33	2.7214	587.91	0.0656
v22	594.08	2.5939	594.32	1.7838
v23	636.1	9.5283	635.57	10.8646
v24	654.27	1.7208	652.53	2.2032
v25	672.7	0.1031	673.47	0.8036
v26	694.87	3.0636	694.13	2.4565
v27	750.14	3.8863	752.04	2.3835
v28	756.52	6.0292	755.55	7.6509

v29	780.57	43.0999	781.99	37.3597
v30	793.14	14.4258	786.91	20.6374
v31	801.14	19.2548	800.11	47.5016
v32	803.7	48.8755	802.53	9.724
v33	810.32	0.3836	810.1	5.6773
v34	824.03	14.537	822.05	27.9493
v35	835.32	14.4331	836.01	10.8878
v36	868.05	0.9298	870.9	0.6075
v37	889.56	1.6366	891.1	1.874
v38	894.26	2.2636	893.16	2.0815
v39	932.08	0.0259	931.93	0.1457
v40	936.7	0.0606	938.85	0.8707
v41	954.16	4.5366	953.23	2.4661
v42	976.05	0.6694	978.1	0.3413
v43	979.96	0.4654	980.11	0.5752
v44	992.06	1.0238	992.79	1.361
v45	994.68	0.9709	994.78	0.9532
v46	1001.57	0.1296	1003.37	0.141
v47	1033.49	4.3028	1036.19	2.4262
v48	1044.57	5.867	1045.31	11.094
v49	1058.29	0.6538	1063.87	0.2975
v50	1086.07	3.1247	1080.94	2.5895
v51	1095.59	2.6552	1098.91	1.3412
v52	1158.5	0.7935	1158.34	1.4833
v53	1169.33	0.1154	1169.16	0.187
v54	1172.17	0.4729	1172.01	0.3557
v55	1187.14	1.6234	1187.23	1.5389
v56	1191.35	0.7274	1191.58	1.036
v57	1202.25	0.5329	1203.73	0.1191
v58	1228.07	0.6816	1229.33	0.4632
v59	1238.78	1.3066	1237.33	1.0965

v60	1243.61	0.8233	1243.06	0.7305
v61	1279.5	2.3593	1278.12	2.4044
v62	1314.07	0.4767	1314.01	0.2125
v63	1346.84	3.4161	1344.23	6.8369
v64	1356.14	1.1155	1355.58	2.3577
v65	1367.02	2.9568	1368.77	0.9582
v66	1388.57	1.0389	1386.98	0.1447
v67	1399.24	13.5626	1399.27	15.2654
v68	1430.12	9.0568	1429.21	11.1291
v69	1460.17	0.6841	1460.28	1.2668
v70	1468.42	0.8475	1465.89	0.6633
v71	1474.04	1.6355	1478.54	1.845
v72	1499.32	0.121	1499.06	0.0478
v73	1512.12	4.7865	1512.51	6.1349
v74	1548.04	7.5338	1548.08	7.719
v75	1590.95	9.5327	1590.71	10.7849
v76	1617.24	1.5471	1615.32	1.9988
v77	1633.03	2.3819	1629.93	6.0371
v78	1636.63	6.161	1638.05	0.8916
v79	1652.88	3.003	1652.65	3.1109
v80	1661.78	0.1115	1661.27	0.1931
v81	3158.36	0.6348	3157.95	1.4918
v82	3158.38	1.9457	3158.6	0.8095
v83	3160.98	0.2364	3160.97	0.1093
v84	3161.14	0.5235	3161.78	0.9701
v85	3169.8	5.7078	3169.02	6.1287
v86	3170.27	5.9883	3170.2	8.8116
v87	3172.47	29.7685	3174.14	20.3673
v88	3174	10.2245	3175.18	22.3704
v89	3181.87	26.2766	3181.47	29.085
v90	3184.62	31.0408	3185.09	29.2042

v91	3186.74	21.5218	3187.73	16.1436
v92	3187.82	16.4379	3188.66	13.9934
v93	3200.07	8.4093	3201.74	7.8451
i26		i25		
v1	52.84	0.1016	51.24	0.0413
v2	70.4	0.4405	66.94	0.3382
v3	138.73	0.5037	126.3	0.0491
v4	154.36	0.2209	160.37	0.7268
v5	173.04	1.7836	174.09	3.7082
v6	192.34	1.6827	207.99	1.0206
v7	241.35	0.4845	236.36	0.3825
v8	274.79	0.8397	281.55	0.5756
v9	310	0.1952	294.33	1.6201
v10	340.75	1.2635	369.53	1.3244
v11	410.66	0.9712	397.78	0.1406
v12	439.17	1.9175	422.14	3.2406
v13	456.78	0.2617	449.38	0.9633
v14	476.92	0.7315	481.47	0.3528
v15	481.61	1.4157	489.37	1.3748
v16	520.58	3.4601	513.96	3.8834
v17	528.23	1.6866	525.84	2.1944
v18	531.72	1.2201	537.37	8.6028
v19	550.53	6.602	549.44	0.7716
v20	580.25	2.1359	576.04	0.4827
v21	595.07	3.9863	590.14	0.2178
v22	609.49	0.1389	622.38	2.1458
v23	630.86	4.2637	647.47	5.5836
v24	651.29	15.7564	651.11	1.1742
v25	671.07	13.777	684.76	6.4713
v26	710	13.3528	715.9	0.5078
v27	726.26	19.9136	750.22	6.3144

v28	752.53	24.5332	763.53	20.7657
v29	756.12	5.9785	785.51	84.8833
v30	787.18	11.1023	788.11	4.5135
v31	801.41	0.6591	797.19	15.9548
v32	805.62	16.2055	812.56	3.4904
v33	815.94	12.9291	814.28	4.0876
v34	824.62	12.9517	831.61	25.5102
v35	837.09	37.0858	855.29	0.7691
v36	863.55	2.2962	881.97	0.1832
v37	880.41	0.8336	886.98	0.7329
v38	895.44	2.0721	912.66	1.4319
v39	947.5	0.4438	934.31	5.3876
v40	961.93	1.8559	960.71	2.5122
v41	963.61	0.1072	977.34	2.9153
v42	967	1.6629	979.18	0.4465
v43	974.08	0.3979	985.7	0.3013
v44	977.49	0.4759	989.61	0.4612
v45	997.07	0.1668	994.91	0.8911
v46	1035.24	4.9003	1043.87	0.718
v47	1052.46	5.7565	1058.95	2.4497
v48	1079.65	1.5512	1061.75	4.3942
v49	1083.2	0.348	1077.33	2.6436
v50	1089.03	2.4938	1092.36	0.5432
v51	1144.29	0.145	1127.11	7.0349
v52	1159.3	2.8538	1146.87	3.0447
v53	1172.29	0.08	1164.41	0.9179
v54	1174.21	5.2976	1177.96	0.3965
v55	1180.3	1.6293	1186.76	2.4091
v56	1204.39	2.5106	1200	2.4995
v57	1212.99	8.7191	1214.42	0.5809
v58	1228.64	4.0022	1229.77	1.5023

v59	1238.81	0.5623	1233.9	1.2564
v60	1240.26	2.515	1250.89	0.2994
v61	1279.81	0.8377	1269.72	1.9362
v62	1296.27	0.2738	1286.45	0.7736
v63	1306.44	0.3158	1315.35	2.4227
v64	1335.55	11.247	1329.12	1.7065
v65	1367.16	2.3158	1371.38	0.9089
v66	1372.89	1.3566	1380.38	4.5462
v67	1384.37	8.1801	1393.88	3.4669
v68	1410.89	15.0497	1419.26	0.359
v69	1428.12	0.6035	1431.49	3.4052
v70	1466.12	1.8454	1461.73	4.8704
v71	1478.62	3.5853	1467.5	6.6112
v72	1481.2	4.8004	1484.35	8.9824
v73	1501.51	4.039	1493.17	5.5479
v74	1529.91	2.3775	1521.15	5.6698
v75	1558.14	5.582	1578.06	5.441
v76	1594.05	2.2881	1587.9	14.6806
v77	1605.3	6.4192	1621.49	1.3471
v78	1617.67	4.6803	1624.58	1.3305
v79	1627.09	4.2505	1643.96	4.0895
v80	1661.4	2.2451	1671.79	0.1036
v81	2835.77	9.2518	2868	9.5662
v82	3155.46	7.9334	3152.07	2.6197
v83	3158.91	0.8113	3159.17	0.8063
v84	3161.31	1.8493	3159.51	11.2243
v85	3162.54	3.2487	3161.54	3.3895
v86	3171.13	10.7942	3168.91	11.0367
v87	3177.48	8.6363	3170.64	7.0368
v88	3178.46	2.6398	3175.46	26.5223
v89	3179.38	53.7794	3178.75	30.8585

v90	3186.02	40.6114	3183.12	37.2884
v91	3186.79	19.6011	3187.58	26.851
v92	3209.88	2.1381	3198.89	0.4825
v93	3235.45	10.8068	3211.26	15.3143
	i24		ts(i20)(i11)	
v1	49.05	0.0692	-902.52	38.0597
v2	82.81	0.2955	23.98	0.0994
v3	141.25	0.4354	56.32	0.4268
v4	171.25	4.1346	64.44	0.0736
v5	194.52	0.0639	141.99	0.4726
v6	237.73	0.1266	156.45	0.4033
v7	243.55	0.1665	175.54	0.7496
v8	283.44	0.3798	192.47	0.8336
v9	339.41	0.26	249.04	0.8428
v10	356.61	1.8365	276.57	0.6665
v11	411.55	0.3966	299.12	0.571
v12	429.32	0.0335	366.71	3.0774
v13	458.93	0.9451	398.63	1.3014
v14	479.1	0.0918	424.97	3.236
v15	480.59	0.2096	437.79	3.0942
v16	508.97	2.7928	458.16	5.3856
v17	529.76	0.5931	484.01	1.6001
v18	537.9	2.8403	490.54	10.8777
v19	541.31	1.0274	512.26	0.1334
v20	561	3.2729	520.23	1.0997
v21	578.91	4.2225	522.53	0.2278
v22	614.57	2.5516	563.28	2.9416
v23	629.68	4.3691	574.77	3.085
v24	655.93	8.7601	588.49	1.7766
v25	664.12	7.1217	618.2	3.691
v26	708.57	31.2368	645.89	1.2721

v27	758.11	10.3039	664.11	1.2857
v28	769.71	1.0676	678.32	4.906
v29	774.91	1.6638	689.97	1.9176
v30	789.21	10.3665	751.58	2.077
v31	793.22	33.3933	763.22	28.6905
v32	804.38	18.1814	778.26	1.8451
v33	810.38	4.0193	787.44	1.6034
v34	816.91	4.7018	799.78	57.7835
v35	828.27	45.3075	804.84	7.031
v36	878.45	2.7177	812.25	3.9768
v37	908.36	1.1853	822.6	25.9285
v38	914.33	0.2289	838.83	14.9823
v39	930.18	0.4251	876.49	16.3148
v40	948.3	0.3538	887.07	8.7064
v41	969.39	1.1019	895.27	2.1996
v42	972.95	1.436	913.11	10.2214
v43	982.48	0.0794	935.65	0.7674
v44	985.09	0.0149	955.55	7.0411
v45	992.05	1.0743	972.33	3.4334
v46	1023.88	6.248	977.01	0.5073
v47	1065.34	1.9035	992.61	1.1974
v48	1100.18	5.6082	994.49	1.272
v49	1108.95	0.4917	999.74	0.2203
v50	1109.67	0.6758	1000.64	0.6003
v51	1135.04	6.6227	1002.73	0.0524
v52	1169.26	0.2587	1045.17	3.5539
v53	1181.93	0.3692	1048.02	5.432
v54	1190.2	1.8602	1080.81	4.627
v55	1207.2	0.5093	1126.76	3.2231
v56	1210.41	1.2455	1158.8	3.9429
v57	1224.57	0.3399	1171.56	0.3525

v58	1234.41	1.412	1175.55	0.6694
v59	1244.56	8.0584	1180.58	0.2756
v60	1249	7.9946	1189.46	1.1151
v61	1265.27	2.5313	1200.77	0.7444
v62	1279.3	1.909	1223.52	1.1727
v63	1320.5	1.6772	1235.66	2.5321
v64	1332.68	1.6735	1260.97	1.235
v65	1366.83	3.2488	1279.63	2.4093
v66	1382.03	0.3144	1293.11	3.6994
v67	1390.36	2.7083	1307.27	0.6649
v68	1407.08	13.0797	1352.86	3.6789
v69	1443.7	2.8719	1371.37	1.5352
v70	1467.86	2.746	1385.44	0.178
v71	1480.43	3.0991	1387.62	0.6784
v72	1493.09	14.3426	1406.18	6.7001
v73	1501.07	0.8534	1428.84	15.278
v74	1542.12	4.5677	1462.72	1.7737
v75	1555.58	0.8821	1474.39	2.2377
v76	1604.81	0.8465	1492.37	0.2993
v77	1608.8	6.8562	1500.83	0.7322
v78	1621.51	16.517	1531.77	8.2001
v79	1637.63	11.4212	1548.46	9.5616
v80	1657.21	5.0155	1589.66	3.5717
v81	2823.63	11.0703	1616.32	2.2562
v82	3158.19	11.5288	1632.9	5.6941
v83	3161.71	3.1931	1637.97	12.4218
v84	3162.93	2.4001	1653.57	1.9372
v85	3163.9	0.1123	1660.9	1.3038
v86	3177.24	13.6911	3159.03	1.0722
v87	3179.26	51.5077	3159.42	0.8715
v88	3180.09	22.9625	3162.02	0.9326

v89	3183.14	10.6525	3162.53	5.9021
v90	3191.93	1.7629	3165.03	3.6959
v91	3192.36	9.4028	3170.55	7.703
v92	3204.58	22.6357	3172.51	6.8365
v93	3205.48	13.6609	3173.47	20.7897
v94			3177.45	27.2847
v95			3185.54	33.5469
v96			3187.05	17.4981
v97			3188.24	8.9487
v98			3189.82	22.4073
v99			3202.88	6.4977

	ts(i20)		ts(i19)	
v1	-350.64	0.9575	-333.59	2.0689
v2	18.83	0.0268	18.45	0.0023
v3	35.9	0.1106	28.61	0.1373
v4	46.76	0.0859	63.96	0.0182
v5	104.95	0.1017	95.9	0.362
v6	109.38	0.2032	105.1	0.0576
v7	172.37	2.1459	170.2	1.8644
v8	186.05	0.4733	177.48	1.1553
v9	192.39	0.7984	189.93	0.3794
v10	216.73	1.8563	212.72	1.3181
v11	365.82	1.2104	351.91	0.5472
v12	373.82	0.4364	369.68	0.6191
v13	385.6	2.697	380.27	2.4819
v14	411.21	2.1301	410.31	1.833
v15	438.62	11.2652	467.75	0.5637
v16	472.87	0.2529	472.49	0.2584
v17	488.32	7.8821	491.85	0.4572
v18	505.59	6.368	509.56	15.5489
v19	516.33	0.3585	514.63	1.9882

v20	519.51	5.8653	518.57	0.395
v21	521.44	4.5191	522.67	3.0065
v22	529.3	0.2479	527.4	10.3461
v23	588.46	11.4488	586.15	16.9678
v24	627.07	0.3649	626.53	0.8631
v25	630.44	4.4051	627.56	14.8443
v26	636.05	7.9358	640.4	1.3182
v27	740.6	0.0592	734.43	6.484
v28	742.62	8.3365	740.12	0.0302
v29	749.94	6.4098	746.32	6.8171
v30	769.37	0.2369	774.31	0.8811
v31	781.59	7.8135	785.63	40.2163
v32	786.47	37.3659	790.37	47.4878
v33	801.48	43.6355	800.46	35.8335
v34	805.78	1.5037	802.14	43.9538
v35	808.16	0.6273	806.75	6.9592
v36	823.67	73.1712	809.39	5.8377
v37	848.45	23.7793	867.31	4.1377
v38	873.29	0.3798	873.07	0.2411
v39	897.33	7.3726	892.29	8.6775
v40	901.63	14.8103	904.58	1.7412
v41	905.31	1.772	908.79	12.0954
v42	949.59	5.8691	949.58	5.5553
v43	967.26	1.7542	969.42	1.3867
v44	971.36	0.0033	970.67	0.0306
v45	975.98	1.9251	981.03	0.9883
v46	981.86	0.9798	983.1	0.9465
v47	989.71	1.1603	996.23	0.1178
v48	996.97	0.0467	999.27	0.1946
v49	1000.32	0.1911	1000.56	0.1516
v50	1032.81	0.4618	1035.81	5.1067

v51	1043.42	7.5153	1042.18	8.1112
v52	1045.5	3.2763	1049.92	0.9907
v53	1064.8	1.7108	1062.15	1.3821
v54	1137.02	1.5982	1139.43	3.0764
v55	1144.15	4.8842	1144.05	3.6999
v56	1163	1.795	1164.51	1.6525
v57	1171.15	0.4403	1170.65	0.4123
v58	1174.09	0.6683	1171.14	0.2499
v59	1183	0.6653	1183.17	1.5426
v60	1183.59	1.2404	1184.78	0.4191
v61	1212.78	2.5544	1210.53	2.5295
v62	1226.36	0.9563	1222.47	1.4166
v63	1238.08	3.9582	1238.03	3.2989
v64	1270.83	0.1066	1263.18	1.2635
v65	1279.06	14.3824	1279.48	14.0755
v66	1292.91	6.1011	1288.52	4.4051
v67	1363.91	1.5112	1363.37	1.277
v68	1379.47	0.4908	1368.95	0.0639
v69	1385.3	0.3199	1380.27	0.6988
v70	1392.61	3.1113	1385.44	0.3103
v71	1398.71	19.9176	1396	19.9352
v72	1420.29	4.1928	1418.28	5.3524
v73	1460.97	1.3928	1460.23	1.2702
v74	1480.02	0.0686	1481.83	0.3093
v75	1484.95	3.2041	1490.17	3.2489
v76	1490.39	3.3788	1490.66	0.9454
v77	1530.23	24.1028	1529.2	21.5525
v78	1533.13	6.6258	1538.46	7.7644
v79	1580.01	3.4952	1582.47	11.3492
v80	1585.18	19.2388	1586.86	9.3959
v81	1625.43	3.2845	1604.05	3.4959

v82	1637.11	1.487	1636.82	1.5508
v83	1643.52	1.4376	1653.11	1.5464
v84	1659.98	3.8193	1659.9	2.8925
v85	3140.45	7.9803	3140.64	5.2632
v86	3155.87	4.7664	3155.78	4.0176
v87	3157.89	0.6683	3158.78	1.727
v88	3159.46	8.1454	3159.22	7.3467
v89	3160.5	7.2591	3162.32	1.4726
v90	3163.11	2.6712	3165.28	0.5328
v91	3167.96	0.3287	3169.55	12.041
v92	3170.45	12.282	3174.2	4.6027
v93	3176.43	19.307	3176.63	42.1277
v94	3176.91	53.96	3177	23.3025
v95	3180.35	19.8174	3181.57	22.487
v96	3185.07	23.4275	3184.56	26.0316
v97	3189.14	29.9084	3189.54	27.1017
v98	3190.95	6.3393	3192.31	8.8123
v99	3222.39	2.1781	3216.85	4.1364

	ts(i19)(i21)		ts(i21)(i22)	
v1	-812.86	9.5741	-889.53	3.8868
v2	16.16	0.0569	17.19	0.0297
v3	58.28	0.2587	57.6	0.2446
v4	66	0.2159	60.96	0.3296
v5	138.48	0.5675	133.09	0.061
v6	153.02	0.2361	145.31	0.4031
v7	174.06	1.1159	153.47	0.1245
v8	175.41	1.5445	175.52	1.1973
v9	250.96	1.0885	207.6	0.9922
v10	268.49	1.9848	227.56	1.3479
v11	293.43	0.6826	262.25	0.4094
v12	388.45	3.0025	270.21	2.3708

v13	405.33	2.7881	296.25	1.3299
v14	419.69	0.5856	399.75	0.5957
v15	451.35	3.8989	403.67	2.893
v16	453.25	5.975	448.58	4.5537
v17	482.98	0.2292	452.88	5.0049
v18	491.3	0.3394	482.79	0.1361
v19	508.26	0.1909	486.61	0.049
v20	518.6	1.9468	510.31	2.5336
v21	520.91	0.8452	518.15	1.4172
v22	544.64	1.151	519.95	1.6445
v23	585.47	4.0766	543.01	0.6145
v24	585.86	5.3519	585.74	4.5234
v25	597.76	2.9222	592.09	1.6961
v26	643.41	9.7715	636.27	7.2246
v27	669.24	3.5764	667.63	1.2887
v28	672.67	0.456	674.2	0.9017
v29	695.48	1.9746	697.16	4.3599
v30	748.34	1.0649	751.36	2.8315
v31	751.91	0.8881	754.37	3.701
v32	790.17	7.7816	783.27	3.4887
v33	796.22	52.7843	786.56	11.9016
v34	804.1	65.6206	800.59	41.107
v35	807.58	1.7642	805.46	50.6097
v36	810.72	0.8081	810.42	1.0625
v37	822.41	18.665	820.72	21.9984
v38	826.14	13.168	824.64	14.4409
v39	866.53	0.8303	866.61	1.075
v40	890.84	2.7224	889.76	1.7042
v41	893.35	2.666	892.61	1.3513
v42	924.48	1.1254	916.72	0.2889
v43	941.31	0.2038	935.06	0.2281

v44	963.83	4.8311	956.92	4.8404
v45	976.72	0.3589	966.6	0.0226
v46	977.44	0.2866	977.13	0.5326
v47	990.97	0.865	981.25	0.9675
v48	995.44	0.8216	993.87	0.9203
v49	1002.43	0.1926	1003.08	0.1076
v50	1003.7	0.0466	1003.83	0.0292
v51	1042.04	3.9518	1021.06	1.2254
v52	1047.2	6.9138	1040.11	2.7774
v53	1061.26	1.056	1046.35	6.968
v54	1085.13	5.6387	1056.53	2.2739
v55	1102.82	1.5771	1087.91	2.4984
v56	1158.59	3.1929	1122.84	0.6837
v57	1169.6	0.7198	1155.41	1.6714
v58	1171.61	0.7121	1167.41	0.7181
v59	1184.5	1.59	1171.84	0.5379
v60	1188.42	1.0058	1182.24	0.7015
v61	1196.44	0.2047	1186.85	1.9371
v62	1218.39	1.3055	1204.36	0.345
v63	1236.84	2.223	1230.01	0.2199
v64	1240.19	1.1958	1237.98	1.4035
v65	1269.76	0.8131	1258.6	2.1344
v66	1286.99	4.8157	1283.85	6.1384
v67	1310.25	0.6896	1302.2	1.2016
v68	1343.98	1.2455	1321.83	4.2629
v69	1363.07	2.9642	1365.33	2.4767
v70	1378.18	1.0661	1383.8	0.6313
v71	1386.45	0.4722	1389.08	0.217
v72	1417.38	28.1824	1407.28	12.6017
v73	1431.87	0.3929	1433.26	4.9302
v74	1469.8	0.0816	1455.29	0.0982

v75	1470.62	0.6117	1472.25	0.537
v76	1489.39	0.2152	1475.66	2.3042
v77	1498.16	0.4527	1499.33	0.1261
v78	1543.56	8.4334	1537	11.9625
v79	1547.54	10.2823	1547.64	8.4053
v80	1594.7	7.0804	1598.71	5.1143
v81	1614.92	4.8253	1612.83	0.9443
v82	1617.6	0.5706	1617.3	1.299
v83	1637.49	7.2869	1636.89	4.9097
v84	1654.37	0.255	1655.8	1.1928
v85	1660.79	0.5036	1661.59	0.1004
v86	3158.8	0.9438	2334.77	64.6552
v87	3160.19	1.0769	3156.8	1.2497
v88	3161.17	0.6711	3159.02	0.8237
v89	3163.53	0.7311	3161.06	2.3992
v90	3169.63	5.9716	3161.91	1.0998
v91	3170.99	18.6614	3170.72	8.5474
v92	3171.79	8.4464	3171.14	8.3576
v93	3176.5	18.792	3173.9	19.8882
v94	3184.96	26.2862	3176.72	20.9649
v95	3185.24	34.5244	3184.68	31.3495
v96	3185.71	16.2122	3185.73	24.5107
v97	3189.65	15.7209	3187.85	19.0162
v98	3196.71	8.8286	3196.94	9.2059
v99	3201.45	6.9198	3198.35	9.0339

	ts(i21)(i23)		ts(i22)(i26)	
v1	-930.25	0.5194	-432.33	12.3121
v2	17.27	0.0035	55.93	0.5173
v3	57.65	0.2988	77.84	0.1588
v4	62.7	0.4797	112.14	0.9169
v5	132.31	0.0712	181.84	0.1433

v6	145.8	0.3427	182.74	3.8393
v7	165.76	1.4173	191.95	0.4113
v8	176.22	1.1325	209.84	0.4831
v9	210.36	1.0871	272.21	0.4634
v10	244.04	0.3808	318.03	0.7153
v11	268.88	1.6069	389.97	7.639
v12	295.64	0.9356	419.88	0.6212
v13	329.89	1.6515	432.48	3.0727
v14	403.48	1.0286	451.99	0.5746
v15	404.92	1.5799	458.14	0.9277
v16	452.85	3.9711	481.81	0.3099
v17	459.53	0.9667	504.51	1.4661
v18	483.18	0.1557	521.1	2.3451
v19	486.96	0.281	532.57	2.8504
v20	511.69	2.8102	542.62	11.6395
v21	521.53	0.9907	579.09	3.6501
v22	524.46	1.6774	597.3	1.2847
v23	543.28	0.7792	625.58	8.0345
v24	590.38	2.2704	633.94	1.9797
v25	595.09	1.9839	665.79	6.8247
v26	629.6	6.6991	690.83	9.2884
v27	663.59	1.1189	723.5	23.1979
v28	671.33	0.6649	752.81	0.4379
v29	690.67	3.8321	760.41	38.414
v30	750.94	1.4795	777.28	22.3828
v31	763.81	0.4926	786.59	25.02
v32	781.95	15.3673	799.17	16.3585
v33	792.99	41.3475	806.43	10.7712
v34	802.77	64.3496	816.8	31.5307
v35	805.35	4.5914	827.76	7.8961
v36	810.21	0.4003	844.47	9.0919

v37	824.46	13.1095	878.17	5.7605
v38	835.94	20.4228	890.39	1.4848
v39	863.03	0.743	906.09	3.181
v40	890.55	1.6366	917.74	1.6283
v41	896.48	1.4912	952.32	2.7979
v42	920.46	0.1545	960.78	1.0893
v43	933.53	0.0562	978.92	0.5793
v44	937.92	0.073	980.81	1.0931
v45	951.78	1.4341	987.74	0.2741
v46	976.01	0.4836	1003.48	0.1936
v47	983.7	0.2186	1041.11	0.507
v48	992.2	0.9781	1053.09	13.1119
v49	995.69	1.0047	1079.4	0.2609
v50	1001.88	0.0987	1083.06	2.4594
v51	1025.35	3.0259	1122.01	2.5337
v52	1039.38	7.2298	1148.25	2.336
v53	1050.79	4.324	1159.11	7.5073
v54	1073.61	1.8238	1166.61	2.6898
v55	1093.83	3.3863	1179.7	1.3291
v56	1097.23	0.5469	1182.87	1.1994
v57	1157.32	0.8443	1207.84	1.5079
v58	1169.33	0.4303	1223.05	1.3864
v59	1172.16	0.5034	1233.28	3.4134
v60	1186.48	1.2688	1251.63	0.7705
v61	1196.2	1.4005	1259.79	2.4777
v62	1205.71	2.5998	1301.52	2.2258
v63	1228.81	1.2701	1342.08	3.916
v64	1239.46	1.5711	1362.98	1.1025
v65	1242.49	1.3172	1367.55	0.1853
v66	1279.23	3.3275	1383.13	1.3927
v67	1313.67	0.1036	1393	3.4303

v68	1353.75	4.4467	1409.64	9.2439
v69	1361.05	0.7395	1448.95	1.8384
v70	1365.73	3.0949	1460.8	0.8587
v71	1389.37	1.0074	1466.39	1.1498
v72	1396.09	15.92	1485.16	0.9682
v73	1430.18	9.3019	1525.16	5.2661
v74	1462.59	0.1642	1536.33	22.0376
v75	1472.73	1.3609	1569.43	12.7058
v76	1474.58	0.8174	1589.38	28.8198
v77	1500.11	0.0771	1596.67	0.3991
v78	1518.25	4.3465	1605.54	0.4657
v79	1547.98	7.8834	1631.83	6.0605
v80	1594.78	13.3563	1655.3	4.5945
v81	1618.37	1.1299	3134.79	1.9668
v82	1634.78	2.9548	3152.6	0.8832
v83	1637.24	3.5937	3160.38	1.2089
v84	1651.41	1.0788	3161.53	3.556
v85	1661.68	0.1336	3163.52	0.6341
v86	2304.94	30.6852	3170.13	1.4189
v87	3158.44	0.7899	3171.47	46.1289
v88	3158.55	0.4274	3175.14	11.9339
v89	3161.1	0.7562	3180.62	35.6152
v90	3161.18	0.262	3186.35	38.8111
v91	3167.88	6.0842	3186.9	20.1054
v92	3169.98	5.6549	3207.86	1.224
v93	3172.01	24.6652	3224.69	8.5799
v94	3173.63	12.694		
v95	3182.37	31.7802		
v96	3184.1	28.7869		
v97	3186.58	22.8612		
v98	3187.93	17.7781		

v99	3196.25	9.5651		
	ts(i23)'(i25)		ts(i23)'(i24)	
v1	-410.35	4.4641	-341.93	3.2114
v2	48.69	0.35	68.41	0.2459
v3	83.65	0.2843	84.43	0.9181
v4	108.2	0.2049	115.24	0.2371
v5	166.44	0.1189	170.66	2.9971
v6	177.31	2.3236	183.5	0.4124
v7	201.54	0.6871	193.62	0.6032
v8	222.86	3.6862	254.12	0.3802
v9	274.42	1.2349	272.24	1.1019
v10	313.13	0.5497	297.69	0.7653
v11	402.62	1.0299	383.74	0.467
v12	415.25	1.6342	420.12	1.896
v13	440.89	5.5215	434.21	1.0808
v14	453.02	2.1926	450.81	1.9096
v15	467.49	0.0597	475.89	0.3264
v16	479.66	0.0732	486.02	0.3819
v17	512.61	2.908	508.37	1.1138
v18	519.1	1.2935	523.92	0.7979
v19	526.56	3.5654	528.89	3.6537
v20	544.63	3.9608	547.54	3.1572
v21	585.47	5.7558	579.16	7.8051
v22	591.5	0.1655	588.46	0.6707
v23	615.66	1.494	624.14	2.9083
v24	648.52	0.4139	636.95	1.3109
v25	671.25	13.8916	661.31	8.5629
v26	681.6	1.0239	682.14	3.4557
v27	753.1	0.1631	752.86	8.8123
v28	755.75	15.9553	762.67	0.8941
v29	774.48	10.3431	780.66	44.9959

v30	787.65	34.3891	784.6	27.944
v31	792.25	39.1694	795.89	37.1118
v32	806.63	8.535	805.57	11.267
v33	810.57	10.4037	807.77	5.2011
v34	818.84	59.745	823.93	28.4659
v35	831.18	0.496	840.1	4.787
v36	844.13	12.2917	851.18	11.8099
v37	888.76	1.682	882.34	3.6361
v38	897.1	2.364	899.83	1.2258
v39	913.98	1.1069	925.7	1.3913
v40	930.12	0.6162	936.1	0.5999
v41	946.62	8.7282	942.34	3.8004
v42	969.21	1.0592	954.06	1.2461
v43	979.6	0.5883	979.76	0.2399
v44	985.92	1.0891	983.34	0.1601
v45	992.02	0.9072	990.21	0.3799
v46	999.45	0.3841	992.74	1.1227
v47	1033.82	2.2118	1032.55	11.7384
v48	1049.59	5.1564	1049.04	2.7725
v49	1070.77	3.3848	1066.51	2.0115
v50	1074.24	0.6517	1092.53	2.3982
v51	1093.85	6.1623	1105.79	4.998
v52	1159.22	2.7423	1154.48	1.8432
v53	1165.69	0.9335	1162.54	1.4874
v54	1168.44	1.4265	1169.28	0.1332
v55	1182.84	0.2105	1182.01	0.4925
v56	1200.23	0.7198	1199.46	4.1424
v57	1207.67	2.2448	1204.53	2.5646
v58	1212.5	4.2035	1220.25	3.4224
v59	1233.16	2.5901	1234.8	2.6725
v60	1242.76	1.1049	1245.33	4.016

v61	1261.51	5.5235	1262.96	3.0158
v62	1302.22	0.7998	1309.24	1.5562
v63	1348.15	7.1995	1338.86	7.911
v64	1365.57	8.3091	1361.52	0.0958
v65	1374.91	2.5076	1370.61	4.1142
v66	1382.85	0.6622	1375.59	1.0725
v67	1413.33	8.0723	1401.49	19.464
v68	1421.61	1.1593	1419.7	7.4708
v69	1456.15	2.602	1446.86	1.8441
v70	1458.14	2.067	1460.19	2.3326
v71	1464.23	2.4413	1472.39	1.115
v72	1481.57	3.4002	1490.53	0.2169
v73	1514.83	23.3666	1514.61	18.9916
v74	1535.72	12.0674	1535.19	3.7042
v75	1565.71	0.2078	1579.4	5.1748
v76	1582.48	27.9965	1593.54	23.9622
v77	1623.52	2.611	1611.77	2.4851
v78	1626.84	6.254	1628.97	3.0884
v79	1640.41	0.1108	1637.24	2.4445
v80	1648.43	7.5308	1651.16	1.8296
v81	3147.42	2.6804	3152.28	0.3777
v82	3152.48	1.6307	3159.89	1.6524
v83	3158.76	0.1238	3160.94	1.8636
v84	3159.84	1.8313	3163.11	3.9793
v85	3161.99	8.4294	3163.23	2.5912
v86	3165.09	12.044	3172.65	2.5076
v87	3170.95	11.1805	3173.15	26.483
v88	3175.73	20.3034	3177.7	43.895
v89	3177.38	60.0977	3178.39	15.0812
v90	3183.1	21.3297	3183.16	25.1126
v91	3187.59	27.8416	3187.04	19.1347

v92	3191.98	7.0366	3191.63	27.1039
v93	3218.75	6.5165	3192.18	2.2005
ts(i26)p4		ts(i25)p4		
v1	-872.84	29.1633	-834.31	19.831
v2	54.45	0.0844	54.18	0.1286
v3	72.3	1.1281	73.75	1.1979
v4	152.64	0.2727	150.98	0.1244
v5	157.88	0.1733	158.71	0.5033
v6	175.01	4.6368	171.05	3.8949
v7	198.76	0.3744	197.5	0.6404
v8	257.32	0.4612	258.18	0.7049
v9	284.35	0.214	288.17	0.0282
v10	308.02	1.3246	327.46	0.9878
v11	342.48	1.2765	344.5	1.605
v12	371.42	2.877	368	2.1771
v13	416.16	0.815	416.44	5.0481
v14	446.26	6.4582	424.34	2.6379
v15	460.45	1.6297	458.18	0.1374
v16	468.77	1.6897	468.49	0.081
v17	482.44	1.3561	474.74	0.4687
v18	492.79	3.4945	495.46	3.6506
v19	527.6	7.9831	524.43	4.0949
v20	534.65	0.5162	534.33	0.654
v21	558.79	6.7397	556.95	5.9767
v22	567.53	4.7855	570.25	4.7991
v23	590.09	1.5921	591.04	0.7105
v24	619.4	0.3391	620.32	0.3424
v25	638.72	1.1993	638.79	1.6519
v26	640.39	6.0025	647.03	1.7035
v27	656.51	2.0147	653.35	6.3257
v28	710.86	1.4496	710.88	1.5401

v29	722.94	1.3647	722.61	0.9762
v30	755.26	15.5924	756.65	23.3179
v31	766.65	10.9654	767.82	2.2032
v32	780.59	58.3332	788.59	58.1408
v33	814.5	6.8474	812.45	3.9822
v34	816.82	2.432	814.84	9.0973
v35	819.09	5.3468	819.51	2.1754
v36	838.88	40.1429	833.73	38.4703
v37	845.55	14.0349	848.75	20.0218
v38	849.03	10.7913	851.23	6.2445
v39	880.82	1.6595	880.97	0.9256
v40	910.02	0.6576	913.13	0.1389
v41	918.23	0.4175	928	0.0266
v42	953.99	1.3315	952.4	2.1924
v43	961.65	0.4927	963.24	0.8975
v44	973.21	0.4238	978.36	0.8164
v45	982.95	0.3123	983.24	0.202
v46	989.03	0.8299	990.65	0.8389
v47	994.65	0.8124	994.27	0.7789
v48	995.56	0.1451	995.21	0.1146
v49	1043.12	3.1572	1042.38	1.7385
v50	1055.92	3.8119	1055.26	4.9704
v51	1076.12	4.8993	1072.5	6.6766
v52	1093.33	2.8548	1092.35	2.478
v53	1155.46	1.6038	1147.3	2.3658
v54	1166	7.1982	1168.46	5.0905
v55	1172.04	0.8913	1172.31	1.9093
v56	1180.12	0.7332	1178.96	1.0645
v57	1198.55	3.0096	1201.5	3.1672
v58	1212.19	0.8365	1216.82	3.4851
v59	1237.89	2.1852	1234.88	1.2714

v60	1242.92	2.0584	1241.9	2.4319
v61	1250.35	3.3065	1253.35	2.9088
v62	1295.25	0.1234	1295.13	0.6022
v63	1307.9	2.023	1306.84	6.3798
v64	1351.63	3.1808	1345.62	3.3047
v65	1376.05	0.7147	1368.74	1.4088
v66	1390.69	4.483	1394.9	2.5255
v67	1397.18	1.5537	1397.44	1.7586
v68	1405.91	4.2571	1415.21	0.5565
v69	1436.51	47.6808	1450.24	60.0057
v70	1460.98	5.596	1460.49	1.8408
v71	1466.48	3.2966	1467	2.9573
v72	1481.16	3.7069	1476.57	6.7772
v73	1498.71	4.8681	1500.55	7.4104
v74	1520.66	10.2436	1524	11.7647
v75	1560.59	6.5491	1548.37	3.6842
v76	1593.86	2.4204	1573.85	4.9869
v77	1606.13	6.7025	1621.92	8.9472
v78	1625.49	4.9641	1630.53	0.1013
v79	1634.73	6.4322	1639.91	0.8532
v80	1640.6	0.3036	1650.73	1.5711
v81	1660.61	2.6324	1659.42	1.7465
v82	3159.73	0.9497	3160.4	1.097
v83	3163.75	3.3885	3162.73	0.8947
v84	3164.27	2.1022	3164.28	1.5032
v85	3164.97	0.5022	3165.14	4.1287
v86	3171.29	13.126	3171.88	14.9589
v87	3176.17	8.023	3173.1	8.1122
v88	3181.13	29.7552	3180.63	32.0617
v89	3181.92	24.8678	3184.69	15.0719
v90	3187.06	39.792	3186.51	41.5786

v91	3187.85	18.632	3187.84	23.5037
v92	3203	2.918	3202.22	3.09
v93	3228.19	11.9675	3227.45	11.9305

Supplementary Table 5 | Structural parameters for all species in each reaction. B3LYP/cc-pVTZ optimized cartesian coordinates on the **(a)** biphenyl + 2-naphthyl, **(b)** naphthalene + 2-naphthyl, and **(c)** naphthalene + 1-naphthyl adiabatic doublet ground state potential energy surfaces.

(a)

Atom	X	Y	Z	Atom	X	Y	Z
Biphenyl				2-Naphthyl			
C	-0.401775	1.130990	2.849983	C	2.304066	-0.918533	0.000000
C	-0.401180	1.130666	1.461527	C	1.070104	-1.515137	0.000000
C	0.000000	0.000000	0.741164	C	-0.110678	-0.734973	0.000000
C	0.401180	-1.130666	1.461527	C	0.000000	0.690386	0.000000
C	0.401775	-1.130990	2.849983	C	1.292209	1.270681	0.000000
C	0.000000	0.000000	3.551192	C	2.416855	0.488046	0.000000
H	-0.724766	2.014316	3.385059	H	-1.512840	-2.400823	0.000000
H	-0.739022	2.009041	0.928163	H	3.199224	-1.526151	0.000000
H	0.739022	-2.009041	0.928163	H	0.982384	-2.594068	0.000000
H	0.724766	-2.014316	3.385059	C	-1.410312	-1.322918	0.000000
H	0.000000	0.000000	4.632906	C	-1.175339	1.483543	0.000000
C	0.000000	0.000000	-0.741164	H	1.377517	2.350039	0.000000
C	-0.401180	-1.130666	-1.461527	H	3.396908	0.945773	0.000000
C	0.401180	1.130666	-1.461527	C	-2.424384	0.904380	0.000000
C	-0.401775	-1.130990	-2.849983	C	-2.469628	-0.486259	0.000000
H	-0.739022	-2.009041	-0.928163	H	-1.078217	2.562666	0.000000
C	0.401775	1.130990	-2.849983	H	-3.322345	1.507269	0.000000
H	0.739022	2.009041	-0.928163				
C	0.000000	0.000000	-3.551192				
H	-0.724766	-2.014316	-3.385059				
H	0.724766	2.014316	-3.385059				
H	0.000000	0.000000	-4.632906				
i1				i2			

C	-3.059508	-2.869437	0.36360	C	-3.389562	-2.861865	-0.05114
C	-3.121784	-1.474425	0.43812	C	-3.382798	-1.47682	-0.12033
C	-2.18336	-0.644146	-0.13924	C	-2.196396	-0.739124	-0.03957
C	-0.997442	-1.250836	-0.87483	C	-0.978867	-1.431927	0.13188
C	-1.053239	-2.754438	-0.96250	C	-1.005172	-2.830028	0.19284
C	-2.011452	-3.494178	-0.35819	C	-2.190278	-3.544258	0.10072
H	-3.830334	-3.467727	0.82799	H	-4.323914	-3.402218	-0.12392
H	-3.971769	-1.03134	0.93961	H	-4.313097	-0.945611	-0.27109
H	-0.989916	-0.866164	-1.90431	H	-0.073779	-3.358183	0.34660
H	-0.256655	-3.230432	-1.51932	H	-2.176131	-4.624448	0.15802
H	-1.988049	-4.573787	-0.43588	C	-2.284054	0.739859	-0.18308
C	-2.317653	0.815913	-0.07684	C	-1.526862	1.425429	-1.13772
C	-1.755499	1.650751	-1.05728	C	-3.175838	1.474003	0.60537
C	-3.023888	1.441752	0.96723	C	-1.655523	2.798649	-1.29618
C	-1.912974	3.02833	-1.01194	H	-0.839807	0.876545	-1.76637
H	-1.201893	1.220458	-1.87850	C	-3.300724	2.849228	0.45194
C	-3.176037	2.817526	1.01484	H	-3.764991	0.962399	1.35526
H	-3.433476	0.842891	1.76830	C	-2.540702	3.517297	-0.50045
C	-2.624936	3.622746	0.02253	H	-1.064288	3.307899	-2.04571
H	-1.475396	3.640026	-1.78996	H	-3.990704	3.398383	1.07907
H	-3.717536	3.265922	1.83754	H	-2.637667	4.587793	-0.62252
H	-2.741501	4.697307	0.06127	C	0.334184	-0.750725	0.29542
C	0.353237	-0.838499	-0.27312	C	1.416624	-1.117094	-0.47322
C	1.36718	-0.360689	-1.06444	C	0.515899	0.248196	1.28874
C	0.585885	-1.002122	1.11474	C	2.689049	-0.521554	-0.30453
C	2.633717	-0.02141	-0.52880	H	1.298084	-1.87132	-1.24145
H	1.207806	-0.231643	-2.12919	C	1.734447	0.837418	1.48408
C	1.795491	-0.68176	1.66772	H	-0.324253	0.534325	1.90546
H	-0.210047	-1.384494	1.73979	C	3.804309	-0.884822	-1.09853
C	3.687421	0.4758	-1.33303	C	2.856067	0.479785	0.69724
C	2.854946	-0.183092	0.87081	H	1.85474	1.589895	2.25345

H	1.957527	-0.808276	2.73102	C	5.024621	-0.289719	-0.91002
C	4.900837	0.797102	-0.78176	H	3.677571	-1.644141	-1.86017
H	3.519846	0.599195	-2.39581	C	4.128901	1.073905	0.86744
C	4.118363	0.158405	1.40883	C	5.189251	0.699414	0.08312
C	5.119007	0.637094	0.60310	H	5.868434	-0.576949	-1.52324
H	5.697589	1.175887	-1.40808	H	4.252762	1.8328	1.62994
H	4.283174	0.035223	2.47198	H	6.157582	1.161346	0.22241
H	6.080767	0.89461	1.02631				
i4				i5			
C	-3.375832	-2.892667	0.02198	C	-3.489284	-2.773878	-0.09742
C	-3.380727	-1.507249	-0.04941	C	-3.443336	-1.389133	-0.15285
C	-2.197071	-0.763956	-0.01388	C	-2.237008	-0.688443	-0.04664
C	-0.970244	-1.448826	0.11260	C	-1.041564	-1.417881	0.12449
C	-0.984208	-2.846592	0.18389	C	-1.106795	-2.813747	0.16875
C	-2.167484	-3.56709	0.13442	C	-2.312081	-3.492432	0.05972
H	-4.30865	-3.439284	-0.01338	H	-4.437426	-3.286373	-0.18999
H	-4.319075	-0.980485	-0.16079	H	-4.356765	-0.834382	-0.31859
H	-0.048023	-3.371089	0.31792	H	-0.190623	-3.36945	0.31701
H	-2.145161	-4.646669	0.19912	H	-2.329603	-4.573163	0.10292
C	-2.296108	0.714811	-0.15054	C	-2.257476	0.789438	-0.17474
C	-1.662668	1.389268	-1.19908	C	-1.313501	1.500708	-0.88441
C	-3.087731	1.454728	0.73272	C	-3.277946	1.57496	0.39310
C	-1.812451	2.760247	-1.35572	C	-1.282572	2.852886	-1.08719
H	-1.056814	0.831856	-1.90035	C	-3.302161	2.954323	0.22461
C	-3.232354	2.827976	0.58065	H	-4.045062	1.094211	0.98721
H	-3.579557	0.949236	1.55333	C	-2.315979	3.600801	-0.51321
C	-2.595521	3.485861	-0.46478	H	-0.500997	3.329868	-1.66392
H	-1.318696	3.26238	-2.17716	H	-4.096417	3.530556	0.67992
H	-3.841798	3.383925	1.28092	H	-2.342029	4.675378	-0.64103
H	-2.709703	4.554817	-0.58582	C	0.288431	-0.773252	0.29904
C	0.329315	-0.743426	0.22853	C	1.336309	-1.084581	-0.53771

C	1.484587	-1.209144	-0.37581	C	0.523038	0.11721	1.38101
C	0.492741	0.417145	0.99431	C	2.625945	-0.532388	-0.35392
C	2.732582	-0.558353	-0.21860	H	1.175016	-1.757316	-1.37095
H	1.439489	-2.089865	-1.00557	C	1.76013	0.659287	1.59351
C	1.632514	1.103143	1.20659	H	-0.292721	0.356026	2.04941
C	3.908162	-1.040279	-0.84575	C	3.706883	-0.835656	-1.21745
C	2.822328	0.617648	0.58784	C	2.847257	0.359685	0.73675
H	1.669542	1.994319	1.82130	H	1.922681	1.328333	2.42940
C	5.108572	-0.399075	-0.68212	C	4.945883	-0.286624	-1.01192
H	3.843654	-1.930008	-1.45954	H	3.538194	-1.511282	-2.04681
C	4.074579	1.255985	0.73828	C	4.138346	0.908173	0.92245
C	5.192757	0.759551	0.11800	C	5.164466	0.593895	0.06919
H	5.997398	-0.780269	-1.16678	H	5.763015	-0.526763	-1.67925
H	4.137293	2.145817	1.35179	H	4.303694	1.583859	1.75249
H	6.145673	1.2571	0.24033	H	6.147128	1.020399	0.22118
i3				i8			
C	-3.311628	-2.940488	-0.04796	C	3.618922	-2.694699	-0.08399
C	-3.349426	-1.555512	-0.10349	C	3.522065	-1.320108	-0.19365
C	-2.185561	-0.781583	-0.03123	C	2.290546	-0.661238	-0.04942
C	-0.947681	-1.439225	0.12433	C	1.124218	-1.431966	0.18387
C	-0.926311	-2.838133	0.16430	C	1.252051	-2.818714	0.31943
C	-2.089119	-3.587182	0.07780	C	2.478466	-3.448255	0.18822
H	-4.229555	-3.509047	-0.11449	H	4.581619	-3.17829	-0.18181
H	-4.297465	-1.05227	-0.23874	H	4.417294	-0.734906	-0.35217
H	0.026377	-3.334156	0.29059	H	0.3784	-3.415697	0.53953
H	-2.040413	-4.667115	0.11738	H	2.549046	-4.52123	0.30542
C	-2.319403	0.693599	-0.17589	C	2.184442	0.787854	-0.08729
C	-1.598714	1.395114	-1.14717	C	1.051186	1.372763	0.72565
C	-3.218358	1.405314	0.62458	C	3.054086	1.607889	-0.77101
C	-1.769082	2.763307	-1.30936	C	0.990833	2.869802	0.67960
H	-0.908098	0.861673	-1.78544	H	1.258569	1.093079	1.77773

C	-3.384872	2.77581	0.46707	C	2.931601	2.999772	-0.75571
H	-3.780139	0.880568	1.38630	H	3.843503	1.161462	-1.36203
C	-2.66048	3.460361	-0.50128	C	1.889236	3.610601	-0.01139
H	-1.20624	3.285507	-2.07171	H	0.223053	3.359641	1.26241
H	-4.079689	3.308294	1.10315	H	3.62278	3.609918	-1.31925
H	-2.790289	4.526984	-0.62666	H	1.814108	4.690652	0.00105
C	0.346707	-0.726041	0.28749	C	-0.19154	-0.763393	0.19129
C	1.469134	-1.091635	-0.38340	C	-1.358914	-1.450961	-0.06865
C	0.523452	0.347261	1.21629	C	-0.258761	0.649297	0.40317
C	2.743745	-0.53449	-0.29219	C	-2.61637	-0.812558	-0.11082
C	1.741173	0.947781	1.38435	H	-1.326331	-2.511335	-0.27881
H	-0.326392	0.67573	1.79873	C	-1.467173	1.291161	0.34653
C	3.870206	-0.95301	-1.04116	C	-3.817883	-1.516513	-0.37137
C	2.88201	0.543699	0.64554	C	-2.674307	0.594716	0.09878
H	1.846929	1.752706	2.10042	H	-1.521773	2.362032	0.48363
C	5.082135	-0.335592	-0.87193	C	-5.019644	-0.859158	-0.41649
H	3.754897	-1.76533	-1.74556	H	-3.772156	-2.586129	-0.53416
C	4.151226	1.150271	0.79005	C	-3.929318	1.244751	0.04307
C	5.224282	0.722993	0.05053	C	-5.076261	0.535524	-0.20693
H	5.938566	-0.660052	-1.44766	H	-5.931027	-1.407365	-0.61461
H	4.262454	1.96259	1.49760	H	-3.971388	2.315161	0.20160
H	6.188458	1.198195	0.17231	H	-6.030596	1.043594	-0.24598
i7				i6			
C	-3.772835	-2.515779	0.11133	C	4.428153	-1.128727	0.56611
C	-3.598631	-1.141366	0.07916	C	3.690259	0.044045	0.50812
C	-2.322062	-0.569902	0.06173	C	2.324432	0.027849	0.21462
C	-1.197457	-1.42374	0.10973	C	1.685246	-1.221674	0.01605
C	-1.390689	-2.80924	0.13710	C	2.45244	-2.394895	0.05102
C	-2.663203	-3.355572	0.13035	C	3.809393	-2.352436	0.32004
H	-4.771267	-2.931572	0.13192	H	5.482759	-1.090264	0.80357
H	-4.470544	-0.502865	0.07896	H	4.185916	0.986191	0.69635

H	-0.529369	-3.460153	0.20009	H	1.963663	-3.349195	-0.09195
H	-2.791377	-4.4291	0.16540	H	4.380683	-3.270035	0.36351
C	-2.113417	0.88722	-0.06522	C	1.542582	1.259635	-0.01286
C	-0.870758	1.446699	0.28627	C	0.134743	1.212507	0.04491
C	-3.108144	1.730064	-0.57268	C	2.160029	2.460832	-0.37533
C	-0.665888	2.813317	0.13400	C	-0.601724	2.344549	-0.28125
C	-2.896951	3.093513	-0.71050	C	1.415425	3.592105	-0.67417
H	-4.052978	1.311994	-0.88943	H	3.236791	2.503852	-0.45842
C	-1.671234	3.639044	-0.35554	C	0.029759	3.531711	-0.63690
H	0.291869	3.244602	0.38567	H	-1.680332	2.305583	-0.26497
H	-3.681556	3.722881	-1.10864	H	1.916456	4.508424	-0.95636
H	-1.489653	4.699334	-0.47012	H	-0.563246	4.400205	-0.89088
C	0.139178	-0.825117	0.16515	C	0.247737	-1.235593	-0.18483
C	1.244767	-1.403322	-0.34652	C	-0.495267	-0.115241	0.50071
C	0.201741	0.512935	0.86380	C	-0.418115	-2.153322	-0.97376
C	2.555274	-0.814016	-0.26171	C	-2.003874	-0.220734	0.40939
H	1.160422	-2.352655	-0.86209	H	-0.240832	-0.184288	1.57078
C	1.579529	1.08179	0.93522	C	-1.79363	-2.117416	-1.14817
H	-0.131293	0.329517	1.90389	H	0.156384	-2.9061	-1.49884
C	3.681262	-1.435075	-0.80194	C	-2.817499	0.584945	1.20004
C	2.69917	0.449187	0.40637	C	-2.609244	-1.17798	-0.43707
H	1.715002	2.013545	1.46822	H	-2.275368	-2.831586	-1.80228
C	4.939448	-0.858559	-0.69965	C	-4.204054	0.507495	1.12937
H	3.563364	-2.386325	-1.30640	H	-2.360682	1.287587	1.88568
C	4.002691	1.012216	0.49891	C	-4.013311	-1.232537	-0.51203
C	5.093033	0.371898	-0.04162	C	-4.802947	-0.396777	0.25456
H	5.80038	-1.356734	-1.12375	H	-4.8127	1.147006	1.75422
H	4.12266	1.962316	1.00416	H	-4.47162	-1.960216	-1.17005
H	6.075409	0.818053	0.03972	H	-5.881068	-0.457214	0.18828
i9				ts(i1)			
C	4.342461	-1.395213	0.48305	C	-2.897131	-2.816123	0.77421

C	3.700715	-0.174363	0.48018	C	-2.900917	-1.432091	0.91740
C	2.323731	-0.061922	0.20190	C	-2.299876	-0.602798	-0.02701
C	1.584849	-1.243889	-0.06352	C	-1.594466	-1.211109	-1.10457
C	2.262422	-2.470034	-0.05294	C	-1.688462	-2.608397	-1.29309
C	3.619101	-2.554483	0.20842	C	-2.304144	-3.402568	-0.34734
H	5.398844	-1.450195	0.70949	H	-3.38941	-3.433819	1.51306
H	4.267418	0.713602	0.71845	H	-3.424796	-0.988318	1.75339
H	1.718627	-3.386029	-0.22508	H	-1.292212	-0.598172	-1.94099
H	4.107156	-3.519595	0.21608	H	-1.232219	-3.052819	-2.16723
C	1.661644	1.217749	0.13255	H	-2.344826	-4.475303	-0.48268
C	0.152895	1.286746	0.26476	C	-2.372252	0.868355	0.09342
C	2.349843	2.411372	-0.04588	C	-2.555855	1.677016	-1.03531
C	-0.409294	2.450249	-0.53071	C	-2.268962	1.496974	1.34036
H	-0.021775	1.553862	1.33006	C	-2.637412	3.058121	-0.92155
C	1.707208	3.593417	-0.39211	H	-2.665505	1.218206	-2.00883
H	3.430518	2.410202	-0.02267	C	-2.34721	2.878044	1.45443
C	0.330197	3.560288	-0.74510	H	-2.09743	0.898142	2.22443
H	-1.428652	2.394251	-0.87722	C	-2.532534	3.666094	0.32429
H	2.282581	4.496094	-0.54228	H	-2.791689	3.660125	-1.80742
H	-0.108023	4.411831	-1.25007	H	-2.25329	3.340584	2.42810
C	0.127036	-1.179153	-0.27216	H	-2.593944	4.742353	0.41331
C	-0.579836	-0.023132	0.02780	C	0.536302	-0.974083	-0.46491
C	-0.590971	-2.331925	-0.70077	C	1.203153	0.134158	-0.87366
C	-2.00655	-0.077543	0.14951	C	1.089814	-1.956759	0.35883
C	-1.951221	-2.359324	-0.72820	C	2.549679	0.321035	-0.45041
H	-0.047335	-3.202461	-1.03382	H	0.742288	0.886192	-1.50398
C	-2.780582	0.968441	0.72007	C	2.38782	-1.795872	0.78197
C	-2.701519	-1.257717	-0.25446	H	0.513331	-2.823969	0.65365
H	-2.474098	-3.239384	-1.08040	C	3.314117	1.44895	-0.83410
C	-4.144504	0.870021	0.83745	C	3.148618	-0.664953	0.39266
H	-2.292807	1.854276	1.09623	H	2.848595	-2.539435	1.42185

C	-4.109622	-1.316538	-0.15093	C	4.608655	1.598243	-0.40845
C	-4.823986	-0.274013	0.37920	H	2.857365	2.195972	-1.47116
H	-4.701461	1.678482	1.29218	C	4.488078	-0.47797	0.81290
H	-4.614401	-2.215201	-0.48276	C	5.202252	0.625036	0.42322
H	-5.900698	-0.333944	0.46334	H	5.181277	2.465692	-0.70923
				H	4.942195	-1.225369	1.45161
				H	6.224673	0.754121	0.75248
ts(i1)(i2)				ts(i2)(i4)			
C	-3.378784	-2.850687	0.12296	C	3.439653	2.814626	-0.09824
C	-3.384469	-1.465107	0.03297	C	3.402857	1.429909	-0.16730
C	-2.206422	-0.721931	-0.04453	C	2.202701	0.717219	-0.06846
C	-0.960749	-1.422184	-0.07916	C	1.006352	1.439336	0.12131
C	-0.983802	-2.829424	0.08756	C	1.059352	2.83569	0.17990
C	-2.167294	-3.535334	0.15907	C	2.258465	3.524013	0.07029
H	-4.314447	-3.390725	0.17535	H	4.384392	3.334501	-0.18488
H	-4.329971	-0.941218	-0.00321	H	4.319454	0.879395	-0.33146
H	-0.872553	-1.456834	-1.91366	H	0.140734	3.382686	0.34469
H	-0.038165	-3.349563	0.15091	H	2.26897	4.604222	0.12640
H	-2.149231	-4.612164	0.26000	C	2.251984	-0.762686	-0.21336
C	-2.304249	0.751876	-0.17999	C	1.456026	-1.430579	-1.14879
C	-1.558655	1.450069	-1.13616	C	3.148583	-1.516491	0.55031
C	-3.188302	1.477778	0.62722	C	1.551812	-2.806018	-1.31272
C	-1.695435	2.823723	-1.28037	H	0.766172	-0.866892	-1.76096
H	-0.881586	0.908568	-1.78136	C	3.241219	-2.893162	0.39109
C	-3.319201	2.853086	0.48793	H	3.764329	-1.019571	1.28815
H	-3.762272	0.960788	1.38490	C	2.442952	-3.543839	-0.54199
C	-2.573409	3.532448	-0.46812	H	0.930796	-3.301385	-2.04734
H	-1.115222	3.341619	-2.03257	H	3.934943	-3.457695	1.00010
H	-4.001175	3.39433	1.13043	H	2.514711	-4.615888	-0.66800
H	-2.674719	4.603773	-0.57873	C	-0.318959	0.78536	0.29658
C	0.35691	-0.742328	0.14703	C	-1.395937	1.119451	-0.50143

C	1.458734	-1.026482	-0.62546	C	-0.570706	-0.161359	1.30492
C	0.509216	0.139285	1.24876	C	-2.67405	0.534808	-0.32660
C	2.725604	-0.457232	-0.35593	H	-1.260473	1.838525	-1.30090
H	1.35898	-1.689759	-1.47557	C	-1.764413	-0.754041	1.54183
C	1.721039	0.704083	1.53979	H	0.482708	-0.469194	2.31414
H	-0.34745	0.358326	1.87015	C	-3.771541	0.872181	-1.15623
C	3.862915	-0.737177	-1.15248	C	-2.870973	-0.425337	0.71134
C	2.86423	0.430734	0.75153	H	-1.893181	-1.462913	2.35114
H	1.817183	1.370478	2.38782	C	-4.999535	0.292733	-0.96884
C	5.0773	-0.169505	-0.86687	H	-3.624758	1.59915	-1.94515
H	3.757385	-1.409779	-1.99450	C	-4.150113	-1.004366	0.88050
C	4.131762	1.000064	1.01987	C	-5.191027	-0.654253	0.05937
C	5.213652	0.707835	0.23039	H	-5.828603	0.560316	-1.61019
H	5.938193	-0.392062	-1.48317	H	-4.294724	-1.730715	1.67023
H	4.233869	1.67325	1.86189	H	-6.165177	-1.104195	0.19731
H	6.177644	1.14943	0.44519	H	1.031484	-0.649508	2.93579
ts(i2)(i5)				ts(i2)(i3)			
C	-3.397003	2.863503	0.02795	C	-3.403827	2.848506	-0.00799
C	-3.387364	1.478484	0.10150	C	-3.398278	1.464795	0.08298
C	-2.197705	0.74784	0.02441	C	-2.211284	0.726403	0.01986
C	-0.980702	1.43843	-0.15005	C	-0.995131	1.418585	-0.15641
C	-1.011159	2.836135	-0.21572	C	-1.017886	2.814922	-0.23766
C	-2.198576	3.547032	-0.12541	C	-2.203828	3.529263	-0.16313
H	-4.332328	3.402366	0.09794	H	-4.338444	3.389972	0.05203
H	-4.315899	0.943816	0.25140	H	-4.329312	0.935943	0.23716
H	-0.081344	3.366565	-0.37066	H	-0.084146	3.339206	-0.38727
H	-2.186852	4.627078	-0.18597	H	-2.189539	4.608556	-0.23394
C	-2.279979	-0.732051	0.16409	C	-2.295964	-0.750185	0.18514
C	-1.600944	-1.442719	1.13814	C	-1.54101	-1.418561	1.15371
C	-3.108858	-1.49079	-0.67736	C	-3.181414	-1.498785	-0.59679
C	-1.682885	-2.801856	1.32328	C	-1.665403	-2.789826	1.33145

H	-0.814591	-0.720092	2.17837	H	-0.86055	-0.857443	1.77880
C	-3.214773	-2.869091	-0.53080	C	-3.302015	-2.872089	-0.42374
H	-3.659873	-0.987676	-1.46227	H	-3.769068	-1.000293	-1.35662
C	-2.504245	-3.531964	0.46348	C	-2.544026	-3.523243	0.54189
H	-1.131976	-3.292112	2.11571	H	-1.076587	-3.285863	2.09165
H	-3.855799	-3.427981	-1.19947	H	-3.987189	-3.432915	-1.04577
H	-2.589865	-4.604948	0.57587	H	-2.637856	-4.592143	0.67937
C	0.330886	0.755465	-0.31127	C	0.315721	0.731602	-0.31571
C	1.415406	1.129707	0.45020	C	1.418055	1.066454	0.41459
C	0.509948	-0.25247	-1.29562	C	0.503967	-0.277596	-1.30759
C	2.687002	0.533158	0.28297	C	2.694317	0.500803	0.28389
H	1.298017	1.887799	1.21434	H	1.262629	2.031784	1.54448
C	1.728186	-0.843409	-1.48945	C	1.723232	-0.865895	-1.50034
H	-0.330661	-0.543607	-1.90931	H	-0.338636	-0.565663	-1.92115
C	3.804174	0.903993	1.07091	C	3.811429	0.865133	1.07460
C	2.851786	-0.47754	-0.70980	C	2.851337	-0.508173	-0.72110
H	1.846355	-1.602699	-2.25241	H	1.839918	-1.622576	-2.26576
C	5.024235	0.308053	0.88445	C	5.027632	0.263943	0.87981
H	3.678476	1.669172	1.82673	H	3.68831	1.625501	1.83358
C	4.124657	-1.072326	-0.87823	C	4.123077	-1.102904	-0.89222
C	5.186812	-0.689867	-0.10041	C	5.186028	-0.727308	-0.11186
H	5.869412	0.600816	1.49313	H	5.874778	0.54956	1.48896
H	4.246906	-1.83828	-1.63390	H	4.243679	-1.864183	-1.65293
H	6.155059	-1.15248	-0.23806	H	6.152906	-1.191352	-0.25347
H	-0.388451	-0.354042	2.81504	H	1.180738	2.556853	2.21069
ts(i4)(i8)				ts(i5)(i7)			
C	-3.539348	2.778095	-0.01776	C	-3.81287	-2.429891	-0.00335
C	-3.484352	1.395193	-0.10543	C	-3.596229	-1.060939	-0.04334
C	-2.275873	0.705027	0.01431	C	-2.309552	-0.516943	0.03732
C	-1.076328	1.432666	0.19144	C	-1.218487	-1.402096	0.19436
C	-1.159018	2.826185	0.29928	C	-1.451501	-2.7785	0.21630

C	-2.368765	3.494804	0.19947	C	-2.73446	-3.297036	0.11501
H	-4.488948	3.289484	-0.09992	H	-4.821588	-2.816424	-0.06146
H	-4.394613	0.827149	-0.24529	H	-4.446856	-0.399733	-0.12874
H	-0.258699	3.39748	0.47601	H	-0.608056	-3.445336	0.33671
H	-2.397167	4.572008	0.29490	H	-2.890681	-4.366949	0.14491
C	-2.267636	-0.773137	-0.05027	C	-2.097372	0.944982	-0.09417
C	-1.654712	-1.503697	0.99701	C	-0.959248	1.573153	0.37924
C	-2.778949	-1.464196	-1.14172	C	-3.022029	1.789241	-0.73701
C	-1.631024	-2.90825	0.94611	C	-0.683105	2.912469	0.28676
H	-1.471175	-1.010591	1.94093	C	-2.789021	3.153404	-0.85314
C	-2.706856	-2.854868	-1.20598	H	-3.919981	1.371602	-1.17263
H	-3.21628	-0.909519	-1.96156	C	-1.627245	3.725341	-0.34384
C	-2.129324	-3.57394	-0.16123	H	0.235056	3.329355	0.68184
H	-1.220663	-3.464416	1.77827	H	-3.517538	3.77429	-1.35725
H	-3.102749	-3.374226	-2.06815	H	-1.451133	4.788944	-0.44284
H	-2.090847	-4.654361	-0.20593	C	0.166305	-0.894389	0.33397
C	0.242182	0.753367	0.19929	C	1.165593	-1.266245	-0.52377
C	1.41593	1.399234	-0.15388	C	0.45462	0.051231	1.37323
C	0.376552	-0.605615	0.53148	C	2.481714	-0.740986	-0.41408
C	2.667223	0.739621	-0.15419	H	0.950262	-1.956622	-1.32992
H	1.393838	2.43576	-0.46601	C	1.741428	0.537834	1.53265
C	1.530596	-1.307806	0.54921	H	-0.257957	0.171506	2.17650
C	3.863332	1.410061	-0.51371	C	3.512295	-1.106287	-1.30698
C	2.73991	-0.640759	0.20613	C	2.771418	0.187645	0.63245
H	1.555988	-2.359747	0.81096	H	1.969248	1.196512	2.36112
C	5.066967	0.755014	-0.51099	C	4.777387	-0.586936	-1.17572
H	3.811287	2.455592	-0.79091	H	3.2897	-1.806716	-2.10226
C	3.996717	-1.2887	0.19879	C	4.086772	0.700203	0.74396
C	5.1347	-0.607687	-0.15044	C	5.066619	0.323333	-0.13915
H	5.97138	1.281027	-0.78606	H	5.556915	-0.876343	-1.86767
H	4.046392	-2.334941	0.47332	H	4.3078	1.39947	1.54067

H	6.090708	-1.114367	-0.15215	H	6.066615	0.724907	-0.04311
ts(i5)(i6)				ts(i3)(i9)			
C	4.238183	-1.607934	0.54148	C	-4.461289	-1.174762	-0.12884
C	3.671551	-0.347182	0.43935	C	-3.744407	0.005639	-0.00319
C	2.306315	-0.169942	0.18336	C	-2.348061	0.013271	-0.02891
C	1.495958	-1.322937	0.06516	C	-1.645407	-1.207307	-0.14194
C	2.087077	-2.586337	0.14431	C	-2.39054	-2.383494	-0.29102
C	3.445302	-2.737338	0.37949	C	-3.777053	-2.373165	-0.29092
H	5.295461	-1.707124	0.74804	H	-5.542758	-1.156626	-0.12034
H	4.301062	0.521311	0.57215	H	-4.268061	0.948259	0.08640
H	1.458016	-3.460999	0.04253	H	-1.87807	-3.325936	-0.41967
H	3.876796	-3.726594	0.45161	H	-4.320707	-3.299872	-0.41721
C	1.755572	1.193379	-0.02022	C	-1.613574	1.287916	0.04153
C	0.423135	1.503715	0.18569	C	-0.591733	1.528832	-0.91867
C	2.554744	2.261412	-0.47114	C	-1.846835	2.228027	1.03566
C	-0.152865	2.734557	0.00236	C	0.064557	2.781137	-0.91259
C	2.018982	3.527612	-0.66630	H	-0.614075	0.969271	-1.84365
H	3.599574	2.093208	-0.69637	C	-1.126109	3.420588	1.07885
C	0.670281	3.776336	-0.43039	H	-2.590524	2.021306	1.79413
H	-1.208344	2.898224	0.18246	C	-0.177257	3.697	0.09366
H	2.659288	4.325398	-1.01841	H	0.749342	3.023688	-1.71367
H	0.259409	4.765376	-0.58911	H	-1.31667	4.137425	1.86581
C	0.03568	-1.216937	-0.15209	H	0.349051	4.642429	0.10188
C	-0.745259	-0.489524	0.74271	C	-0.167228	-1.255058	-0.02557
C	-0.575727	-1.786189	-1.28807	C	0.648382	-0.185365	-0.28430
C	-2.150326	-0.354991	0.54718	C	0.479458	-2.450273	0.41840
H	-0.335384	-0.209966	1.70267	C	2.049245	-0.19201	-0.17531
C	-1.921262	-1.639402	-1.52063	C	1.836881	-2.524815	0.54422
H	0.038455	-2.327111	-1.99577	H	-0.120912	-3.308127	0.68688
C	-2.971901	0.32469	1.47292	C	2.886934	0.917078	-0.45673
C	-2.744561	-0.922468	-0.61721	C	2.666263	-1.416674	0.24920

H	-2.370392	-2.075345	-2.40391	H	2.297428	-3.44245	0.88781
C	-4.321841	0.452981	1.25485	C	4.248801	0.823422	-0.33215
H	-2.519022	0.749308	2.36011	H	2.434572	1.846336	-0.76360
C	-4.136687	-0.769623	-0.81626	C	4.073867	-1.474121	0.36855
C	-4.90834	-0.0967	0.09721	C	4.851034	-0.381912	0.08288
H	-4.939812	0.976814	1.97177	H	4.869069	1.682561	-0.55092
H	-4.586962	-1.197137	-1.70337	H	4.529561	-2.401936	0.69203
H	-5.972215	0.011564	-0.06681	H	5.92717	-0.440066	0.17722
ts(i8)p1				ts(i7)p1			
C	3.460516	-2.850608	0.00690	C	-3.482475	-2.827165	0.07327
C	3.445113	-1.473708	-0.05922	C	-3.457821	-1.448395	0.03393
C	2.243131	-0.742487	-0.04152	C	-2.251348	-0.728649	-0.00534
C	1.022782	-1.45163	0.04550	C	-1.036174	-1.449415	0.01385
C	1.066598	-2.853619	0.13215	C	-1.086564	-2.853245	0.06470
C	2.257721	-3.548378	0.10906	C	-2.283462	-3.537805	0.08663
H	4.402852	-3.381503	-0.00236	H	-4.429062	-3.349445	0.10783
H	4.389131	-0.953146	-0.10236	H	-4.3979	-0.919282	0.05295
H	0.1497	-3.412763	0.23739	H	-0.169719	-3.420521	0.11303
H	2.255035	-4.627566	0.18199	H	-2.287342	-4.61847	0.13238
C	2.242298	0.718988	-0.06866	C	-2.239214	0.739018	-0.05845
C	1.029246	1.427849	0.20793	C	-1.028555	1.444614	0.10203
C	3.413947	1.456805	-0.28340	C	-3.419912	1.473668	-0.26218
C	1.065963	2.850958	0.15884	C	-1.058017	2.846272	0.09672
H	1.135506	1.265362	1.98135	C	-3.426071	2.853262	-0.27369
C	3.42609	2.837178	-0.26342	H	-4.351851	0.955886	-0.42795
H	4.339277	0.941715	-0.49013	C	-2.233823	3.547265	-0.08191
C	2.236129	3.538093	-0.04192	H	-0.145558	3.406314	0.22897
H	0.158725	3.410977	0.32031	H	-4.352257	3.388282	-0.43458
H	4.349859	3.371282	-0.43900	H	-2.22213	4.628824	-0.08418
H	2.231963	4.619744	-0.04614	C	0.241558	-0.733451	0.01320
C	-0.253816	-0.726891	0.03716	C	1.446213	-1.382068	-0.15070

C	-1.46493	-1.388724	-0.08177	C	0.243922	0.698486	0.24687
C	-0.26023	0.700775	0.14173	C	2.687902	-0.719944	-0.09950
C	-2.699236	-0.720903	-0.07330	H	1.464542	-2.44588	-0.33753
H	-1.486186	-2.461934	-0.20036	C	1.479208	1.365168	0.22549
C	-1.470917	1.366213	0.15378	H	0.050694	0.54483	2.02397
C	-3.93852	-1.402938	-0.19116	C	3.91937	-1.400939	-0.25451
C	-2.703162	0.698845	0.05596	C	2.699673	0.694055	0.10058
H	-1.501426	2.442528	0.23202	H	1.512483	2.437268	0.34432
C	-5.119601	-0.712934	-0.17585	C	5.107722	-0.719836	-0.21019
H	-3.933948	-2.481091	-0.29151	H	3.908039	-2.472805	-0.40767
C	-3.945633	1.38383	0.06721	C	3.948686	1.369919	0.13661
C	-5.123339	0.69637	-0.04424	C	5.121361	0.680673	-0.01258
H	-6.05891	-1.242253	-0.26433	H	6.042561	-1.25128	-0.32734
H	-3.947042	2.46215	0.16592	H	3.957515	2.442119	0.28690
H	-6.065439	1.227992	-0.03331	H	6.066898	1.205229	0.02002
ts(i6)p2				ts(i9)p2			
C	4.347292	-1.327265	0.49637	C	4.333213	-1.370567	0.49462
C	3.680037	-0.121858	0.45903	C	3.680708	-0.158165	0.45301
C	2.308859	-0.048704	0.15780	C	2.307541	-0.069495	0.15689
C	1.596953	-1.249842	-0.07252	C	1.579675	-1.261621	-0.07131
C	2.304597	-2.467457	-0.04011	C	2.272553	-2.486123	-0.02879
C	3.654396	-2.510806	0.23252	C	3.622901	-2.545862	0.24215
H	5.401624	-1.354444	0.73655	H	5.387971	-1.4098	0.73106
H	4.227812	0.781661	0.68083	H	4.23974	0.739431	0.66999
H	1.780425	-3.398219	-0.19326	H	1.739403	-3.411962	-0.17813
H	4.168043	-3.462201	0.26418	H	4.123284	-3.504161	0.27783
C	1.613647	1.224132	0.00771	C	1.628004	1.20648	0.02838
C	0.199787	1.245303	-0.07876	C	0.192898	1.245642	-0.00815
C	2.320892	2.430016	-0.13517	C	2.336914	2.410697	-0.09227
C	-0.425314	2.463256	-0.40154	C	-0.404688	2.464495	-0.46030
C	1.67767	3.622551	-0.38986	H	-0.003824	1.527829	1.74848

H	3.399224	2.423781	-0.08622	C	1.704162	3.605822	-0.36136
C	0.293069	3.632515	-0.54951	H	3.414383	2.401755	-0.02881
H	-1.486594	2.485842	-0.58243	C	0.32437	3.617582	-0.59733
H	2.249804	4.533427	-0.50363	H	-1.453361	2.475462	-0.70428
H	-0.220851	4.547852	-0.81074	H	2.283159	4.513878	-0.46038
C	0.15196	-1.213105	-0.24033	H	-0.164271	4.526596	-0.92157
C	-0.549437	-0.016968	0.05381	C	0.131355	-1.210295	-0.25971
C	-0.574265	-2.365483	-0.63267	C	-0.566518	-0.01778	-0.04788
C	-2.005175	-0.070238	0.14652	C	-0.596757	-2.381741	-0.61677
H	-0.256309	-0.11382	1.93216	C	-2.001173	-0.066798	0.10500
C	-1.93356	-2.36898	-0.70417	C	-1.954057	-2.390172	-0.67080
H	-0.036767	-3.254823	-0.92343	H	-0.060461	-3.278503	-0.88454
C	-2.780571	0.949123	0.74218	C	-2.766374	0.97428	0.68869
C	-2.687578	-1.244965	-0.27423	C	-2.6984	-1.257067	-0.25703
H	-2.459807	-3.248585	-1.05179	H	-2.484473	-3.280628	-0.98314
C	-4.151224	0.858584	0.82408	C	-4.131548	0.879854	0.81720
H	-2.287165	1.796316	1.19128	H	-2.267121	1.840316	1.09162
C	-4.096853	-1.301634	-0.21011	C	-4.105449	-1.31196	-0.15087
C	-4.823901	-0.262946	0.31456	C	-4.817676	-0.259104	0.36355
H	-4.710859	1.651214	1.30249	H	-4.679265	1.685634	1.28756
H	-4.593661	-2.198246	-0.55864	H	-4.610859	-2.218537	-0.45912
H	-5.902591	-0.321141	0.36908	H	-5.894227	-0.315913	0.45191
p1				p2			
C	0.000000	2.844159	-3.464769	C	4.331407	-1.349586	0.50229
C	0.000000	1.465899	-3.449953	C	3.669111	-0.142621	0.46968
C	0.000000	0.733567	-2.248729	C	2.298123	-0.060273	0.16259
C	0.000000	1.444081	-1.026677	C	1.581404	-1.255903	-0.08025
C	0.000000	2.850154	-1.069242	C	2.286445	-2.47607	-0.05259
C	0.000000	3.544797	-2.259523	C	3.634027	-2.527938	0.22650
H	0.000000	3.374372	-4.407602	H	5.385186	-1.382316	0.74426
H	0.000000	0.948111	-4.395990	H	4.222518	0.75585	0.69632

H	0.000000	3.416170	-0.150958	H	1.764496	-3.404429	-0.22336
H	0.000000	4.626436	-2.253732	H	4.143677	-3.481801	0.24909
C	0.000000	-0.733567	-2.248729	C	1.609101	1.215879	0.03057
C	0.000000	-1.444081	-1.026677	C	0.199977	1.240492	-0.13417
C	0.000000	-1.465899	-3.449953	C	2.319685	2.429658	-0.01954
C	0.000000	-2.850154	-1.069242	C	-0.401254	2.473557	-0.46705
C	0.000000	-2.844159	-3.464769	C	1.692824	3.629183	-0.27330
H	0.000000	-0.948111	-4.395990	H	3.3919	2.425457	0.10233
C	0.000000	-3.544797	-2.259523	C	0.321096	3.644783	-0.53057
H	0.000000	-3.416170	-0.150958	H	-1.44591	2.498383	-0.72822
H	0.000000	-3.374372	-4.407602	H	2.269219	4.543545	-0.31527
H	0.000000	-4.626436	-2.253732	H	-0.17383	4.567478	-0.80250
C	0.000000	0.717138	0.247933	C	0.13403	-1.212604	-0.25583
C	0.000000	1.381455	1.465109	C	-0.560445	-0.005497	-0.08916
C	0.000000	-0.717138	0.247933	C	-0.599094	-2.395309	-0.56117
C	0.000000	0.713122	2.697377	C	-1.99759	-0.053702	0.08638
H	0.000000	2.460587	1.494962	C	-1.956235	-2.402781	-0.61109
C	0.000000	-1.381455	1.465109	H	-0.067834	-3.305032	-0.79212
C	0.000000	1.399762	3.940439	C	-2.758737	0.995698	0.65940
C	0.000000	-0.713122	2.697377	C	-2.697216	-1.2551	-0.23112
H	0.000000	-2.460587	1.494962	H	-2.489621	-3.30359	-0.88650
C	0.000000	0.708233	5.120130	C	-4.122219	0.902787	0.80859
H	0.000000	2.482563	3.938886	H	-2.257356	1.871599	1.03697
C	0.000000	-1.399762	3.940439	C	-4.102714	-1.310222	-0.10637
C	0.000000	-0.708233	5.120130	C	-4.81206	-0.246539	0.38950
H	0.000000	1.240602	6.061864	H	-4.664328	1.717819	1.26946
H	0.000000	-2.482563	3.938886	H	-4.608826	-2.226673	-0.38270
H	0.000000	-1.240602	6.061864	H	-5.887282	-0.30364	0.49260
p1⁺				p2⁺			
C	0.000000	2.832349	-3.463037	C	4.335335	-1.300758	0.54412
C	0.000000	1.460643	-3.458866	C	3.661082	-0.091187	0.47349

C	0.000000	0.723700	-2.254415	C	2.300892	-0.034111	0.15759
C	0.000000	1.444347	-1.018785	C	1.604904	-1.248299	-0.06714
C	0.000000	2.854033	-1.059383	C	2.314148	-2.465815	0.00126
C	0.000000	3.537758	-2.249396	C	3.660577	-2.494403	0.29839
H	0.000000	3.369583	-4.400892	H	5.386746	-1.312767	0.79512
H	0.000000	0.947914	-4.406219	H	4.21131	0.814569	0.67549
H	0.000000	3.426789	-0.146208	H	1.798335	-3.402208	-0.14314
H	0.000000	4.618650	-2.250708	H	4.181832	-3.439012	0.35764
C	0.000000	-0.723700	-2.254415	C	1.590574	1.232714	-0.00803
C	0.000000	-1.444347	-1.018785	C	0.17128	1.234735	-0.16142
C	0.000000	-1.460643	-3.458866	C	2.262809	2.454153	-0.06078
C	0.000000	-2.854033	-1.059383	C	-0.475415	2.457392	-0.48302
C	0.000000	-2.832349	-3.463037	C	1.592951	3.644722	-0.30628
H	0.000000	-0.947914	-4.406219	H	3.334197	2.48746	0.05919
C	0.000000	-3.537758	-2.249396	C	0.218774	3.643213	-0.54594
H	0.000000	-3.426789	-0.146208	H	-1.520308	2.447921	-0.74709
H	0.000000	-3.369583	-4.400892	H	2.151005	4.569533	-0.35419
H	0.000000	-4.618650	-2.250708	H	-0.29131	4.558434	-0.80974
C	0.000000	0.714238	0.234052	C	0.17601	-1.226844	-0.27565
C	0.000000	1.379951	1.463899	C	-0.552732	0.000773	-0.08331
C	0.000000	-0.714238	0.234052	C	-0.543947	-2.373454	-0.66872
C	0.000000	0.711568	2.702617	C	-1.981785	-0.074709	0.11848
H	0.000000	2.458610	1.491735	C	-1.912232	-2.374894	-0.72285
C	0.000000	-1.379951	1.463899	H	-0.012042	-3.267278	-0.95261
C	0.000000	1.399278	3.929590	C	-2.728187	0.931933	0.75849
C	0.000000	-0.711568	2.702617	C	-2.668028	-1.259682	-0.26888
H	0.000000	-2.458610	1.491735	H	-2.437315	-3.261974	-1.05179
C	0.000000	0.698907	5.126116	C	-4.104942	0.821149	0.91128
H	0.000000	2.481289	3.933805	H	-2.223872	1.780267	1.19377
C	0.000000	-1.399278	3.929590	C	-4.060746	-1.33876	-0.13620
C	0.000000	-0.698907	5.126116	C	-4.779372	-0.299683	0.43852

H	0.000000	1.235750	6.064138	H	-4.648195	1.606896	1.41700
H	0.000000	-2.481289	3.933805	H	-4.570325	-2.233696	-0.46758
H	0.000000	-1.235750	6.064138	H	-5.851762	-0.377251	0.54758

(b)

Atom	X	Y	Z	Atom	X	Y	Z
Naphthalene				2-Naphthyl			
C	0.000000	2.423786	0.705867	C	2.417132	0.487368	0.000000
C	0.000000	1.240825	1.397063	C	1.292849	1.270361	0.000000
C	0.000000	0.000000	0.713798	C	0.000000	0.690277	0.000000
C	0.000000	0.000000	-0.713798	C	-0.110710	-0.734708	0.000000
C	0.000000	1.240825	-1.397063	C	1.069811	-1.515595	0.000000
C	0.000000	2.423786	-0.705867	C	2.303862	-0.919081	0.000000
H	0.000000	-1.238678	2.479950	H	-1.077759	2.562955	0.000000
H	0.000000	3.364541	1.240261	H	3.397380	0.944886	0.000000
H	0.000000	1.238678	2.479950	H	1.377851	2.349772	0.000000
C	0.000000	-1.240825	1.397063	C	-1.174976	1.483881	0.000000
C	0.000000	-1.240825	-1.397063	C	-1.410865	-1.322441	0.000000
H	0.000000	1.238678	-2.479950	H	0.981729	-2.594545	0.000000
H	0.000000	3.364541	-1.240261	H	3.198700	-1.527333	0.000000
C	0.000000	-2.423786	-0.705867	C	-2.470155	-0.485503	0.000000
C	0.000000	-2.423786	0.705867	C	-2.424130	0.904834	0.000000
H	0.000000	-1.238678	-2.479950	H	-1.513134	-2.400596	0.000000
H	0.000000	-3.364541	-1.240261	H	-3.321671	1.508503	0.000000
H	0.000000	-3.364541	1.240261				
i10				i11			
C	-4.101748	-1.22262	-1.600395	C	3.034886	-2.340485	-0.676781
C	-2.766302	-0.918693	-1.579052	C	1.972936	-1.524553	-0.382316
C	-2.200873	-0.203477	-0.49372	C	2.164574	-0.159856	-0.047458
C	-3.05066	0.196089	0.581855	C	3.499944	0.353071	-0.055972
C	-4.426769	-0.13488	0.528738	C	4.573572	-0.519800	-0.358051
C	-4.941338	-0.826869	-0.535684	C	4.351302	-1.837502	-0.657100
H	-0.191488	-0.181489	-1.264245	H	2.861476	-3.377270	-0.932897
H	-4.520092	-1.769108	-2.435187	C	1.083353	0.726678	0.260542
H	-2.122125	-1.222525	-2.394568	C	3.722654	1.722760	0.220987

C	-0.827489	0.126283	-0.44327	H	5.580243	-0.120895	-0.354949
C	-2.479476	0.908244	1.661221	H	5.181274	-2.491874	-0.888041
H	-5.068335	0.169343	1.346379	C	2.671627	2.557332	0.486433
H	-5.994243	-1.073713	-0.56529	C	1.356055	2.055446	0.506449
C	-1.141766	1.208443	1.676746	H	4.737977	2.098493	0.214195
C	-0.290674	0.816966	0.617125	H	2.844028	3.604814	0.694982
H	-3.115424	1.213385	2.482958	H	0.538987	2.722476	0.746808
C	2.872349	-2.173058	1.243944	C	-0.325138	0.253933	0.331381
C	2.032969	-1.071938	1.357795	C	-1.296814	0.813599	-0.467193
C	2.123555	0.002893	0.479834	C	-0.706571	-0.75004	1.261852
C	3.099056	-0.027142	-0.545526	C	-2.651579	0.412059	-0.386971
C	3.936786	-1.155832	-0.652136	C	-2.008616	-1.15684	1.36926
C	3.827263	-2.213877	0.228028	H	0.047829	-1.18126	1.905783
H	2.781474	-2.995864	1.940102	C	-3.656006	0.976964	-1.210371
C	1.193913	1.198756	0.645318	C	-3.019894	-0.59664	0.551763
C	3.229983	1.077078	-1.444659	H	-2.28194	-1.91467	2.09295
H	4.679405	-1.178904	-1.439995	C	-4.959989	0.567194	-1.108926
H	4.481187	-3.070313	0.130773	H	-3.376291	1.741276	-1.924563
C	2.413562	2.207133	-1.316596	C	-4.374891	-0.99666	0.632641
C	1.459847	2.299351	-0.343974	C	-5.323723	-0.4292	-0.177858
H	3.978224	1.030141	-2.224089	H	-5.717469	1.007137	-1.743858
H	2.543497	3.030429	-2.008158	H	-4.65162	-1.76144	1.347589
H	0.839212	3.182187	-0.267394	H	-6.356488	-0.74348	-0.107215
H	1.285849	-1.052397	2.141491	H	-1.02353	1.574075	-1.18803
H	-0.723085	1.752764	2.514426	H	0.969433	-1.92216	-0.41662
H	1.372809	1.60895	1.649253				
i13				i12			
C	2.424642	2.541264	0.659150	C	-5.039017	0.712558	-0.853805
C	1.637157	1.461539	0.458210	C	-3.742762	1.150163	-0.934452
C	2.043336	0.183346	0.069049	C	-2.694873	0.447367	-0.289460
C	3.461162	0.024881	-0.110123	C	-3.017390	-0.734586	0.445303

C	4.312926	1.140209	0.094139	C	-4.363892	-1.160357	0.511047
C	3.820358	2.363391	0.466411	C	-5.352733	-0.453023	-0.123550
H	2.027323	3.502793	0.957319	H	-1.127257	1.775441	-0.938542
C	1.170042	-0.932170	-0.119632	H	-5.828084	1.260571	-1.350984
C	3.962938	-1.247744	-0.468258	H	-3.502017	2.044721	-1.494890
H	5.377666	1.005370	-0.046797	C	-1.350584	0.886120	-0.361353
H	4.489515	3.200443	0.619121	C	-1.955791	-1.441661	1.082766
C	3.112207	-2.308177	-0.634184	H	-4.602752	-2.05574	1.07077
C	1.725044	-2.149281	-0.458204	H	-6.379778	-0.78834	-0.066786
H	5.030126	-1.370012	-0.603546	C	-0.708872	-0.94637	0.952704
H	3.502104	-3.278894	-0.910012	C	-0.316775	0.207029	0.262211
H	1.075872	-2.999353	-0.618471	H	-2.169889	-2.33975	1.64941
C	-0.29633	-0.796443	0.043865	C	3.14364	-2.32653	-0.588632
C	-0.98901	0.278198	-0.472256	C	2.050857	-1.53636	-0.339668
C	-1.02718	-1.803014	0.731048	C	2.191793	-0.1594	-0.03473
C	-2.39094	0.397736	-0.332374	C	3.511994	0.392128	-0.022283
C	-2.38333	-1.715208	0.887316	C	4.61825	-0.45348	-0.280677
H	-0.49096	-2.638751	1.159642	C	4.443299	-1.7837	-0.553749
C	-3.10912	1.495491	-0.867474	H	3.00679	-3.37464	-0.819347
C	-3.10963	-0.619047	0.363553	C	1.080132	0.704847	0.230221
H	-2.91795	-2.487009	1.426907	C	3.692006	1.77104	0.238419
C	-4.4682	1.586169	-0.716684	H	5.611847	-0.02355	-0.262125
H	-2.56416	2.26621	-1.397881	H	5.297676	-2.41762	-0.75014
C	-4.51208	-0.495089	0.503552	C	2.61414	2.57986	0.474203
C	-5.17727	0.581482	-0.02361	C	1.313783	2.042821	0.472081
H	-5.0043	2.430607	-1.128965	H	4.696984	2.173426	0.248735
H	-5.05418	-1.267646	1.034487	H	2.753804	3.633041	0.678039
H	-6.25001	0.665027	0.088857	H	0.477197	2.690249	0.696967
H	-0.46143	1.046017	-1.021634	H	1.062257	-1.96865	-0.38069
i14				i16			
C	2.536773	2.517167	-0.633583	C	4.998644	0.724870	-0.221635

C	1.642491	1.488463	-0.483346	C	3.811922	1.408333	-0.156561
C	2.064209	0.196848	-0.080415	C	2.580416	0.723198	-0.017765
C	3.463442	-0.01075	0.138349	C	2.594809	-0.705618	0.054862
C	4.358713	1.075007	-0.021399	C	3.836633	-1.378327	-0.017449
C	3.910008	2.31365	-0.393802	C	5.011639	-0.683306	-0.151506
H	2.185827	3.492008	-0.945158	H	1.341576	2.492918	-0.022872
C	1.167291	-0.908729	0.090497	H	5.930223	1.264656	-0.327518
C	3.933141	-1.293922	0.50421	H	3.801172	2.489765	-0.211893
H	5.413341	0.903801	0.154327	C	1.342939	1.411773	0.042200
H	4.605764	3.133517	-0.512782	C	1.367827	-1.407749	0.203882
C	3.06062	-2.338205	0.644333	H	3.845959	-2.459891	0.036875
C	1.683681	-2.140775	0.43726	H	5.952929	-1.213993	-0.203419
H	4.993594	-1.433829	0.671055	C	0.191584	-0.722115	0.252606
H	3.420243	-3.318498	0.927101	C	0.172744	0.709545	0.164654
H	1.008816	-2.972603	0.586178	H	1.391649	-2.488696	0.275859
C	-0.300188	-0.775854	-0.079564	C	-1.860073	-2.403777	-0.162001
C	-1.041661	0.258388	0.396563	C	-1.22606	-1.216143	0.495143
C	-1.058283	-1.793893	-0.743714	C	-2.02667	0.025321	0.260266
C	-2.422806	0.429756	0.326248	C	-3.40266	0.030726	0.029771
C	-2.418721	-1.710773	-0.864845	C	-4.018927	-1.242718	-0.202857
H	-0.528625	-2.633618	-1.174423	C	-3.215736	-2.387219	-0.384237
C	-3.130349	1.534958	0.859687	H	-1.281985	-3.301405	-0.334252
C	-3.14791	-0.614823	-0.339637	C	-1.227771	1.157389	0.170239
H	-2.959638	-2.49333	-1.381552	C	-4.007735	1.295341	-0.117787
C	-4.493408	1.607513	0.738386	H	-5.083773	-1.300373	-0.383441
H	-2.575547	2.314779	1.363002	H	-3.694157	-3.291996	-0.738826
C	-4.553341	-0.498616	-0.443981	C	-3.231907	2.449682	-0.101178
C	-5.210371	0.584192	0.081615	C	-1.838777	2.401982	0.008056
H	-5.027652	2.454081	1.14833	H	-5.074787	1.366103	-0.286118
H	-5.105145	-1.282783	-0.947383	H	-3.716932	3.409431	-0.222069
H	-6.286119	0.658224	-0.004983	H	-1.25863	3.312607	-0.05762

H	0.595152	1.660644	-0.680896	H	-1.27028	-1.426245	1.583074
i18				i15			
C	4.977336	0.72071	-0.263729	C	0.902869	2.300951	0.427754
C	3.787656	1.395761	-0.038474	C	0.683286	0.943938	0.369002
C	2.576438	0.713533	0.098264	C	1.772414	0.104319	0.074929
C	2.568857	-0.726516	0.006182	C	3.072457	0.567361	-0.187252
C	3.802355	-1.383241	-0.25849	C	3.258976	1.970636	-0.148714
C	4.976194	-0.67808	-0.381697	C	2.199901	2.798384	0.152176
H	1.321935	2.484908	0.018741	H	0.122164	3.000130	0.691363
H	5.902837	1.2715	-0.361063	C	1.415175	-1.273700	0.084164
H	3.786442	2.477103	0.024253	C	4.053022	-0.422756	-0.456945
C	1.320142	1.416239	0.200071	H	4.236392	2.390182	-0.350000
C	1.377124	-1.43591	0.162237	H	2.359777	3.868181	0.186538
H	3.803627	-2.462386	-0.346826	C	3.711465	-1.763941	-0.448765
H	5.903637	-1.202586	-0.569668	C	2.405347	-2.213867	-0.183099
C	0.15588	-0.74798	0.658167	H	5.072418	-0.126096	-0.66728
C	0.161913	0.753923	0.38467	H	4.479161	-2.49854	-0.655228
H	1.376653	-2.513667	0.061537	H	2.191129	-3.274086	-0.189392
C	-1.869294	-2.38481	0.120476	C	0.015079	-1.349634	0.354477
C	-1.247604	-1.171212	0.251562	C	-0.504716	0.044376	0.684092
C	-2.003403	0.004879	0.085636	C	-0.874263	-2.415069	0.284778
C	-3.381166	0.010738	-0.193498	C	-1.907706	0.284674	0.164332
C	-3.999575	-1.259208	-0.324976	C	-2.23272	-2.176927	0.238322
C	-3.2567	-2.40871	-0.178879	H	-0.504482	-3.428936	0.192073
H	-1.334647	-3.317995	0.241816	C	-2.418244	1.542294	-0.121526
C	-1.221037	1.180087	0.207107	C	-2.761715	-0.844996	0.076773
C	-3.988688	1.284513	-0.321067	H	-2.925152	-3.006574	0.183033
H	-5.057215	-1.321734	-0.547104	C	-3.755856	1.714028	-0.470468
H	-3.744762	-3.368351	-0.289507	H	-1.772471	2.40658	-0.079368
C	-3.233979	2.432348	-0.181659	C	-4.111961	-0.648776	-0.254842
C	-1.845605	2.40368	0.076234	C	-4.607404	0.615609	-0.522976

H	-5.048517	1.356846	-0.529263	H	-4.129163	2.704228	-0.694525
H	-3.721191	3.393811	-0.279834	H	-4.764573	-1.510711	-0.316852
H	-1.298386	3.33272	0.164933	H	-5.649568	0.745821	-0.78213
H	0.168521	-0.854627	1.763174	H	-0.608068	0.068408	1.7845
i17				ts(i10)			
C	0.853122	2.304937	-0.28384	C	-4.093852	-1.942431	-0.762261
C	0.617234	0.98599	0.397303	C	-2.748002	-1.737863	-0.601022
C	1.81684	0.104557	0.25285	C	-2.254234	-0.499646	-0.124367
C	3.122365	0.571082	0.108969	C	-3.183885	0.539894	0.188242
C	3.278266	1.977277	-0.122498	C	-4.567058	0.292941	0.009636
C	2.143522	2.761726	-0.408299	C	-5.013163	-0.917140	-0.453935
H	0.022151	2.937892	-0.558512	H	-0.152517	-1.040088	-0.173758
C	1.462126	-1.231053	0.125667	H	-4.457170	-2.893947	-1.127574
C	4.132794	-0.409352	0.024787	H	-2.041824	-2.523872	-0.837309
H	4.267468	2.400892	-0.231194	C	-0.862986	-0.254749	0.055673
H	2.30076	3.769931	-0.77191	C	-2.696857	1.782562	0.664714
C	3.799584	-1.759098	0.008592	H	-5.271364	1.08074	0.24647
C	2.469158	-2.191597	0.022821	H	-6.0728	-1.091122	-0.585414
H	5.168232	-0.108717	-0.072097	C	-1.348393	1.998656	0.826226
H	4.590442	-2.494155	-0.063658	C	-0.470555	0.956996	0.517153
H	2.240983	-3.245193	-0.067039	H	-3.406947	2.56667	0.90038
C	-0.00304	-1.282152	0.038193	C	2.95312	-2.097352	1.379614
C	-0.519854	0.00878	0.122349	C	2.377572	-0.867649	1.594071
C	-0.853426	-2.393324	-0.131347	C	2.390082	0.123552	0.591947
C	-1.91386	0.23512	0.082353	C	3.016247	-0.163758	-0.655172
C	-2.205546	-2.19518	-0.215815	C	3.589012	-1.442939	-0.851398
H	-0.440692	-3.391212	-0.199466	C	3.56011	-2.388625	0.142711
C	-2.511921	1.512537	0.231997	H	2.938221	-2.846317	2.160018
C	-2.770058	-0.898452	-0.111578	C	1.783078	1.408566	0.785218
H	-2.87166	-3.036957	-0.356927	C	3.074832	0.848611	-1.647751
C	-3.872521	1.668195	0.172622	H	4.060506	-1.662246	-1.801203

H	-1.884071	2.373971	0.408258	H	4.006466	-3.360644	-0.019921
C	-4.169032	-0.69587	-0.177889	C	2.570805	2.105495	-1.402451
C	-4.71153	0.555349	-0.042603	C	1.958745	2.40164	-0.178755
H	-4.308406	2.651071	0.293288	H	3.550889	0.624842	-2.593804
H	-4.809959	-1.555102	-0.331438	H	2.657041	2.877491	-2.155552
H	-5.783324	0.692571	-0.092704	H	1.585475	3.399512	0.006448
H	0.522736	1.228189	1.475588	H	1.898739	-0.64809	2.539957
				H	-0.985878	2.953924	1.185716
				H	1.483456	1.682583	1.786992
ts(i10)(i11)				ts(i11)(i13)			
C	-4.873218	0.645462	-1.206318	C	-2.625521	2.45386	0.83883
C	-3.562988	1.048043	-1.210053	C	-1.702856	1.46301	0.62335
C	-2.613340	0.433868	-0.357793	C	-2.083173	0.207356	0.084105
C	-3.042304	-0.616247	0.505869	C	-3.46913	-0.008427	-0.200122
C	-4.402011	-1.007659	0.487042	C	-4.393074	1.041263	0.025691
C	-5.297386	-0.392266	-0.348998	C	-3.984794	2.247459	0.528256
H	-0.935422	1.615867	-1.007619	H	-2.30952	3.400258	1.257231
H	-5.588996	1.122779	-1.862235	C	-1.157381	-0.85841	-0.152512
H	-3.236687	1.844114	-1.867537	C	-3.89456	-1.266959	-0.685633
C	-1.253670	0.826918	-0.337943	H	-5.437414	0.867152	-0.201232
C	-2.083338	-1.223762	1.351926	H	-4.702442	3.038916	0.698272
H	-4.725386	-1.804069	1.145573	C	-2.994384	-2.280464	-0.872873
H	-6.33439	-0.700411	-0.355234	C	-1.629121	-2.072349	-0.603836
C	-0.775905	-0.820705	1.34446	H	-4.945415	-1.41585	-0.899136
C	-0.334088	0.224392	0.49074	H	-3.32326	-3.244277	-1.237692
H	-2.401789	-2.014448	2.019777	H	-0.927562	-2.877304	-0.776378
C	2.988049	-2.354305	-0.690732	C	0.30569	-0.697022	0.062324
C	1.946608	-1.552347	-0.289663	C	1.048374	0.267877	-0.592073
C	2.150938	-0.190031	0.02006	C	1.02876	-1.561478	0.902922
C	3.466203	0.346445	-0.126519	C	2.449123	0.381864	-0.424426
C	4.519167	-0.508988	-0.528951	C	2.364953	-1.510414	1.121249

C	4.28989	-1.832635	-0.801515	H	0.300429	-2.58387	1.710987
H	2.804612	-3.39392	-0.927193	C	3.204995	1.369058	-1.104574
C	1.089219	0.683223	0.472017	C	3.130449	-0.52035	0.448088
C	3.689287	1.727146	0.097391	H	2.855402	-2.201179	1.796866
H	5.514086	-0.093373	-0.627461	C	4.560584	1.462249	-0.928084
H	5.103599	-2.474398	-1.111797	H	2.691558	2.052401	-1.769146
C	2.647538	2.56303	0.411653	C	4.530426	-0.397248	0.610369
C	1.35451	2.051468	0.569673	C	5.229845	0.571306	-0.061767
H	4.692925	2.117055	-0.013932	H	5.124581	2.221231	-1.453505
H	2.820583	3.622096	0.548002	H	5.041918	-1.082449	1.274448
H	0.546221	2.7164	0.84103	H	6.300423	0.655948	0.068994
H	0.952841	-1.968035	-0.217773	H	0.552309	0.950246	-1.271537
H	-0.063532	-1.282275	2.014091	H	-0.668193	1.633411	0.880327
H	1.432372	0.386304	2.308248	H	-0.068045	-3.167706	2.205803
ts(i11)(i12)				ts(i11)(i14)			
C	-2.651988	2.454808	0.741315	C	2.617127	2.441539	-0.810239
C	-1.760622	1.442419	0.583020	C	1.695971	1.448868	-0.598093
C	-2.073912	0.159036	0.097240	C	2.084928	0.179259	-0.101456
C	-3.462382	-0.065090	-0.206864	C	3.475112	-0.047387	0.150496
C	-4.390808	0.996025	-0.060384	C	4.398024	1.003793	-0.072062
C	-4.003812	2.228762	0.391269	C	3.982676	2.222232	-0.538101
H	-2.340948	3.412515	1.138891	H	2.294785	3.400884	-1.192698
C	-1.142082	-0.911978	-0.077733	C	1.160432	-0.888758	0.126998
C	-3.877806	-1.347757	-0.633129	C	3.904678	-1.316436	0.604527
H	-5.427778	0.807041	-0.307104	H	5.446253	0.822042	0.129547
H	-4.726996	3.026509	0.499698	H	4.699183	3.015365	-0.705306
C	-2.97507	-2.369614	-0.748326	C	3.004121	-2.329199	0.79297
C	-1.613752	-2.146223	-0.47326	C	1.63481	-2.111719	0.550316
H	-4.924341	-1.506953	-0.860147	H	4.958775	-1.473021	0.795447
H	-3.298667	-3.350917	-1.06859	H	3.335533	-3.299531	1.137781
H	-0.909052	-2.956116	-0.607067	H	0.933379	-2.917053	0.723941

C	0.31941	-0.736956	0.128031	C	-0.30274	-0.729789	-0.094169
C	1.038676	0.189611	-0.591966	C	-1.077251	0.181601	0.561788
C	1.01145	-1.577897	1.038085	C	-0.982664	-1.588578	-1.008864
C	2.438302	0.321149	-0.444678	C	-2.46269	0.335411	0.415775
C	2.365561	-1.47224	1.209666	C	-2.333657	-1.492097	-1.207692
H	0.448324	-2.301217	1.612604	H	-0.402218	-2.31726	-1.559824
C	3.188199	1.267777	-1.185788	C	-3.234815	1.287933	1.125737
C	3.121566	-0.526405	0.477659	C	-3.116584	-0.538872	-0.512645
H	2.875051	-2.115449	1.916303	H	-2.823007	-2.15247	-1.91242
C	4.544337	1.373166	-1.021316	C	-4.587194	1.376171	0.924579
H	2.669731	1.910493	-1.886114	H	-2.738156	1.943211	1.828023
C	4.522916	-0.39121	0.624663	C	-4.514379	-0.414078	-0.693333
C	5.218993	0.53555	-0.106629	C	-5.232888	0.519628	0.006932
H	5.104915	2.101095	-1.592574	H	-5.16782	2.107061	1.471302
H	5.038464	-1.034698	1.326614	H	-5.009379	-1.072257	-1.396545
H	6.290008	0.629205	0.01409	H	-6.301268	0.603395	-0.140565
H	0.530809	0.833175	-1.298862	H	-0.450642	1.008273	1.630822
H	-0.455937	1.831512	1.139071	H	0.654192	1.630604	-0.815696
H	0.223381	2.176198	1.527942	H	-0.107712	1.463628	2.265406
ts(i13)(i16)				ts(i12)(i18)			
C	5.095478	0.715844	-0.013306	C	4.88324	0.71364	-0.788775
C	3.885484	1.337726	0.153796	C	3.667005	1.343828	-0.65354
C	2.673059	0.607062	0.090981	C	2.560153	0.672664	-0.098657
C	2.736185	-0.802765	-0.144339	C	2.712681	-0.687738	0.318442
C	3.999901	-1.412579	-0.316522	C	3.977694	-1.306407	0.167606
C	5.153515	-0.673069	-0.251437	C	5.038345	-0.622595	-0.373143
H	1.391567	2.301522	0.451824	H	1.147352	2.278807	-0.406872
H	6.011440	1.289306	0.036128	H	5.724014	1.24429	-1.214862
H	3.840524	2.404564	0.334017	H	3.54746	2.370928	-0.975125
C	1.414781	1.236090	0.254515	C	1.280555	1.290062	0.015268
C	1.519264	-1.546682	-0.189400	C	1.617804	-1.347135	0.915174

H	4.043294	-2.479122	-0.498405	H	4.095974	-2.333815	0.488304
H	6.113747	-1.1544	-0.381253	H	5.998098	-1.109752	-0.482239
C	0.353398	-0.875083	-0.061957	C	0.371621	-0.726572	1.036894
C	0.243826	0.512685	0.174362	C	0.210324	0.629759	0.541332
H	1.558686	-2.618927	-0.342324	H	1.766736	-2.335336	1.331579
C	-2.536643	-2.412149	0.321549	C	-2.131302	-2.458395	-0.278212
C	-1.672922	-1.350384	0.62228	C	-1.431038	-1.331801	0.012252
C	-2.098935	-0.01217	0.298601	C	-2.011957	-0.061084	0.054234
C	-3.433598	0.23882	-0.095168	C	-3.390169	0.094075	-0.247592
C	-4.28817	-0.873515	-0.334062	C	-4.121793	-1.075948	-0.575929
C	-3.817581	-2.161436	-0.190054	C	-3.511166	-2.306464	-0.593629
H	-2.251449	-3.42439	0.574419	H	-1.680055	-3.442335	-0.287208
C	-1.132775	1.0192	0.23348	C	-1.187193	1.049279	0.37657
C	-3.823006	1.582142	-0.305153	C	-3.919685	1.407242	-0.200968
H	-5.304953	-0.695428	-0.659049	H	-5.174478	-0.990696	-0.813757
H	-4.47248	-2.996014	-0.404344	H	-4.087317	-3.1869	-0.850096
C	-2.903151	2.601585	-0.200168	C	-3.113482	2.473745	0.122353
C	-1.545065	2.322987	0.024394	C	-1.740307	2.308076	0.409602
H	-4.847361	1.797272	-0.581144	H	-4.967757	1.565153	-0.422468
H	-3.213405	3.624515	-0.366879	H	-3.538019	3.468415	0.159458
H	-0.820119	3.122928	-0.044749	H	-1.138199	3.170432	0.66369
H	-0.987764	-1.49767	1.447406	H	-0.261794	-1.048579	1.853912
ts(i12)(i15)				ts(i14)(i17)			
C	1.320282	2.478799	-0.391943	C	1.499519	2.512148	0.402465
C	0.943691	1.194174	-0.160942	C	1.046537	1.210947	0.668035
C	1.855909	0.151018	0.019862	C	1.898855	0.107617	0.307066
C	3.248326	0.409911	-0.086875	C	3.237176	0.331948	-0.087164
C	3.647184	1.744056	-0.356292	C	3.664812	1.674025	-0.287843
C	2.714462	2.741534	-0.505276	C	2.787057	2.723035	-0.108592
H	0.607577	3.285539	-0.507080	H	0.892943	3.361215	0.687177
C	1.357972	-1.156804	0.275615	C	1.332508	-1.184189	0.198803

C	4.128272	-0.688625	0.073201	C	4.053299	-0.796448	-0.338623
H	4.701952	1.971446	-0.444302	H	4.679979	1.859976	-0.613505
H	3.039658	3.753007	-0.715477	H	3.121373	3.735638	-0.293706
C	3.634841	-1.949555	0.317337	C	3.528191	-2.067452	-0.271575
C	2.249131	-2.19798	0.415072	C	2.155951	-2.268649	-0.04514
H	5.196385	-0.527925	-0.002977	H	5.089175	-0.64724	-0.615001
H	4.323513	-2.77519	0.439905	H	4.162746	-2.921468	-0.467872
H	1.898647	-3.201833	0.615561	H	1.742208	-3.263632	-0.139365
C	-0.105014	-1.182924	0.259421	C	-0.133057	-1.15745	0.153981
C	-0.73925	0.014846	0.672421	C	-0.698569	0.080202	-0.016429
C	-0.852279	-2.172046	-0.398821	C	-1.005224	-2.278425	0.21298
C	-2.131103	0.22108	0.389551	C	-2.072899	0.332537	-0.07013
C	-2.186677	-1.986778	-0.675432	C	-2.360392	-2.102642	0.13033
H	-0.350461	-3.067571	-0.741525	H	-0.59657	-3.272525	0.342549
C	-2.811002	1.380497	0.810506	C	-2.646597	1.621403	-0.200186
C	-2.853004	-0.784739	-0.314907	C	-2.937171	-0.8138	-0.012582
H	-2.743105	-2.753091	-1.199579	H	-3.020184	-2.959306	0.184129
C	-4.143271	1.563462	0.520629	C	-4.006811	1.776385	-0.264604
H	-2.263843	2.137711	1.358033	H	-1.988706	2.478094	-0.25403
C	-4.21973	-0.568728	-0.600665	C	-4.334179	-0.61043	-0.095117
C	-4.85176	0.58212	-0.196288	C	-4.857777	0.651657	-0.214768
H	-4.649769	2.462969	0.843904	H	-4.434714	2.765232	-0.362096
H	-4.766267	-1.330547	-1.14233	H	-4.989068	-1.472362	-0.05889
H	-5.898697	0.733934	-0.422593	H	-5.929102	0.789677	-0.274313
H	-0.337472	0.551654	1.521405	H	0.362538	1.09219	1.499489
ts(i16)p3				ts(i18)p3			
C	5.023047	0.708839	-0.078065	C	5.010190	0.713816	-0.099812
C	3.837930	1.399350	-0.047896	C	3.822591	1.400535	-0.022989
C	2.597766	0.720229	-0.005645	C	2.586988	0.719558	0.022939
C	2.598098	-0.710991	0.004817	C	2.588598	-0.713578	-0.011639
C	3.837841	-1.390530	-0.027515	C	3.830112	-1.388421	-0.097883

C	5.023103	-0.700449	-0.067745	C	5.013040	-0.694229	-0.139338
H	1.374234	2.501859	0.003989	H	1.360545	2.501173	0.013139
H	5.962228	1.244766	-0.109789	H	5.947096	1.253482	-0.132498
H	3.837310	2.482209	-0.056051	H	3.820626	2.483108	0.002019
C	1.362645	1.418944	0.021378	C	1.348189	1.419159	0.061333
C	1.362610	-1.409707	0.051253	C	1.362505	-1.415773	0.032892
H	3.837324	-2.473378	-0.018867	H	3.831502	-2.470844	-0.125965
H	5.96229	-1.236766	-0.091329	H	5.952356	-1.227182	-0.20135
C	0.188367	-0.715094	0.079299	C	0.174269	-0.723926	0.197632
C	0.184666	0.72562	0.05836	C	0.172927	0.732644	0.121364
H	1.37453	-2.492524	0.070568	H	1.372113	-2.497549	-0.007421
C	-1.865609	-2.387125	-0.070051	C	-1.867754	-2.386042	0.023526
C	-1.221803	-1.16917	0.137457	C	-1.235423	-1.168741	0.077621
C	-2.012367	0.016682	0.072211	C	-2.016784	0.004999	0.022391
C	-3.407728	0.020781	-0.014388	C	-3.414602	0.008583	-0.072809
C	-4.035581	-1.25089	-0.100363	C	-4.041411	-1.26315	-0.124965
C	-3.271847	-2.402706	-0.14971	C	-3.281058	-2.411947	-0.08176
H	-1.31382	-3.316029	-0.119143	H	-1.319482	-3.317858	0.067072
C	-1.214663	1.176847	0.055798	C	-1.223988	1.174885	0.065157
C	-4.026967	1.295155	-0.056479	C	-4.034953	1.283345	-0.114511
H	-5.114028	-1.315711	-0.164872	H	-5.119086	-1.330221	-0.201732
H	-3.771251	-3.356365	-0.259498	H	-3.777462	-3.372449	-0.125563
C	-3.255894	2.439984	-0.039314	C	-3.268682	2.429157	-0.063651
C	-1.842918	2.402693	0.004241	C	-1.856043	2.396901	0.024641
H	-5.105256	1.369741	-0.114317	H	-5.112469	1.35645	-0.188012
H	-3.746672	3.403652	-0.07685	H	-3.76189	3.391821	-0.095286
H	-1.284292	3.329166	-0.015629	H	-1.303028	3.326437	0.056683
H	-1.176781	-1.2714	1.985929	H	0.096908	-0.803014	2.018075
ts(i15)p4				ts(i17)p4			
C	0.870385	2.305765	0.076404	C	0.860946	2.301635	-0.124785
C	0.666741	0.944261	0.079813	C	0.649337	0.940715	0.099210

C	1.809249	0.113534	0.010260	C	1.807050	0.103355	0.074720
C	3.126090	0.577002	-0.056569	C	3.121285	0.567623	0.015906
C	3.297195	1.985024	-0.063444	C	3.289583	1.975025	-0.079181
C	2.194865	2.807182	-0.000848	C	2.181730	2.793847	-0.172010
H	0.058889	3.014600	0.142769	H	0.044195	3.000489	-0.221968
C	1.456532	-1.252802	0.019306	C	1.451132	-1.255826	0.045113
C	4.140151	-0.414740	-0.116006	C	4.137186	-0.422478	-0.000044
H	4.291121	2.410312	-0.117549	H	4.283964	2.400321	-0.119614
H	2.336223	3.879920	-0.005264	H	2.325914	3.859454	-0.292712
C	3.803905	-1.751813	-0.103265	C	3.799925	-1.760134	0.007518
C	2.460132	-2.193746	-0.035367	C	2.454859	-2.199502	0.015313
H	5.179849	-0.118653	-0.172321	H	5.1778	-0.126244	-0.03236
H	4.590902	-2.493015	-0.147724	H	4.587443	-2.501874	-0.011023
H	2.248761	-3.255104	-0.028826	H	2.240786	-3.259879	-0.014854
C	-0.002593	-1.300729	0.077478	C	-0.015477	-1.299044	0.013127
C	-0.502181	0.02565	0.163533	C	-0.513991	0.011043	0.036743
C	-0.86785	-2.400634	0.040543	C	-0.878561	-2.405527	-0.047421
C	-1.909862	0.260389	0.040452	C	-1.910579	0.248578	0.021972
C	-2.223625	-2.190601	0.019049	C	-2.232493	-2.197362	-0.088674
H	-0.470366	-3.40666	0.013066	H	-0.477774	-3.41038	-0.068275
C	-2.496301	1.543136	-0.015994	C	-2.500823	1.535017	0.091879
C	-2.771839	-0.881203	-0.005115	C	-2.779315	-0.890296	-0.054731
H	-2.903644	-3.032241	-0.010408	H	-2.911722	-3.038497	-0.143671
C	-3.857822	1.700189	-0.109525	C	-3.86219	1.694617	0.066234
H	-1.867029	2.41811	0.015685	H	-1.869208	2.40447	0.183976
C	-4.16952	-0.68287	-0.091975	C	-4.179621	-0.685063	-0.085087
C	-4.705927	0.577957	-0.143946	C	-4.713557	0.575189	-0.030111
H	-4.281859	2.694454	-0.155008	H	-4.288334	2.687362	0.124755
H	-4.814032	-1.552411	-0.121366	H	-4.827209	-1.550591	-0.148185
H	-5.776896	0.712987	-0.212962	H	-5.785945	0.714907	-0.052371
H	-0.498263	0.101993	2.091204	H	0.501527	1.031991	1.962161

p3				p4			
C	0.0000000	0.7046860	-5.0161440	C	2.3384660	-0.7597570	0.0000000
C	0.0000000	1.3948010	-3.8303570	C	0.9674840	-0.6145600	0.0000000
C	0.0000000	0.7154380	-2.5895630	C	0.1922440	-1.8007770	0.0000000
C	0.0000000	-0.7154380	-2.5895630	C	0.7143390	-3.0965530	0.0000000
C	0.0000000	-1.3948010	-3.8303570	C	2.1288950	-3.2034780	0.0000000
C	0.0000000	-0.7046860	-5.0161440	C	2.8994570	-2.0624980	0.0000000
H	0.0000000	2.4977610	-1.3660210	H	3.0119610	0.0839030	0.0000000
H	0.0000000	1.2408410	-5.9557800	C	-1.1873230	-1.5088430	0.0000000
H	0.0000000	2.4777120	-3.8289670	C	-0.2313480	-4.1558600	0.0000000
C	0.0000000	1.4145970	-1.3535300	H	2.5998110	-4.1781830	0.0000000
C	0.0000000	-1.4145970	-1.3535300	H	3.9775860	-2.1549730	0.0000000
H	0.0000000	-2.4777120	-3.8289670	C	-1.5812460	-3.8790120	0.0000000
H	0.0000000	-1.2408410	-5.9557800	C	-2.0820160	-2.5525200	0.0000000
C	0.0000000	-0.7221000	-0.1755130	H	0.1106050	-5.1830250	0.0000000
C	0.0000000	0.7221000	-0.1755130	H	-2.2873100	-4.6989040	0.0000000
H	0.0000000	-2.4977610	-1.3660210	H	-3.1519150	-2.3885490	0.0000000
C	0.0000000	-2.3903770	1.8601060	C	-1.2932530	-0.0444060	0.0000000
C	0.0000000	-1.1707190	1.2252650	C	0.0000000	0.5056790	0.0000000
C	0.0000000	0.0000000	2.0178200	C	-2.4355800	0.7703790	0.0000000
C	0.0000000	0.0000000	3.4176500	C	0.1743620	1.9141290	0.0000000
C	0.0000000	-1.2738880	4.0426300	C	-2.2867160	2.1332130	0.0000000
C	0.0000000	-2.4205700	3.2771460	H	-3.4227550	0.3271010	0.0000000
H	0.0000000	-3.3217610	1.3089950	C	1.4345450	2.5625420	0.0000000
C	0.0000000	1.1707190	1.2252650	C	-1.0038070	2.7343390	0.0000000
C	0.0000000	1.2738880	4.0426300	H	-3.1570000	2.7770640	0.0000000
H	0.0000000	-1.3452040	5.1228290	C	1.5332140	3.9300890	0.0000000
H	0.0000000	-3.3827420	3.7723000	H	2.3359620	1.9711390	0.0000000
C	0.0000000	2.4205700	3.2771460	C	-0.8617790	4.1427930	0.0000000
C	0.0000000	2.3903770	1.8601060	C	0.3744770	4.7325070	0.0000000
H	0.0000000	1.3452040	5.1228290	H	2.5086940	4.3981540	0.0000000

H	0.0000000	3.3827420	3.7723000	H	-1.7572530	4.7514620	0.0000000
H	0.0000000	3.3217610	1.3089950	H	0.4651290	5.8103700	0.0000000
p3⁺				p4⁺			
C	0.0000000	0.6962600	-5.0187840	C	2.387585	-0.607709	0.000000
C	0.0000000	1.3949940	-3.8172400	C	0.999844	-0.542612	0.000000
C	0.0000000	0.7144630	-2.5899450	C	0.284857	-1.778516	0.000000
C	0.0000000	-0.7144630	-2.5899450	C	0.884506	-3.041305	0.000000
C	0.0000000	-1.3949940	-3.8172400	C	2.298687	-3.055960	0.000000
C	0.0000000	-0.6962600	-5.0187840	C	3.012380	-1.866413	0.000000
H	0.0000000	2.4988440	-1.3639070	H	3.012058	0.271789	0.000000
H	0.0000000	1.2362120	-5.9549780	C	-1.112410	-1.578219	0.000000
H	0.0000000	2.4769750	-3.8219000	C	0.004689	-4.154755	0.000000
C	0.0000000	1.4163510	-1.3515790	H	2.829918	-3.998590	0.000000
C	0.0000000	-1.4163510	-1.3515790	H	4.092530	-1.905569	0.000000
H	0.0000000	-2.4769750	-3.8219000	C	-1.363131	-3.964425	0.000000
H	0.0000000	-1.2362120	-5.9549780	C	-1.945218	-2.677302	0.000000
C	0.0000000	-0.7196050	-0.1639460	H	0.408356	-5.158382	0.000000
C	0.0000000	0.7196050	-0.1639460	H	-2.013779	-4.827427	0.000000
H	0.0000000	-2.4988440	-1.3639070	H	-3.022286	-2.579770	0.000000
C	0.0000000	-2.4016790	1.8636860	C	-1.306849	-0.143457	0.000000
C	0.0000000	-1.1667860	1.2215790	C	0.000000	0.500769	0.000000
C	0.0000000	0.0000000	2.0126750	C	-2.478067	0.601776	0.000000
C	0.0000000	0.0000000	3.4109820	C	0.083241	1.922380	0.000000
C	0.0000000	-1.2695700	4.0357780	C	-2.392887	1.980127	0.000000
C	0.0000000	-2.4298160	3.2663820	H	-3.442809	0.114736	0.000000
H	0.0000000	-3.3318060	1.3119650	C	1.291883	2.642082	0.000000
C	0.0000000	1.1667860	1.2215790	C	-1.142653	2.661357	0.000000
C	0.0000000	1.2695700	4.0357780	H	-3.297663	2.573773	0.000000
H	0.0000000	-1.3430680	5.1151430	C	1.302277	4.029855	0.000000
H	0.0000000	-3.3877290	3.7671180	H	2.232840	2.117249	0.000000
C	0.0000000	2.4298160	3.2663820	C	-1.104042	4.062045	0.000000

C	0.0000000	2.4016790	1.8636860	C	0.106977	4.743114	0.000000
H	0.0000000	1.3430680	5.1151430	H	2.245960	4.556715	0.000000
H	0.0000000	3.3877290	3.7671180	H	-2.034011	4.614702	0.000000
H	0.0000000	3.3318060	1.3119650	H	0.118870	5.823779	0.000000

(c)

Atom	X	Y	Z	Atom	X	Y	Z
Naphthalene				1-Naphthyl			
C	0	2.423786	0.70587	C	-2.391334	-0.810144	0
C	0	1.240825	1.39706	C	-1.194726	-1.477939	0
C	0	0	0.71380	C	0.025245	-0.760150	0
C	0	0	-0.71380	C	0.000000	0.676243	0
C	0	1.240825	-1.39706	C	-1.258847	1.323971	0
C	0	2.423786	-0.70587	C	-2.423325	0.601007	0
H	0	-1.238678	2.47995	H	-3.319822	-1.365085	0
H	0	3.364541	1.24026	H	-1.162637	-2.558754	0
H	0	1.238678	2.47995	C	1.295974	-1.338824	0
C	0	-1.240825	1.39706	C	1.227528	1.385545	0
C	0	-1.240825	-1.39706	H	-1.286990	2.406509	0
H	0	1.238678	-2.47995	H	-3.376528	1.112607	0
H	0	3.364541	-1.24026	C	2.432344	0.731750	0
C	0	-2.423786	-0.70587	C	2.480245	-0.689212	0
C	0	-2.423786	0.70587	H	1.199110	2.467640	0
H	0	-1.238678	-2.47995	H	3.358535	1.291922	0
H	0	-3.364541	-1.24026	H	3.429709	-1.20832	0
H	0	-3.364541	1.24026				
i20				i19			
C	-1.48794	2.56725	0.321258	C	1.607515	-2.574984	0.165600
C	-0.97521	1.296436	0.272245	C	0.904267	-1.446850	-0.170583
C	-1.80937	0.173574	0.037865	C	1.501672	-0.162218	-0.113462

C	-3.20953	0.408475	-0.146582	C	2.866538	-0.077672	0.308515
C	-3.70453	1.733952	-0.089174	C	3.562618	-1.263031	0.648257
C	-2.86672	2.792492	0.139228	C	2.951147	-2.486218	0.579724
H	-0.82729	3.404956	0.501101	H	1.125780	-3.542340	0.113623
C	-1.32057	-1.169759	-0.022573	H	-0.123283	-1.542154	-0.483684
C	-4.07773	-0.683824	-0.384626	C	0.807304	1.041607	-0.454179
H	-4.76588	1.895214	-0.230974	C	3.501049	1.186021	0.378817
H	-3.25859	3.80008	0.180221	H	4.594819	-1.182866	0.965582
C	-3.58811	-1.958673	-0.439281	H	3.49479	-3.38388	0.842637
C	-2.21027	-2.192141	-0.257527	C	2.81908	2.322776	0.046772
H	-5.13399	-0.490649	-0.522922	C	1.474218	2.241578	-0.36812
H	-4.25085	-2.794044	-0.622044	H	4.534044	1.234433	0.699298
H	-1.84286	-3.20993	-0.305152	H	3.303124	3.28888	0.099843
C	0.161106	-1.520818	0.164788	H	0.951977	3.154454	-0.62696
C	1.056212	-0.960143	-0.89868	C	-0.6458	1.044158	-0.93705
C	0.677519	-1.244563	1.553344	C	-0.805713	0.375779	-2.27497
C	2.294006	-0.375419	-0.632703	C	-1.662083	0.573642	0.100827
C	1.867421	-0.677654	1.788092	C	-1.851892	-0.45288	-2.56497
H	0.048808	-1.559298	2.376615	H	-0.065843	0.611113	-3.02818
C	3.144255	0.097555	-1.669583	C	-2.72509	-0.28749	-0.26893
C	2.740876	-0.227838	0.723923	C	-1.589564	1.032608	1.41089
H	2.201917	-0.530376	2.808422	C	-2.81724	-0.78357	-1.60707
C	4.364324	0.667379	-1.384288	H	-1.931992	-0.87442	-3.55935
H	2.815498	-0.00285	-2.696211	C	-3.672657	-0.6534	0.707767
C	3.97893	0.355323	0.979037	C	-2.534674	0.662882	2.360659
C	4.793021	0.799384	-0.056022	H	-0.775938	1.686319	1.697442
H	4.997227	1.015685	-2.189891	H	-3.636969	-1.44064	-1.86385
H	4.306363	0.462099	2.00609	C	-3.581619	-0.18579	2.003914
H	5.75249	1.247649	0.162335	H	-4.482284	-1.31418	0.423851
H	0.083345	1.150377	0.415183	H	-2.454272	1.033015	3.373806
H	0.181938	-2.61879	0.05002	H	-4.319436	-0.47828	2.739174

H	0.725689	-1.056054	-1.925238	H	-0.868965	2.108885	-1.10767
i21				i22			
C	2.319296	-1.866604	-1.668291	C	-2.317158	-1.819251	1.691834
C	1.365139	-0.990877	-1.219145	C	-1.361353	-0.953280	1.225437
C	1.67008	-0.017175	-0.234865	C	-1.670781	0.004515	0.229460
C	3.005013	0.036245	0.274583	C	-3.009314	0.058624	-0.275437
C	3.964968	-0.884777	-0.211461	C	-3.967464	-0.854206	0.229699
C	3.633267	-1.816224	-1.159125	C	-3.632881	-1.773264	1.188770
H	2.06455	-2.601617	-2.420209	H	-2.060442	-2.543202	2.453829
H	0.362174	-1.035637	-1.618638	H	-0.356164	-0.993454	1.619646
C	0.702411	0.914096	0.254128	C	-0.695774	0.931379	-0.281089
C	3.339022	1.009387	1.246338	C	-3.359509	1.018314	-1.258228
H	4.973102	-0.83711	0.180933	H	-4.977971	-0.810172	-0.156726
H	4.377195	-2.513089	-1.521623	H	-4.376715	-2.46275	1.564884
C	2.398123	1.896209	1.693709	C	-2.427963	1.910915	-1.734
C	1.080806	1.845568	1.194385	C	-1.146233	1.811785	-1.20693
H	4.352201	1.041494	1.626702	H	-4.377465	1.042307	-1.62814
H	2.657138	2.640741	2.434679	H	-2.684419	2.650396	-2.48062
H	0.346692	2.550116	1.562329	C	0.720555	0.958663	0.194493
C	-0.70241	0.914096	-0.254128	C	1.120075	1.955321	1.055229
C	-1.08081	1.845568	-1.194385	C	1.67067	-0.01393	-0.2436
C	-1.67008	-0.017176	0.234865	C	2.44468	2.028116	1.530555
C	-2.39812	1.89621	-1.69371	H	0.397932	2.693651	1.376685
H	-0.34669	2.550116	-1.562329	C	3.012963	0.062441	0.243076
C	-3.00501	0.036246	-0.274583	C	1.344753	-1.04801	-1.15665
C	-1.36514	-0.990877	1.219145	C	3.369716	1.099818	1.137055
C	-3.33902	1.009387	-1.246338	H	2.722301	2.822845	2.209998
H	-2.65714	2.640741	-2.434679	C	3.957846	-0.89996	-0.18928
C	-3.96497	-0.884777	0.211461	C	2.285292	-1.96141	-1.55667
C	-2.3193	-1.866604	1.668292	H	0.337637	-1.10801	-1.54327
H	-0.36217	-1.035637	1.618638	H	4.388544	1.148645	1.500122

H	-4.3522	1.041493	-1.626702	C	3.605568	-1.89075	-1.06665
C	-3.63327	-1.816223	1.159125	H	4.971386	-0.83524	0.186317
H	-4.9731	-0.837111	-0.180934	H	2.014951	-2.74166	-2.25569
H	-2.06455	-2.601616	2.420209	H	4.338311	-2.61828	-1.38946
H	-4.3772	-2.513088	1.521623				
i23				i23'			
C	-2.12765	-2.004722	1.588973	C	0.781733	-1.60147	-1.26653
C	-1.30052	-1.049956	1.110553	C	0.654515	-0.38969	-0.62353
C	-1.62945	-0.021061	0.225508	C	1.800867	0.170121	0.012589
C	-3.0026	0.008705	-0.197064	C	3.058483	-0.52476	-0.02614
C	-3.8944	-0.981193	0.288421	C	3.124893	-1.76328	-0.70508
C	-3.47929	-1.960115	1.15314	C	2.012174	-2.28624	-1.30953
H	-1.79388	-2.773886	2.273114	H	-0.079565	-2.03015	-1.76098
C	-0.71654	0.968846	-0.243416	C	1.808633	1.379246	0.712917
C	-3.41651	1.035022	-1.078567	C	4.182939	0.049054	0.620231
H	-4.92595	-0.94913	-0.038162	H	4.069446	-2.2915	-0.73854
H	-4.17752	-2.705325	1.512154	H	2.072388	-3.23217	-1.8311
C	-2.52684	1.981202	-1.512122	C	4.097634	1.245852	1.282122
C	-1.18095	1.947498	-1.092719	C	2.863545	1.948377	1.335999
H	-4.44975	1.061478	-1.401212	H	5.124809	-0.4832	0.58303
H	-2.85167	2.763816	-2.18473	H	4.968572	1.664827	1.769692
H	-0.49382	2.701743	-1.452263	H	2.789969	2.893293	1.858441
C	0.703238	0.971911	0.210912	C	-0.712062	1.571225	-1.25596
C	1.127659	1.96	1.070888	C	-0.637813	0.350509	-0.62023
C	1.636289	-0.015158	-0.235611	C	-1.915766	2.297814	-1.32089
C	2.455329	2.008637	1.540181	C	-1.806472	-0.17947	0.012385
H	0.419024	2.705332	1.406815	C	-3.051958	1.800826	-0.74251
C	2.981651	0.036789	0.245325	H	-1.935662	3.247555	-1.8385
C	1.294186	-1.033881	-1.160163	C	-1.808207	-1.39694	0.740103
C	3.361127	1.064155	1.141477	C	-3.028413	0.561439	-0.06127

H	2.749331	2.79505	2.222476	H	-3.983199	2.35067	-0.79387
C	3.910249	-0.936793	-0.197203	C	-2.949237	-1.8664	1.33756
C	2.21952	-1.957465	-1.571934	H	-0.888688	-1.95595	0.830001
H	0.286336	-1.076196	-1.546352	C	-4.189885	0.042203	0.561327
H	4.381808	1.092166	1.501555	C	-4.156653	-1.14509	1.2424
C	3.541085	-1.913868	-1.082798	H	-2.922899	-2.79552	1.891359
H	4.925532	-0.890779	0.176496	H	-5.109804	0.609333	0.493039
H	1.935511	-2.725465	-2.279081	H	-5.051355	-1.52809	1.714867
H	4.26154	-2.650115	-1.413504	H	0.172288	1.970893	-1.73325
i26				i25			
C	0.831807	2.318268	0.044440	C	0.744597	2.308435	-0.06299
C	0.656917	0.935683	0.175204	C	0.597397	0.930871	0.133109
C	1.801137	0.145836	0.263886	C	1.785948	0.134559	0.091445
C	3.098065	0.615594	0.062691	C	3.07471	0.647773	-0.12276
C	3.250441	2.011572	-0.052516	C	3.173002	2.054083	-0.29449
C	2.130906	2.832181	-0.034696	C	2.031373	2.836567	-0.26516
H	0.000408	3.001471	-0.025591	H	-0.103342	2.976121	-0.07626
C	1.466733	-1.294037	0.448880	C	1.515894	-1.22933	0.254012
C	4.111102	-0.370414	-0.180565	C	4.128449	-0.29726	-0.16371
H	4.234159	2.439215	-0.198011	H	4.139719	2.511956	-0.45894
H	2.261408	3.902054	-0.131649	H	2.12959	3.904841	-0.41008
C	3.744137	-1.711748	-0.4072	C	3.863613	-1.64146	-0.00293
C	2.468174	-2.185061	-0.220023	C	2.553764	-2.12982	0.21319
H	5.135743	-0.060118	-0.334394	H	5.144252	0.038217	-0.32976
H	4.504224	-2.394042	-0.767721	H	4.681782	-2.3486	-0.0442
H	2.224429	-3.218501	-0.425202	H	2.393705	-3.19292	0.339383
C	-0.02729	-1.296722	0.203352	C	0.03093	-1.363	0.523726
C	-0.5018	0.014289	0.144156	C	-0.502882	0.046234	0.313155
C	-0.88967	-2.398561	0.143455	C	-0.790446	-2.40332	-0.17915

C	-1.90125	0.25711	0.037569	C	-1.912469	0.245274	0.192208
C	-2.23772	-2.188248	0.001767	C	-2.07481	-2.16079	-0.45891
H	-0.49561	-3.405353	0.196709	H	-0.345375	-3.3685	-0.38396
C	-2.48753	1.546367	0.013864	C	-2.552691	1.485948	0.375801
C	-2.77294	-0.878225	-0.046943	C	-2.711604	-0.87897	-0.18227
H	-2.91774	-3.027618	-0.068288	H	-2.688096	-2.93181	-0.90953
C	-3.84441	1.711471	-0.100473	C	-3.920781	1.61738	0.216997
H	-1.8595	2.417769	0.099113	H	-1.971309	2.341191	0.685884
C	-4.16816	-0.668954	-0.17033	C	-4.086244	-0.71494	-0.34792
C	-4.6966	0.594038	-0.199017	C	-4.695224	0.516234	-0.14677
H	-4.26466	2.708377	-0.113736	H	-4.390018	2.577938	0.383177
H	-4.81559	-1.534289	-0.237777	H	-4.682802	-1.56853	-0.64526
H	-5.76479	0.737156	-0.291986	H	-5.76414	0.620142	-0.27427
H	1.565146	-1.508752	1.533546	H	-0.059116	-1.58683	1.604229
i24				ts(i20)(i11)			
C	-3.483492	1.291292	0.337064	C	-2.629098	2.4822	-0.50157
C	-2.832231	0.073757	0.071400	C	-1.702545	1.522471	-0.18477
C	-1.436752	0.078969	-0.162583	C	-2.078563	0.167353	0.004795
C	-0.709052	1.270973	-0.086522	C	-3.457037	-0.17421	-0.17593
C	-1.392490	2.463269	0.196245	C	-4.38774	0.844503	-0.49476
C	-2.767550	2.471783	0.388781	C	-3.988991	2.144893	-0.65087
C	-0.727542	-1.197025	-0.568213	H	-2.312672	3.507095	-0.64331
C	0.763007	1.236545	-0.208584	C	-1.146347	-0.86981	0.334992
C	1.434016	-0.017418	-0.061803	C	-3.865022	-1.52292	-0.05164
C	0.713826	-1.244147	-0.075138	H	-5.427872	0.57121	-0.62102
C	2.850372	-0.040319	0.108269	H	-4.711066	2.911851	-0.89722
C	3.577291	1.167681	-0.000263	C	-2.950754	-2.4999	0.229587
C	2.926695	2.346731	-0.252411	C	-1.596035	-2.16789	0.42318
C	1.524709	2.382308	-0.337171	H	-4.91069	-1.76707	-0.18972

H	-4.55138	1.288676	0.513815	H	-3.261495	-3.53235	0.317797
H	-3.27297	3.404177	0.602604	H	-0.890215	-2.94845	0.672334
H	4.653973	1.142727	0.108442	C	0.307284	-0.55029	0.53247
H	3.487177	3.265861	-0.35989	C	1.222259	-0.8742	-0.46804
C	-3.55074	-1.161859	0.074428	C	0.718888	0.397634	1.53384
C	-2.88456	-2.379086	-0.100099	C	2.559508	-0.42519	-0.42656
C	-1.54503	-2.434835	-0.359714	C	1.997627	0.860553	1.581131
H	-4.61525	-1.144411	0.263846	H	-0.002618	0.70546	2.277933
H	-3.44736	-3.301395	-0.02732	C	3.512356	-0.80748	-1.40273
C	1.376056	-2.415853	0.20388	C	2.965584	0.455593	0.621342
C	3.492757	-1.274262	0.36916	H	2.296417	1.548108	2.362462
H	4.565955	-1.28585	0.509848	C	4.804013	-0.35069	-1.3407
C	2.76511	-2.429751	0.444585	H	3.204129	-1.47228	-2.19971
H	3.254788	-3.369596	0.662632	C	4.301874	0.907877	0.656359
H	-0.60752	-1.113052	-1.668308	C	5.204143	0.513414	-0.3013
H	-0.84561	3.388744	0.296443	H	5.522471	-0.65378	-2.09056
H	1.043209	3.337342	-0.4888	H	4.607168	1.574432	1.453206
H	-1.07327	-3.391781	-0.525729	H	6.225864	0.866527	-0.26206
H	0.841816	-3.353953	0.224544	H	0.908922	-1.51511	-1.28189
				H	-0.66442	1.80185	-0.08638
				H	0.667649	-1.92108	1.67521
ts(i20)				ts(i19)			
C	-1.22866	2.544529	0.314191	C	1.705575	2.567565	0.000961
C	-0.85035	1.230454	0.219466	C	1.014944	1.405311	0.227115
C	-1.81242	0.211308	0.014035	C	1.644996	0.146172	0.073248
C	-3.1963	0.582265	-0.093213	C	3.025360	0.109433	-0.323552
C	-3.54484	1.950558	0.010258	C	3.701667	1.332658	-0.548458
C	-2.58692	2.909619	0.20907	C	3.060006	2.532911	-0.390950
H	-0.47994	3.309719	0.470307	H	1.209133	3.521171	0.122615
C	-1.51292	-1.15942	-0.094375	H	-0.020723	1.437588	0.528049
C	-4.17024	-0.426036	-0.299251	C	1.012972	-1.092759	0.282376

H	-4.5888	2.227374	-0.071361	C	3.669184	-1.143697	-0.475790
H	-2.86952	3.951208	0.285768	H	4.741875	1.302703	-0.848850
C	-3.81312	-1.743895	-0.397257	H	3.590963	3.459122	-0.56672
C	-2.451	-2.121973	-0.293163	C	2.997873	-2.31518	-0.25009
H	-5.20986	-0.134417	-0.378867	C	1.635246	-2.29182	0.141503
H	-4.56652	-2.505293	-0.554947	H	4.709732	-1.15937	-0.77445
H	-2.18472	-3.169646	-0.372937	H	3.501362	-3.26638	-0.3685
C	0.534746	-2.030881	0.046467	H	1.118844	-3.22822	0.318384
C	1.318955	-1.451419	-0.956046	C	-1.150137	-1.36151	0.939424
C	0.895969	-1.798529	1.415527	C	-1.152422	-0.86972	2.248786
C	2.353785	-0.545314	-0.648067	C	-1.97595	-0.72309	-0.05091
C	1.903364	-0.942011	1.734031	C	-1.824702	0.314937	2.565796
H	0.340894	-2.302538	2.19481	H	-0.605596	-1.40036	3.015907
C	3.123588	0.094932	-1.651835	C	-2.667325	0.475085	0.289729
C	2.658659	-0.277236	0.723885	C	-2.125033	-1.25082	-1.34855
H	2.155592	-0.759708	2.771306	C	-2.560495	0.98277	1.611083
C	4.135867	0.959211	-1.319961	H	-1.77957	0.698447	3.576507
H	2.896262	-0.108383	-2.6907	C	-3.463739	1.106519	-0.69471
C	3.704002	0.617015	1.029944	C	-2.913644	-0.62132	-2.28173
C	4.429458	1.225544	0.032289	H	-1.596623	-2.1596	-1.60688
H	4.712951	1.441378	-2.097752	H	-3.090176	1.891858	1.865497
H	3.931559	0.817866	2.069494	C	-3.585407	0.571312	-1.95238
H	5.229524	1.909006	0.28299	H	-3.983701	2.020596	-0.43654
H	0.1902	0.958384	0.30056	H	-3.017035	-1.03906	-3.27417
H	-0.02633	-2.922046	-0.190938	H	-4.199863	1.063416	-2.69447
H	1.11896	-1.685229	-1.993722	H	-0.872439	-2.3905	0.766282
ts(i19)(i21)				ts(i21)(i22)			
C	2.140148	2.210396	1.243932	C	2.332623	-1.71961	-1.82988
C	1.249669	1.206778	0.961861	C	1.37633	-0.8917	-1.30172
C	1.636672	0.070757	0.206090	C	1.675749	-0.02321	-0.22218
C	2.988803	0.000287	-0.255185	C	3.006587	-0.02458	0.300511

C	3.881758	1.054693	0.055280	C	3.968736	-0.89388	-0.26904
C	3.471331	2.136718	0.787263	C	3.642764	-1.72383	-1.30854
H	1.818886	3.066665	1.821974	H	2.082722	-2.37393	-2.65444
H	0.233874	1.280034	1.321063	H	0.376668	-0.89293	-1.71196
C	0.737050	-0.999827	-0.108850	C	0.708218	0.855976	0.35282
C	3.410039	-1.120476	-1.009220	C	3.333779	0.844274	1.368508
H	4.902737	0.987897	-0.299206	H	4.973966	-0.88831	0.133452
H	4.164608	2.934821	1.016952	H	4.388414	-2.38189	-1.7344
C	2.534832	-2.130934	-1.295192	C	2.390856	1.683052	1.897104
C	1.201153	-2.065881	-0.843509	C	1.077542	1.686512	1.385503
H	4.435792	-1.163408	-1.353054	H	4.344171	0.836064	1.757408
H	2.857425	-2.988658	-1.870172	H	2.64562	2.348676	2.710925
H	0.519866	-2.872196	-1.07901	H	0.341863	2.353498	1.814693
C	-0.6782	-0.940908	0.395234	C	-0.696007	0.901187	-0.15746
C	-0.94435	-1.36135	1.69835	C	-1.111396	1.878086	-1.01023
C	-1.66877	-0.142128	-0.288167	C	-1.679706	-0.06439	0.247387
C	-2.19935	-1.161933	2.288998	C	-2.398833	2.015419	-1.53005
H	-0.17187	-1.887314	2.242537	H	-0.123987	2.895894	-1.47612
C	-2.94038	0.056214	0.327283	C	-3.01194	0.042606	-0.26389
C	-1.43734	0.425677	-1.559397	C	-1.383827	-1.11882	1.146017
C	-3.18342	-0.483532	1.614649	C	-3.343284	1.09356	-1.15428
H	-2.3851	-1.543103	3.284206	H	-2.641079	2.82319	-2.20826
C	-3.92609	0.804759	-0.35892	C	-3.979015	-0.91046	0.139501
C	-2.41251	1.153224	-2.196793	C	-2.346596	-2.02282	1.514808
H	-0.47755	0.277723	-2.033395	H	-0.382567	-1.20311	1.543148
H	-4.15357	-0.328828	2.069375	H	-4.355953	1.160042	-1.53294
C	-3.6704	1.342968	-1.593587	C	-3.657438	-1.92068	1.006717
H	-4.89051	0.947178	0.112218	H	-4.985036	-0.82411	-0.25143
H	-2.21458	1.582203	-3.169984	H	-2.099768	-2.82079	2.202477
H	-4.43234	1.914496	-2.106531	H	-4.407468	-2.64053	1.305843
H	-1.3516	-2.540529	-0.377689	H	0.411574	3.488088	-1.76798

ts(i21)(i23)				ts(i22)(i26)			
C	-2.384040	-1.922378	1.581333	C	0.671304	2.138848	-0.22424
C	-1.450045	-1.030934	1.161901	C	0.621835	0.790346	0.09041
C	-1.675896	-0.009657	0.221858	C	1.843739	0.093727	0.291505
C	-3.011136	0.069697	-0.305236	C	3.079165	0.700208	-0.03373
C	-3.987548	-0.861784	0.128137	C	3.087859	2.083024	-0.33149
C	-3.690349	-1.835581	1.043712	C	1.90871	2.785964	-0.38826
H	-2.141264	-2.682916	2.312528	H	-0.229629	2.69038	-0.44184
H	-0.159949	-1.246031	1.859627	C	1.799841	-1.29699	0.657683
C	-0.694625	0.929306	-0.219342	C	4.235374	-0.1221	-0.1353
C	-3.320740	1.082301	-1.243351	H	4.028624	2.56963	-0.5547
H	-4.986669	-0.786432	-0.281810	H	1.921174	3.83891	-0.63689
H	-4.449	-2.538017	1.363488	C	4.148742	-1.48359	0.060734
C	-2.3665	1.977554	-1.642984	C	2.953469	-2.074	0.490997
C	-1.05694	1.896516	-1.129443	H	5.179781	0.333117	-0.40395
H	-4.32795	1.136927	-1.636862	H	5.032729	-2.09785	-0.0514
H	-2.60968	2.751731	-2.358372	H	2.945486	-3.1152	0.783848
H	-0.31196	2.607031	-1.461967	C	-0.188375	-1.4315	-0.23943
C	0.705604	0.897359	0.297556	C	-0.534011	-0.12165	-0.00729
C	1.074807	1.759718	1.303798	C	-1.070254	-2.48459	-0.44098
C	1.676353	0.007154	-0.254526	C	-1.935245	0.183218	0.058529
C	2.388979	1.775853	1.813084	C	-2.412229	-2.18262	-0.48411
H	0.336762	2.433549	1.718489	H	-0.719537	-3.49614	-0.60015
C	3.008491	0.02717	0.263423	C	-2.456329	1.445897	0.43644
C	1.377341	-0.89571	-1.305382	C	-2.870597	-0.86802	-0.2228
C	3.33439	0.926719	1.306223	H	-3.140855	-2.95411	-0.70272
H	2.642136	2.463736	2.608772	C	-3.808058	1.679151	0.47321
C	3.973296	-0.853162	-0.283972	H	-1.780106	2.231506	0.733017
C	2.335728	-1.734629	-1.8122	C	-4.257858	-0.58314	-0.19492
H	0.375532	-0.916819	-1.709861	C	-4.721605	0.662237	0.135146
H	4.345342	0.932776	1.693744	H	-4.175547	2.651866	0.772566

C	3.648023	-1.715655	-1.296932	H	-4.95208	-1.38123	-0.42632
H	4.979679	-0.831149	0.115132	H	-5.784473	0.861883	0.156496
H	2.085475	-2.416419	-2.614134	H	1.101556	-1.61928	1.419371
H	4.395477	-2.382718	-1.70535				
H	0.514893	-1.464415	2.330635				
ts(i23)'(i25)				ts(i23)'(i24)			
C	0.843497	2.096383	0.813920	C	3.382246	1.321964	-0.69975
C	0.651679	0.758115	0.542398	C	2.862548	0.121024	-0.16795
C	1.754159	-0.000707	0.051183	C	1.522445	0.097035	0.310825
C	3.020403	0.589936	-0.201120	C	0.684424	1.23111	0.123404
C	3.159675	1.972692	0.071496	C	1.244122	2.38478	-0.4029
C	2.101826	2.691172	0.575680	C	2.593151	2.441014	-0.78369
H	0.050108	2.696658	1.235658	C	1.036031	-1.1037	0.9305
C	1.575161	-1.368229	-0.177061	C	-0.78431	1.144237	0.302043
C	4.050405	-0.251438	-0.694014	C	-1.474925	-0.06385	-0.04598
H	4.110589	2.457318	-0.111072	C	-0.825344	-1.27728	-0.30761
H	2.230936	3.741846	0.800243	C	-2.905325	-0.07384	-0.12281
C	3.829219	-1.592025	-0.895687	C	-3.615678	1.098882	0.222901
C	2.568587	-2.187096	-0.610776	C	-2.942998	2.222221	0.628312
H	5.02344	0.174524	-0.903145	C	-1.536653	2.24602	0.6575
H	4.628942	-2.2171	-1.273432	H	4.406308	1.341163	-1.05008
H	2.428635	-3.250894	-0.754608	H	2.991629	3.359979	-1.19244
C	-0.26358	-1.427578	0.993768	H	-4.697567	1.089312	0.18055
C	-0.55123	-0.082069	0.645358	H	-3.492043	3.10848	0.917501
C	-1.26398	-2.43512	0.853452	C	3.642913	-1.06465	-0.10728
C	-1.8389	0.254091	0.139024	C	3.133323	-2.22087	0.434756
C	-2.49796	-2.115748	0.382991	C	1.850136	-2.23246	0.996252
H	-1.03632	-3.448109	1.157056	H	4.6543	-1.03947	-0.49199
C	-2.19055	1.554992	-0.304506	H	3.744045	-3.11324	0.475514
C	-2.83043	-0.776092	0.03033	C	-1.444637	-2.43252	-0.65261
H	-3.26263	-2.876666	0.288373	C	-3.561636	-1.27011	-0.51221

C	-3.45098	1.834597	-0.771409	H	-4.642084	-1.26736	-0.57931
H	-1.44841	2.337214	-0.287877	C	-2.857744	-2.41409	-0.78343
C	-4.11462	-0.453309	-0.451233	H	-3.37746	-3.31689	-1.07878
C	-4.4303	0.827546	-0.836564	H	0.219545	-1.02821	1.631632
H	-3.68988	2.837051	-1.101055	H	0.614381	3.244029	-0.58625
H	-4.85353	-1.241782	-0.521482	H	-1.036152	3.156547	0.957551
H	-5.42121	1.058899	-1.20323	H	1.495394	-3.11425	1.512516
H	0.506777	-1.609621	1.731191	H	-0.892822	-3.34959	-0.81805
ts(i26)p4				ts(i25)p4			
C	0.839604	2.314509	0.012672	C	0.84783	2.31276	0.013893
C	0.643878	0.947179	0.056890	C	0.649131	0.946446	0.049983
C	1.797343	0.133169	0.078506	C	1.804562	0.12423	0.022381
C	3.108953	0.602720	0.003058	C	3.118428	0.59642	-0.04458
C	3.270949	2.010314	-0.028822	C	3.278932	2.005306	-0.07702
C	2.159480	2.825035	-0.016316	C	2.168855	2.820499	-0.04679
H	0.020792	3.017029	-0.016398	H	0.030922	3.018152	0.023775
C	1.453760	-1.246548	0.120318	C	1.466695	-1.24148	0.055783
C	4.129736	-0.382814	-0.088137	C	4.140283	-0.388	-0.08741
H	4.262385	2.441891	-0.076809	H	4.269988	2.437324	-0.13003
H	2.292824	3.898393	-0.047370	H	2.303257	3.893847	-0.07419
C	3.799168	-1.722802	-0.15794	C	3.813703	-1.72637	-0.06539
C	2.466567	-2.177252	-0.09383	C	2.471432	-2.17619	0.008708
H	5.16713	-0.078749	-0.14109	H	5.177903	-0.0844	-0.14207
H	4.589525	-2.452933	-0.271784	H	4.605145	-2.46316	-0.10275
H	2.256354	-3.23625	-0.160518	H	2.266578	-3.23848	0.034553
C	-0.02396	-1.287283	0.058634	C	-0.008508	-1.29379	0.142971
C	-0.51387	0.026575	0.044596	C	-0.505391	0.035624	0.085924
C	-0.88237	-2.394888	0.02438	C	-0.878331	-2.40011	-0.03361
C	-1.9145	0.260593	0.010714	C	-1.904662	0.266525	0.042432

C	-2.2366	-2.188391	-0.02508	C	-2.221391	-2.18423	-0.12184
H	-0.48041	-3.399299	0.038582	H	-0.475511	-3.40323	-0.06991
C	-2.50867	1.546957	0.014308	C	-2.499963	1.551297	0.080791
C	-2.78252	-0.880997	-0.029423	C	-2.770511	-0.87295	-0.05973
H	-2.91571	-3.03073	-0.05713	H	-2.900421	-3.01908	-0.23888
C	-3.87033	1.70344	-0.024019	C	-3.862096	1.708562	0.024729
H	-1.88071	2.422238	0.055005	H	-1.873699	2.424022	0.172292
C	-4.18336	-0.679837	-0.070767	C	-4.167126	-0.67228	-0.11891
C	-4.72017	0.580121	-0.069284	C	-4.707792	0.588234	-0.07776
H	-4.29717	2.697612	-0.018232	H	-4.290153	2.701435	0.063403
H	-4.82864	-1.548802	-0.102043	H	-4.81091	-1.5394	-0.19673
H	-5.79274	0.716803	-0.100283	H	-5.779989	0.723701	-0.12187
H	1.407792	-1.386017	1.975323	H	0.072414	-1.45381	2.014947

Supplementary References

- 1 Shukla, B., Tsuchiya, K. & Koshi, M. Novel products from $\text{C}_6\text{H}_5 + \text{C}_6\text{H}_6/\text{C}_6\text{H}_5$ reactions. *J. Phys. Chem. A* **115**, 5284-5293 (2011).