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Supplementary Information for

Unconventional Gas-Phase Synthesis of Biphenyl and its Atropisomeric Methyl-Substituted Derivatives

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Precursor synthesis and characterization

The synthesis of (2-bromoethynyl)benzene was performed analogue to a reported procedure[1] with an increase in the concentration of the starting materials due to the large scale of precursor needed. Regarding the purification, batches performed with less than 10 g of phenylacetylene could be purified by either column chromatography or distillation for both precursors whereas larger batches (20–50 g) decomposed before affording the desired product and, thus, had to be purified by column chromatography. A solution of phenylacetylene (8.0 mL, 7.44 g, 72 mmol) in MeOH (50 mL) was cooled down to 0 °C and KOH (10.0 g, 180 mmol) was added. After 20 min of stirring at 0 °C, N-bromosuccinimide (15.3 g, 86 mmol) was added to the mixture in portions and stirred at 0 °C for 15 min. The cold bath was replaced by a rt water bath and the mixture was stirred for 30 min. Then, Et_2O (200 mL) was added and the mixture was extracted with brine (3 x 100 mL), dried over $MgSO_4$, filtered and evaporated to afford a brown oil/liquid. This liquid was purified by column chromatography (SiO_2; hexane) to afford the product as a light-yellow oil (9.63 g, 73%). ^{1}H NMR (200 MHz, $CDCl_3$) δ: 7.44 (dd, 2H), 7.31 (m, 3H) ppm. ^{13}C NMR (50 MHz, $CDCl_3$) δ: 132.10, 128.78, 128.44, 122.78, 80.19 and 49.93 ppm. MS: m/z 180.0 [M^+] 101.1 [M^+–Br]. The characteristic C≡C stretching vibration was found at 2202 cm^{-1} whereas for the starting material it is observed at 2110 cm^{-1}. The provided characterization is in accordance with the literature.[2] ^{1}H and ^{13}C NMR data were recorded with a Bruker DPX-200 NMR spectrometer referenced towards $CDCl_3$ (7.26 ppm for ^{1}H NMR and 77.16 ppm for ^{13}C NMR). The GC-MS data were recorded with an Agilent 7820A GC spectrometer. IR data were recorded with a Bruker Equinox 55 FT-IR spectrometer.

Table S1 Peak velocities (v_p), speed ratios (S), collision energies (E_c), and center-of-mass angles (Θ_{CM}) for the reactions of phenylethynyl radicals (C_6H_5CC) with 1,3-butadiene-d_6 (C_4D_6), isoprene ($CH_2C(CH_3)CHCH_2$), and 1,3-pentadiene ($CH_2CHCHCHCH_3$).

Beam	v_p (m s^{-1})	S	E_c (kJ mol^{-1})	Θ_{CM} (°)
$CD_2CDCDCD_2$ (X^1A_g)	750 ± 10	8.0 ± 0.2		
C_6H_5CC (X^2A_1) / He	1760 ± 18	9.3 ± 0.6	68.9 ± 1.5	15.0 ± 0.4
C_6H_5CC (X^2A_1) / Ne	898 ± 6	13.5 ± 1.2	25.8 ± 0.5	27.1 ± 0.5
$CH_2C(CH_3)CHCH_2$ (X^1A')	721 ± 20	8.5 ± 0.6		
C_6H_5CC (X^2A_1) / He	1749 ± 10	10.1 ± 0.6	72.7 ± 1.3	16.3 ± 0.5
C_6H_5CC (X^2A_1) / Ne	895 ± 9	14.3 ± 1.2	26.8 ± 0.6	29.2 ± 0.6
$CH_2CHCHCHCH_3$ (X^1A')	711 ± 20	8.5 ± 0.7		
C_6H_5CC (X^2A_1) / He	1778 ± 13	10.2 ± 0.6	74.5 ± 1.5	15.8 ± 0.5
C_6H_5CC (X^2A_1) / Ne	898 ± 8	14.6 ± 1.0	26.7 ± 0.9	28.8 ± 0.9

Table S2 RRKM rate constants (s^{-1}) for the reaction of phenylethynyl radicals with 1,3-butadiene-d_6 computed with *w*B97X-D/cc-pVTZ zero-point energy corrected CCSD(T)/cc-pVTZ energies, and *w*B97X-D/cc-pVTZ harmonic frequencies at collision energies of 0.0, 25.8, and 68.9 kJ mol^{-1} relative to the entrance channel.

	0	**25.8**	**68.9**
k_1 (i1 → i3)	2.93×10^{5}	7.16×10^{5}	2.43×10^{6}
k_{-1} (i3 → i1)	7.32×10^{6}	2.17×10^{7}	9.72×10^{7}
k_2 (i1 → i2)	2.71×10^{-3}	6.96×10^{-2}	3.60
k_{-2} (i2 → i1)	1.21×10^{-1}	2.65	1.10×10^{2}
k_3 (i1 → p2+D)	2.78	4.08×10^{1}	1.19×10^{3}
k_4 (i2 → p2+D)	1.37×10^{3}	1.19×10^{4}	1.85×10^{5}
k_5 (i2 → i4)	4.49×10^{9}	5.61×10^{9}	7.63×10^{9}
k_{-5} (i4 → i2)	2.83×10^{4}	8.47×10^{4}	4.12×10^{5}
k_6 (i3 → i4)	1.45×10^{4}	5.77×10^{4}	3.79×10^{5}
k_{-6} (i4 → i3)	8.22×10^{-2}	5.50×10^{-1}	7.81
k_7 (i4 → p1+D)	3.67×10^{8}	5.99×10^{8}	1.24×10^{9}
k_{36} (i1 → i21)	1.32×10^{7}	2.75×10^{7}	7.62×10^{7}
k_{-36} (i21 → i1)	1.17×10^{7}	3.00×10^{7}	1.12×10^{8}

k_{37} (i21 → i22)	8.27×10^{-2}	8.24×10^{-1}	1.66×10^{1}
k_{-37} (i22 → i21)	7.39×10^{-5}	1.13×10^{-3}	4.31×10^{-2}
k_{38} (i22 → p10+D)	5.57×10^{4}	1.67×10^{5}	8.06×10^{6}
k_{49} (i28 → i29)	1.38×10^{8}	2.69×10^{8}	6.52×10^{8}
k_{-49} (i29 → i28)	4.51×10^{10}	7.26×10^{10}	1.35×10^{11}
k_{50} (i29 → i1)	7.92×10^{11}	9.77×10^{11}	1.29×10^{12}
k_{-50} (i1 → i29)	1.31×10^{6}	3.18×10^{6}	1.07×10^{7}
k_{59} (i2 → p13 + phenylacetylene)	3.24		

Table S3 RRKM rate constants (s^{-1}) for the reaction of phenylethynyl radicals with isoprene computed with *w*B97X-D/cc-pVTZ zero-point energy corrected CCSD(T)/cc-pVTZ energies, and *w*B97X-D/cc-pVTZ harmonic frequencies at collision energies of 0.0, 26.8 and 72.7 kJ mol^{-1} relative to the entrance channel.

	0.0	**26.8**	**72.7**
k_8 (i5 → i7)	1.41×10^{5}	3.50×10^{5}	1.24×10^{6}
k_{-8} (i7 → i5)	4.47×10^{6}	1.44×10^{7}	7.49×10^{7}
k_9 (i5 → i6)	2.36×10^{-3}	6.03×10^{-2}	3.29
k_{-9} (i6 → i5)	2.32	4.63×10^{1}	1.78×10^{3}
k_{10} (i5 → p4+H)	2.21×10^{-1}	3.53	1.20×10^{2}
k_{11} (i5 → p4+H)	9.40×10^{1}	1.44×10^{3}	4.29×10^{4}
k_{12} (i6 → i8)	3.62×10^{11}	3.95×10^{11}	4.45×10^{11}
k_{-12} (i8 → i6)	1.08×10^{4}	3.39×10^{4}	1.84×10^{5}
k_{13} (i7 → i8)	2.35×10^{4}	9.02×10^{4}	5.89×10^{5}
k_{-13} (i8 → i7)	4.33×10^{-2}	2.89×10^{-1}	4.35
k_{14} (i8 → p3+H)	4.77×10^{8}	7.79×10^{8}	1.64×10^{9}
k_{39} (i5 → i23)	9.68×10^{6}	1.96×10^{7}	5.27×10^{7}

k_{-39} (i23 → i5)	5.15×10^{6}	1.39×10^{7}	5.73×10^{7}
k_{40} (i23 → i24)	1.26×10^{-1}	1.22	2.51×10^{1}
k_{-40} (i24 → i23)	3.27×10^{-5}	4.98×10^{-4}	2.04×10^{-2}
k_{41} (i24 → p11+H)	3.75×10^{4}	1.13×10^{5}	5.78×10^{5}
k_{15} (i9 → i11)	7.29×10^{4}	1.83×10^{5}	6.56×10^{5}
k_{-15} (i11 → i9)	3.13×10^{6}	9.75×10^{6}	4.82×10^{7}
k_{16} (i9 → i10)	6.07×10^{-3}	1.35×10^{-1}	6.54
k_{-16} (i10 → i9)	1.12	2.06×10^{1}	7.55×10^{2}
k_{17} (i9 → p6+H)	3.00	3.61×10^{1}	9.14×10^{2}
k_{18} (i10 → p6+H)	1.30×10^{2}	1.62×10^{3}	3.97×10^{4}
k_{19} (i10 → i12)	2.44×10^{10}	2.97×10^{10}	3.92×10^{10}
k_{-19} (i12 → i10)	9.13×10^{3}	2.86×10^{4}	1.54×10^{5}
k_{-20} (i11 → i12)	8.66×10^{3}	3.66×10^{4}	2.63×10^{5}
k_{-20} (i12 → i11)	2.86×10^{-2}	2.02×10^{-1}	3.25
k_{21} (i12 → p5+H)	7.67×10^{8}	1.26×10^{9}	2.66×10^{9}

k_{42} (i9 → i23)	5.18×10^{6}	1.07×10^{7}	2.96×10^{7}
k_{-42} (i23 → i9)	6.94×10^{6}	1.82×10^{7}	7.20×10^{7}
k_{43} (i23 → i25)	4.14×10^{-1}	3.48	6.13×10^{1}
k_{-43} (i25 → i23)	9.91×10^{-5}	1.32×10^{-3}	4.66×10^{-2}
k_{44} (i25 → p11′+H)	5.90×10^{4}	1.75×10^{5}	8.74×10^{5}
k_{51} (i30 → i31)	6.25×10^{7}	1.31×10^{8}	3.55×10^{8}
k_{-51} (i31 → i30)	4.15×10^{10}	7.10×10^{10}	1.45×10^{11}
k_{52} (i31 → i5)	5.82×10^{11}	7.23×10^{11}	9.71×10^{11}
k_{-52} (i5 → i31)	1.02×10^{6}	2.36×10^{6}	7.60×10^{6}
k_{53} (i32 → i33)	1.29×10^{8}	2.55×10^{8}	6.35×10^{8}
k_{-53} (i33 → i32)	2.44×10^{10}	4.20×10^{10}	8.71×10^{10}
k_{54} (i33 → i9)	1.41×10^{12}	1.71×10^{12}	2.23×10^{12}
k_{-54} (i9 → i33)	6.94×10^{5}	1.64×10^{6}	5.43×10^{6}

Table S4 RRKM rate constants (s^{-1}) for the reaction of phenylethynyl radicals with 1,3-pentadiene computed with wB97XD/cc-pVTZ zero-point energy corrected CCSD(T)/cc-pVTZ energies, and *w*B97X-D/cc-pVTZ harmonic frequencies at collision energies of 0.0, 26.7 and 74.5 kJ mol^{-1} relative to the entrance channel.

	0.0	**26.7**	**74.5**
k_{22} (i13 → i15)	2.06×10^{5}	4.95×10^{5}	1.77×10^{6}
k_{-22} (i15 → i13)	1.90×10^{7}	5.41×10^{7}	2.51×10^{8}
k_{23} (i13 → i14)	1.13×10^{-2}	2.67×10^{-1}	1.59×10^{1}
k_{-23} (i14 → i13)	2.63×10^{-1}	5.22	2.39×10^{2}
k_{24} (i13 → p8+H)	7.43	9.43×10^{1}	2.87×10^{3}
k_{25} (i14 → p8+H)	6.52×10^{1}	8.21×10^{2}	2.32×10^{4}
k_{26} (i14 → i16)	8.50×10^{9}	1.01×10^{10}	1.30×10^{10}
k_{-26} (i16 → i14)	3.56×10^{4}	1.05×10^{5}	5.49×10^{5}
k_{27} (i15 → i16)	2.25×10^{4}	9.39×10^{4}	7.34×10^{5}
k_{-27} (i16 → i15)	4.76×10^{-2}	3.49×10^{-1}	6.58
k_{28} (i16 → p7+H)	6.84×10^{8}	1.10×10^{9}	2.33×10^{9}

k_{45} (i13 → i26)	2.18×10^{7}	4.36×10^{7}	1.21×10^{8}
k_{-45} (i26 → i13)	3.16×10^{7}	7.84×10^{7}	3.00×10^{8}
k_{46} (i26 → i27)	1.20×10^{-1}	1.22	3.00×10^{1}
k_{-46} (i27 → i26)	9.32×10^{-5}	1.48×10^{-3}	7.36×10^{-2}
k_{47} (i27 → p12+H)	2.39×10^{4}	7.66×10^{4}	4.52×10^{5}
k_{29} (i17 → i19)	1.51×10^{5}	3.98×10^{5}	1.61×10^{6}
k_{-29} (i19 → i17)	2.10×10^{6}	6.85×10^{6}	3.82×10^{7}
k_{30} (i17 → i18)	2.72×10^{-2}	6.46×10^{-1}	3.82×10^{1}
k_{-30} (i18 → i17)	1.84×10^{-1}	3.83	1.85×10^{2}
k_{31} (i17 → p9+H)	1.10×10^{1}	1.47×10^{2}	4.72×10^{3}
k_{32} (i18 → p9+H)	8.18×10^{1}	9.61×10^{2}	2.52×10^{4}
k_{33} (i18 → i20)	9.93×10^{9}	1.23×10^{10}	1.69×10^{10}
k_{-33} (i20 → i18)	5.80×10^{3}	1.81×10^{4}	1.04×10^{5}

k_{34} (i19 → i20)	3.32×10^{4}	1.27×10^{5}	8.81×10^{5}
k_{-34} (i20 → i19)	1.89×10^{-2}	1.29×10^{-1}	2.21
k_{35} (i20 → p3+H)	3.98×10^{8}	6.48×10^{8}	1.40×10^{9}
k_{48} (i17 → i26)	1.18×10^{7}	2.56×10^{7}	7.91×10^{7}
k_{-48} (i26 → i17)	4.25×10^{6}	1.18×10^{7}	5.34×10^{7}
k_{55} (i34 → i35)	5.13×10^{7}	1.08×10^{8}	3.02×10^{8}
k_{-55} (i35 → i34)	2.98×10^{10}	5.17×10^{10}	1.11×10^{11}
k_{56} (i35 → i13)	7.61×10^{11}	9.45×10^{11}	1.28×10^{12}
k_{-56} (i13 → i35)	1.49×10^{6}	3.68×10^{6}	1.36×10^{7}
k_{57} (i36 → i37)	1.65×10^{7}	3.55×10^{7}	1.03×10^{8}
k_{-57} (i37 → i36)	4.22×10^{10}	7.32×10^{10}	1.57×10^{11}
k_{58} (i37 → i17)	9.67×10^{11}	1.17×10^{12}	1.54×10^{12}
k_{-58} (i17 → i37)	8.03×10^{6}	1.78×10^{7}	5.99×10^{7}

Table S5 Predicted energies of species participating on the adiabatic doublet ground state potential energy surfaces for reactions of **(a)** phenylethynyl + 1,3-butadiene-d_6, **(b)** phenylethynyl + isoprene, and **(c)** phenylethynyl + 1,3-pentadiene. The energies are computed at the CCSD(T)/cc-pVTZ//*w*B97X-D/cc-pVTZ level of theory with *w*B97X-D/cc-pVTZ zero-point energy corrections.

(a)

	*w*B97X-D/ cc-pVTZ + E_{zpc} [a]	E_{zpc} [b]	CCSD(T)/ cc-pVTZ	E[c] (kJ/mol)
Phenylethynyl (C_{2v}, $^2B_1$)	-307.568246	0.098128	-307.091736	
1,3-Butadiene-d_6 (C_{2h}, ^1A_g)	-155.923156	0.066690	-155.695410	
Phenylethynyl + 1,3-Butadiene-d_6	-463.491402	0.164818	-462.787146	0.0
i1 (C_1, ^2A)	-463.598479	0.168608	-462.898159	-282
vdW(i1) (C_1, ^2A)	-463.498285	0.165573	-462.793821	-16
i2 (C_s, $^2A'$)	-463.595274	0.168587	-462.887969	-255
i3 (C_s, $^2A'$)	-463.611518	0.172618	-462.912385	-308
i4 (C_1, ^2A)	-463.670160	0.172375	-462.966964	-452
i21 (C_1, ^2A)	-463.616542	0.170556	-462.913413	-316
i22 (C_1, ^2A)	-463.661655	0.171404	-462.957306	-430
i28 (C_1, ^2A)	-463.568238	0.167908	-462.871539	-213
i29 (C_1, ^2A)	-463.569512	0.168294	-462.862622	-189
tsi1vdW (C_1, ^2A)	-463.498232	0.165422	-462.793505	-15
tsi1i3 (C_1, ^2A)	-463.556519	0.168366	-462.854733	-168
tsi1i2 (C_1, ^2A)	-463.522238	0.164108	-462.809702	-61
tsi1p2 (C_1, ^2A)	-463.521780	0.163138	-462.815650	-79
tsi3i4 (C_1, ^2A)	-463.550953	0.168180	-462.844216	-141
tsi2i4 (C_1, ^2A)	-463.582154	0.168627	-462.875743	-223
tsi2p2 (C_1, ^2A)	-463.519938	0.163247	-462.820733	-92
tsi4p1 (C_1, ^2A)	-463.618329	0.167597	-462.913531	-325
tsi1i21 (C_1, ^2A)	-463.564091	0.167485	-462.860298	-185
tsi21i22 (C_1, ^2A)	-463.531495	0.167466	-462.824424	-91
tsi22p10 (C_1, ^2A)	-463.570035	0.165855	-462.870741	-217
tsi1i29 (C_1, ^2A)	-463.563395	0.167218	-462.854922	-172
tsi2p12 (C_1, ^2A)	-463.515799	0.164623	-462.8092631	-59

D	-0.502669	0.000000	-0.499810	
p1 (D_2, ^1A)	-463.125188	0.166695	-462.426635	
p2 (C_s, $^1A'$)	-463.026086	0.162543	-462.327788	
phenylacetylene (C_{2v}, $^1A_1$)	-308.274325	0.107761	-307.8108257	
p13 (C_1, ^2A)	-155.243032	0.056343	-155.0059924	
p10 (C_1, ^1A)	-463.071536	0.165255	-462.374622	
p1 + D	-463.627857	0.166695	-462.926445	-361
p2 + D	-463.528755	0.162543	-462.827598	-112
p10 + D	-463.574205	0.165255	-462.874432	-228
p13 + phenylacetylene	-463.517357	0.164104	-462.8168181	-80

(b)

	*w*B97X-D/ cc-pVTZ + E_{zpc} [a]	E_{zpc} [b]	CCSD(T)/ cc-pVTZ	E[c] (kJ/mol)
phenylethynyl(C_{2v}, $^2B_1$)	-307.568246	0.098128	-307.091736	
Isoprene (C_s, $^1A'$)	-195.195944	0.114251	-194.939888	
Phenylacetylenyl + Isoprene	-502.764190	0.212379	-502.031624	0.0
i5 (C_1, ^2A)	-502.868400	0.215639	-502.139237	-274
vdW(i5) (C_1, ^2A)	-502.771936	0.213210	-502.039091	-17
i7 (C_1, ^2A)	-502.885113	0.220221	-502.157577	-310
i6 (C_1, ^2A)	-502.859919	0.216318	-502.125427	-236
i8 (C_1, ^2A)	-502.945260	0.219636	-502.213137	-458
i23(C_1, ^2A)	-502.891376	0.218054	-502.159314	-320
i24(C_1, ^2A)	-502.937699	0.218689	-502.204290	-437
i9 (C_1, ^2A)	-502.871802	0.215800	-502.142372	-282
vdW(i9) (C_1, ^2A)	-502.772305	0.213142	-502.039425	-18
i11(C_1, ^2A)	-502.885531	0.220066	-502.157776	-311
i10 (C_1, ^2A)	-502.865429	0.216084	-502.130773	-251
i12 (C_1, ^2A)	-502.942922	0.219579	-502.211193	-453
i25(C_1, ^2A)	-502.938731	0.218730	-502.204787	-438
i30 (C_1, ^2A)	-502.843257	0.214450	-502.117145	-219
i31 (C_1, ^2A)	-502.843890	0.215945	-502.108464	-192
i32 (C_1, ^2A)	-502.839000	0.214445	-502.114729	-213
i33 (C_1, ^2A)	-502.843325	0.215831	-502.108869	-194
tsi5vdW (C_1, ^2A)	-502.771920	0.213101	-502.038874	-17
tsi5i7 (C_1, ^2A)	-502.828539	0.215561	-502.098306	-167
tsi5i6 (C_1, ^2A)	-502.795293	0.210260	-502.053581	-63
tsi5i23 (C_1, ^2A)	-502.837622	0.214667	-502.105168	-187
tsi5p4 (C_1, ^2A)	-502.794082	0.208473	-502.057487	-78
tsi7i8 (C_1, ^2A)	-502.827265	0.214614	-502.090733	-149

tsi6i8 (C_1, ^2A)	-502.855408	0.215857	-502.120866	-225
tsi6p4 (C_1, ^2A)	-502.792127	0.208415	-502.055250	-72
tsi8p3 (C_1, ^2A)	-502.895350	0.212445	-502.159413	-335
tsi23i24 (C_1, ^2A)	-502.807506	0.213346	-502.070045	-98
tsi24p11 (C_1, ^2A)	-502.846966	0.210146	-502.115885	-227
tsi9vdW (C_1, ^2A)	-502.772097	0.213154	-502.039118	-18
tsi9i11 (C_1, ^2A)	-502.830204	0.215523	-502.099468	-170
tsi9i10 (C_1, ^2A)	-502.797412	0.210056	-502.055378	-68
tsi9i23 (C_1, ^2A)	-502.839061	0.214471	-502.106099	-190
tsi9p6 (C_1, ^2A)	-502.798333	0.207938	-502.061581	-90
tsi11i12 (C_1, ^2A)	-502.825337	0.214321	-502.088646	-145
tsi10i12 (C_1, ^2A)	-502.854925	0.215721	-502.120385	-224
tsi10p6 (C_1, ^2A)	-502.795546	0.208035	-502.058768	-83
tsi12p5 (C_1, ^2A)	-502.893911	0.212317	-502.157697	-331
tsi23i25 (C_1, ^2A)	-502.808791	0.213275	-502.072369	-105
tsi25p11′ (C_1, ^2A)	-502.847955	0.210174	-502.116939	-230
tsi30i31 (C_1, ^2A)	-502.824927	0.214028	-502.090902	-151
tsi32i33 (C_1, ^2A)	-502.823275	0.213992	-502.090983	-152
tsi31i5 (C_1, ^2A)	-502.837087	0.214801	-502.100599	-175
tsi33i9 (C_1, ^2A)	-502.837807	0.214661	-502.101651	-178
H	-0.502156	0.000000	-0.499810	
p3 (C_1, ^1A)	-502.400500	0.210639	-501.670030	
p4 (C_s, $^1A'$)	-502.299779	0.206644	-501.569713	
p5 (C_1, ^1A)	-502.400447	0.210632	-501.669942	
p6 (C_s, $^1A'$)	-502.302220	0.206888	-501.572642	
p11(C_1, ^1A)	-502.349213	0.209151	-501.620255	
p11′(C_1, ^1A)	-502.349690	0.209009	-501.619947	
p3 + H	-502.902656	0.210639	-502.169840	-367

p4 + H	-502.801935	0.206644	-502.069523	-115
p5 + H	-502.902603	0.210632	-502.169752	-367
p6 + H	-502.804376	0.206888	-502.072452	-122
p11+H	-502.851369	0.209151	-502.120065	-241
p11′+H	-502.851846	0.209009	-502.119757	-240

(c)

	*w*B97X-D/ cc-pVTZ + E_{zpc} [a]	E_{zpc} [b]	CCSD(T)/ cc-pVTZ	E[c] (kJ/mol)
Phenylethynyl (C_{2v}, $^2B_1$)	-307.568246	0.098128	-307.091736	
1,3-pentadiene (C_s, $^1A'$)	-195.196422	0.114016	-194.939183	
Phenylethynyl + 1,3-pentadiene	-502.764668	0.212144	-502.030919	0.0
i13 (C_1, ^2A)	-502.871723	0.216014	-502.141710	-281
vdW(i13) (C_1, ^2A)	-502.772608	0.213044	-502.038693	-18
i14 (C_1, ^2A)	-502.867396	0.216122	-502.131100	-253
i15 (C_1, ^2A)	-502.879890	0.220571	-502.153977	-301
i16 (C_1, ^2A)	-502.938571	0.220126	-502.208502	-445
i17 (C_1, ^2A)	-502.867249	0.216159	-502.139817	-275
vdW(i17) (C_1, ^2A)	-502.773504	0.213311	-502.039458	-19
i18 (C_1, ^2A)	-502.866526	0.215470	-502.131357	-255
i19 (C_1, ^2A)	-502.880644	0.220537	-502.154487	-302
i20 (C_1, ^2A)	-502.943152	0.219536	-502.211146	-454
i26 (C_1, ^2A)	-502.887110	0.218459	-502.156757	-314
i27 (C_1, ^2A)	-502.931230	0.219410	-502.199621	-424
i34 (C_1, ^2A)	-502.841898	0.214535	-502.115268	-215
i35 (C_1, ^2A)	-502.843291	0.215830	-502.107118	-190
i36 (C_1, ^2A)	-502.844046	0.214831	-502.116645	-218
i37 (C_1, ^2A)	-502.842699	0.215833	-502.107565	-192
tsi13vdW (C_1, ^2A)	-502.772461	0.213083	-502.038454	-17
tsi13i14 (C_1, ^2A)	-502.797192	0.210277	-502.054226	-66
tsi13i15 (C_1, ^2A)	-502.831062	0.215982	-502.100354	-172
tsi13i26 (C_1, ^2A)	-502.839580	0.215048	-502.106795	-192
tsi13p8 (C_1, ^2A)	-502.798354	0.207967	-502.060223	-88
tsi14i16 (C_1, ^2A)	-502.857046	0.216085	-502.121864	-228

tsi14p8 (C_1, ^2A)	-502.796332	0.208071	-502.058212	-82
tsi15i16 (C_1, ^2A)	-502.821969	0.214961	-502.086831	-139
tsi16p7 (C_1, ^2A)	-502.889072	0.212828	-502.157211	-330
tsi17vdW (C_1, ^2A)	-502.773187	0.213038	-502.038972	-19
tsi17i26 (C_1, ^2A)	-502.833887	0.214860	-502.102559	-181
tsi1718 (C_1, ^2A)	-502.795457	0.210186	-502.053901	-65
tsi17i19 (C_1, ^2A)	-502.825463	0.216078	-502.096528	-162
tsi17p9 (C_1, ^2A)	-502.795072	0.208052	-502.059087	-85
tsi18i20 (C_1, ^2A)	-502.854724	0.215598	-502.120010	-225
tsi18p9 (C_1, ^2A)	-502.796214	0.207755	-502.059037	-85
tsi19i20 (C_1, ^2A)	-502.825114	0.214623	-502.089243	-147
tsi20p3 (C_1, ^2A)	-502.894099	0.212392	-502.157953	-333
tsi25i27 (C_1, ^2A)	-502.803118	0.213563	-502.068118	-94
tsi27p12 (C_1, ^2A)	-502.841697	0.210835	-502.111031	-214
tsi13i35 (C_1, ^2A)	-502.836881	0.214697	-502.099392	-173
tsi34i35 (C_1, ^2A)	-502.824142	0.213967	-502.089408	-149
tsi17i37 (C_1, ^2A)	-502.836739	0.214640	-502.100608	-176
tsi36i37 (C_1, ^2A)	-502.824349	0.214108	-502.089664	-149
H	-0.502669	0.000000	-0.499810	
p3 (C_1, ^1A)	-502.400475	0.210664	-501.670027	
p7 (C_1, ^1A)	-502.398180	0.210952	-501.667936	
p8 (C_s, $^1A'$)	-502.302864	0.206900	-501.572104	
p9 (C_s, $^1A'$)	-502.302255	0.206558	-501.572483	
p12 (C_1, ^1A)	-502.34429	0.209234	-501.614879	
p3 + H	-502.903144	0.210664	-502.169837	-369
p7 + H	-502.900849	0.210952	-502.167746	-362
p8 + H	-502.805533	0.206900	-502.071914	-121
p9 + H	-502.804924	0.206558	-502.072293	-123

p12 + H	-502.846959	0.209234	-502.114689	-228

[a] wB97XD/cc-pVTZ energy with zero-point energy correction in hartree.
[b] zero-point energy by wB97XD/cc-pVTZ in hartree.
[c] relative energy by CCSD(T)/cc-pVTZ with wB97XD/cc-pVTZ zero-point energy correction.

Table S6 *w*B97X-D/cc-pVTZ optimized cartesian coordinates on the **(a)** phenylethynyl + 1,3-butadiene-d_6, **(b)** phenylethynyl + isoprene, and **(c)** phenylethynyl + 1,3-pentadiene adiabatic doublet ground state potential energy surfaces.

(a)

Atom	X	Y	Z	Atom	X	Y	Z
Phenylethynyl				**1,3-Butadiene-d_6**			
C	0.000000	0.000000	2.063239	C	0.603602	1.736137	0.000000
C	0.000000	0.000000	3.335500	C	0.603602	0.407600	0.000000
C	0.000000	0.000000	0.669896	D	1.524507	2.302178	0.000000
C	0.000000	1.216831	-0.046161	D	-0.322962	2.297576	0.000000
C	0.000000	-1.216831	-0.046161	D	1.547781	-0.128064	0.000000
C	0.000000	1.210125	-1.423103	C	-0.603602	-0.407600	0.000000
H	0.000000	2.143623	0.509225	C	-0.603602	-1.736137	0.000000
C	0.000000	-1.210125	-1.423103	D	-1.547781	0.128064	0.000000
H	0.000000	-2.143623	0.509225	D	-1.524507	-2.302178	0.000000
C	0.000000	0.000000	-2.111120	D	0.322962	-2.297576	0.000000
H	0.000000	2.142392	-1.969839				
H	0.000000	-2.142392	-1.969839				
H	0.000000	0.000000	-3.192694				
i1				**i3**			
C	3.581539	-0.452531	-0.140154	C	0.000000	0.671262	0.000000
C	3.315342	0.816849	0.322194	C	1.064176	1.442133	0.000000
C	4.280286	1.742021	0.653769	C	-1.356631	1.358019	0.000000
D	2.716013	-2.383256	0.095857	C	-1.269922	2.854665	0.000000
D	4.61364	-0.763892	-0.257136	C	-0.143316	3.549760	0.000000
D	2.273525	1.100696	0.430608	C	1.221643	2.903237	0.000000
C	0.027802	-0.705735	-0.247471	D	-1.932668	1.028945	0.871702
D	4.01341	2.724873	1.012775	D	-1.932668	1.028945	-0.871702
D	5.333589	1.509434	0.56414	D	-2.215127	3.384947	0.000000
D	2.723449	-1.802911	-1.543768	D	-0.171171	4.632932	0.000000
C	2.55564	-1.483848	-0.508969	D	1.793219	3.233281	-0.873181
C	-1.330254	-0.27912	-0.107942	D	1.793219	3.233281	0.873181
C	-2.130488	-0.786425	0.916898	C	0.059343	-0.807100	0.000000
C	-1.872418	0.652909	-0.994259	C	1.292349	-1.465116	0.000000
C	-3.443425	-0.369561	1.049242	C	-1.096679	-1.584000	0.000000
H	-1.712381	-1.507533	1.605194	C	1.364670	-2.843826	0.000000
C	1.167436	-1.061933	-0.366135	H	2.199699	-0.874688	0.000000
C	-3.185920	1.066217	-0.856215	C	-1.025047	-2.970258	0.000000

H	-1.254206	1.047048	-1.788683	H	-2.069789	-1.113389	0.000000
C	-3.974916	0.556957	0.164468	C	0.203093	-3.606521	0.000000
H	-4.054303	-0.769468	1.847042	H	2.331280	-3.329674	0.000000
H	-3.595377	1.788914	-1.548773	H	-1.937347	-3.551616	0.000000
H	-5.001102	0.881283	0.270178	H	0.259277	-4.686499	0.000000
i2				**i4**			
C	1.303018	-0.884851	0.000000	C	-2.923759	-1.127837	0.202580
C	0.916421	-2.131254	0.000000	C	-3.557707	0.051425	0.045945
C	-0.479923	-2.593687	0.000000	C	-1.437840	-1.250716	0.125674
C	-1.559421	-1.806595	0.000000	C	-0.704151	0.053578	-0.033262
C	-2.920091	-2.308624	0.000000	C	-1.426507	1.211630	-0.207761
C	-4.000540	-1.532379	0.000000	C	-2.820874	1.242339	-0.183963
D	-0.617242	-3.670008	0.000000	D	-3.487229	-2.035970	0.372672
D	-1.434224	-0.727594	0.000000	D	-4.637842	0.096198	0.093277
D	-3.039084	-3.387808	0.000000	D	-1.187358	-1.921862	-0.710720
D	-3.916557	-0.452410	0.000000	D	-1.061514	-1.782876	1.009583
D	-4.997295	-1.950430	0.000000	D	-0.903972	2.142554	-0.381070
D	1.673573	-2.912437	0.000000	D	-3.339479	2.178441	-0.332386
C	1.282107	0.492255	0.000000	C	0.761189	0.035714	-0.014951
C	1.287918	1.223161	1.216821	C	1.513751	1.202628	0.181656
C	1.287918	1.223161	-1.216821	C	1.469467	-1.161226	-0.177397
C	1.287918	2.599650	1.204216	C	2.894533	1.175234	0.191678
H	1.287835	0.679867	2.151320	H	1.012791	2.144344	0.354792
C	1.287918	2.599650	-1.204216	C	2.854303	-1.187803	-0.168151
H	1.287835	0.679867	-2.151320	H	0.936988	-2.089447	-0.326599
C	1.288502	3.299419	0.000000	C	3.576880	-0.020709	0.013007
H	1.287122	3.140591	2.140963	H	3.444285	2.093246	0.350902
H	1.287122	3.140591	-2.140963	H	3.369717	-2.129148	-0.304253
H	1.290436	4.380338	0.000000	H	4.657902	-0.041018	0.023472
i21				**i22**			
C	0.277590	0.000001	-0.000411	C	-1.534716	-0.341688	0.059370
C	1.570473	-0.000024	-0.000185	C	-1.842691	0.974557	-0.318043
C	2.464178	-0.000246	-1.243762	C	-3.256279	1.146362	-0.353613
C	3.848974	-0.000121	-0.661794	C	-2.854936	-1.058344	0.271020
C	3.848713	0.000134	0.662333	D	-1.129900	1.731248	-0.601675
C	2.463688	0.000242	1.243753	D	-3.750249	2.068625	-0.622231
D	2.279095	0.876332	-1.868674	D	-2.938849	-1.445821	1.290117
D	2.279113	-0.877063	-1.868344	D	-2.954155	-1.917388	-0.398728

D	4.736029	-0.000233	-1.279686
D	4.735523	0.000263	1.280574
D	2.278371	-0.876331	1.868603
D	2.278354	0.877067	1.868243
C	-1.091408	0.000001	-0.000205
C	-1.828800	-1.217644	0.000057
C	-1.828800	1.217646	-0.000281
C	-3.204007	-1.204400	0.000245
H	-1.287056	-2.153226	0.000110
C	-3.204006	1.204402	-0.000089
H	-1.287055	2.153228	-0.000487
C	-3.905871	0.000001	0.000176
H	-3.744989	-2.141359	0.000450
H	-3.744988	2.141362	-0.000142
H	-4.986739	0.000002	0.000325

tsi1i3

C	0.541129	-0.478928	-0.168941
C	1.541134	-1.147934	-0.448694
C	3.005422	-1.186650	-0.349273
C	3.540949	0.222965	-0.212484
C	2.831718	1.223510	0.328696
C	1.566612	1.062823	1.002843
D	3.448124	-1.660036	-1.226546
D	3.291885	-1.806780	0.507454
D	4.493723	0.429813	-0.681886
D	3.203076	2.236213	0.205815
D	1.496699	0.378459	1.836652
D	0.916876	1.925922	1.080276
C	-0.879681	-0.229332	-0.114429
C	-1.741164	-1.206889	0.383383
C	-1.413905	0.979217	-0.560052
C	-3.106408	-0.979598	0.428385
H	-1.328609	-2.144429	0.728868
C	-2.778661	1.201481	-0.514877
H	-0.748434	1.739324	-0.945780
C	-3.629318	0.223725	-0.019489
H	-3.764065	-1.746082	0.815388
H	-3.180587	2.141405	-0.867996

C	1.013136	-0.421453	0.109628
C	1.313519	0.918905	0.385075
C	2.077384	-1.268490	-0.229670
C	2.609984	1.392248	0.287993
H	0.531071	1.584087	0.719219
C	3.371084	-0.793111	-0.330367
H	1.872928	-2.313272	-0.427891
C	3.644660	0.544114	-0.078568
H	2.816640	2.430074	0.513197
H	4.171073	-1.467825	-0.604288
H	4.656467	0.918108	-0.153670
C	-3.878789	-0.007857	-0.014628
D	-4.943912	-0.168532	0.042534
C	-0.323877	-0.979809	0.192824
D	-0.361990	-2.051908	0.357282

tsi1i2

C	0.242819	-0.367381	-0.066523
C	-0.958060	-0.599292	0.081435
C	-2.372094	-0.827895	0.064595
C	-3.341854	0.161053	-0.038060
C	-4.734539	-0.124157	0.006602
C	-5.711589	0.794054	-0.100465
D	-2.670027	-1.870376	0.082797
D	-3.024944	1.192126	-0.137779
D	-5.014656	-1.167225	0.125726
D	-5.483775	1.845547	-0.222411
D	-6.753910	0.511946	-0.071631
D	-1.547858	-0.758951	1.230190
C	1.626150	-0.115989	-0.038313
C	2.113697	1.198947	0.036082
C	2.548718	-1.173315	-0.095049
C	3.473704	1.439118	0.056722
H	1.412122	2.020413	0.076426
C	3.905781	-0.917795	-0.070282
H	2.184051	-2.189028	-0.158157
C	4.377546	0.386167	0.005000
H	3.833102	2.457665	0.114621
H	4.603320	-1.743426	-0.112045

H	-4.695649	0.399856	0.017347	H	5.440895	0.580224	0.021789
tsi1p2				**tsi3i4**			
C	-3.550100	-0.632289	-0.102648	C	-0.699002	-0.075753	0.394519
C	-3.485869	0.802288	0.011752	C	-1.398514	-1.246740	0.287669
C	-4.563401	1.588557	-0.006783	C	-1.541409	1.146347	0.697491
D	-2.630557	-2.520834	-0.247630	C	-2.770035	1.147674	-0.181794
D	-4.532964	-1.078934	-0.195701	C	-3.334884	0.015678	-0.601309
D	-2.500190	1.241425	0.116398	C	-2.724996	-1.256674	-0.193112
C	0.018298	-0.656561	-0.030845	D	-0.982097	2.070066	0.561516
D	-4.480118	2.662726	0.078895	D	-1.852936	1.154378	1.749845
D	-5.560021	1.176661	-0.109520	D	-3.200440	2.104793	-0.450139
D	-2.562768	-2.099297	1.863994	D	-4.222131	0.018803	-1.219710
C	-2.478046	-1.464324	-0.069515	D	-3.349471	-2.130584	-0.042960
C	1.377160	-0.224223	-0.016675	D	-1.769998	-1.803840	-0.880312
C	2.416277	-1.157013	-0.041692	C	0.744291	-0.013707	0.187610
C	1.686225	1.137174	0.022934	C	1.502903	-1.194009	0.216678
C	3.733245	-0.733921	-0.027509	C	1.421536	1.184071	-0.069991
H	2.178875	-2.211112	-0.071368	C	2.864355	-1.175418	-0.013151
C	-1.128578	-1.020041	-0.041581	H	0.998855	-2.123214	0.443185
C	3.005614	1.552804	0.037120	C	2.786475	1.199151	-0.301529
H	0.883527	1.860993	0.042286	H	0.880933	2.118718	-0.113714
C	4.032076	0.620153	0.011862	C	3.517160	0.021940	-0.275256
H	4.530382	-1.464411	-0.046906	H	3.424409	-2.100421	0.022213
H	3.233878	2.609382	0.067998	H	3.281537	2.139142	-0.505917
H	5.062547	0.947776	0.023038	H	4.584060	0.036793	-0.450955
tsi2i4				**tsi2p2**			
C	-0.536709	-0.396640	-0.144780	C	-0.043346	-0.703341	0.131083
C	-1.467024	-1.246131	-0.543027	C	-1.160598	-1.153343	0.286844
C	-2.898865	-1.151667	-0.328547	C	-2.544080	-1.489381	0.186512
C	-3.586016	-0.023555	-0.034423	C	-3.521410	-0.596550	-0.019406
C	-2.949704	1.228513	0.251213	C	-3.338722	0.835108	-0.164368
C	-1.788618	1.308895	0.938776	C	-4.342859	1.681218	-0.375889
D	-1.153133	-2.066509	-1.189834	D	-2.794002	-2.536226	0.293235
D	-3.468651	-2.031753	-0.599711	D	-4.538317	-0.966849	-0.083762
D	-4.664226	-0.041864	-0.144508	D	-2.323695	1.208760	-0.094859
D	-3.382740	2.124807	-0.180237	D	-4.173814	2.743768	-0.480090
D	-1.253550	2.244987	1.030177	D	-5.366532	1.334670	-0.451902
D	-1.502568	0.529734	1.628943	D	-0.823881	-2.260906	1.858333

C	0.861815	-0.199308	-0.110109	C	1.298639	-0.247374	0.049901
C	1.702008	-1.129691	0.530129	C	2.307192	-1.095355	-0.417992
C	1.445611	0.954709	-0.663706	C	1.628580	1.054854	0.438097
C	3.065912	-0.918659	0.591326	C	3.613140	-0.647080	-0.493358
H	1.263049	-2.013305	0.972878	H	2.053089	-2.102301	-0.717403
C	2.809916	1.152806	-0.598332	C	2.936960	1.494700	0.358144
H	0.807272	1.681975	-1.146608	H	0.850764	1.710386	0.804035
C	3.628095	0.219942	0.028578	C	3.932016	0.646912	-0.107214
H	3.697446	-1.646930	1.082312	H	4.386576	-1.310557	-0.855154
H	3.242765	2.041766	-1.037105	H	3.182402	2.503165	0.661535
H	4.695814	0.381802	0.081111	H	4.954343	0.993878	-0.168091
tsi4p1				**tsi1i21**			
C	2.842192	-1.119146	0.328878	C	-0.252582	-0.306718	-0.462730
C	3.525381	0.011645	-0.067948	C	-1.471754	-0.375258	-0.472919
C	1.443630	-1.102547	0.415398	C	-2.795472	-0.681370	-1.059668
C	0.720567	0.023913	-0.024972	C	-3.892782	0.078211	-0.371060
C	1.431425	1.151007	-0.416289	C	-3.642153	0.627388	0.811518
C	2.818463	1.153849	-0.426985	C	-2.348815	0.406516	1.452317
D	3.380359	-2.012570	0.613468	D	-2.971773	-1.759934	-0.993312
D	4.605956	0.007654	-0.108079	D	-2.773513	-0.443013	-2.125460
D	0.913632	-2.022636	0.621483	D	-4.849222	0.178358	-0.866658
D	0.892820	2.028975	-0.747773	D	-4.385644	1.254181	1.296058
D	3.349487	2.040878	-0.744300	D	-1.780682	1.253252	1.816807
D	1.244236	-0.833550	2.238060	D	-2.176687	-0.523185	1.979157
C	-0.757500	0.012407	-0.02303	C	1.136601	-0.138457	-0.242659
C	-1.477200	1.119649	0.422839	C	1.775112	1.056122	-0.599520
C	-1.464789	-1.105789	-0.46146	C	1.897055	-1.161719	0.337485
C	-2.862044	1.110525	0.4272	C	3.129958	1.218650	-0.377783
H	-0.945059	1.986593	0.791447	H	1.193597	1.848993	-1.048840
C	-2.849537	-1.115304	-0.458793	C	3.251601	-0.990163	0.554474
H	-0.925225	-1.968117	-0.830647	H	1.410407	-2.086669	0.613857
C	-3.553619	-0.006853	-0.014276	C	3.873876	0.198500	0.198957
H	-3.402647	1.976401	0.78488	H	3.609766	2.147053	-0.656564
H	-3.380388	-1.989355	-0.811146	H	3.826332	-1.788332	1.004460
H	-4.634979	-0.014401	-0.010771	H	4.933547	0.329084	0.370022
tsi21i22				**tsi22p10**			
C	0.417689	-0.577196	-0.528431	C	1.529818	-0.340322	-0.106827
C	1.569898	0.075328	-0.580705	C	1.797906	0.998583	0.418084

C	2.177647	1.322657	-0.018996	C	3.134210	1.182084	0.429309
C	3.297404	0.680765	0.790995	C	2.848379	-0.942146	-0.361755
C	3.475604	-0.621131	0.520541	D	1.052336	1.684065	0.783828
C	2.541004	-1.053466	-0.530670	D	3.649347	2.062799	0.781270
D	1.474055	1.887526	0.593795	D	2.995903	-1.898815	-0.836377
D	2.590435	2.006620	-0.767120	D	2.938342	-2.091766	1.456772
D	3.904101	1.254824	1.477698	C	-0.989524	-0.423853	-0.183515
D	4.243618	-1.238524	0.963149	C	-1.304808	0.905095	-0.471901
D	2.935689	-1.472238	-1.454300	C	-2.014118	-1.276117	0.233052
D	1.338453	-1.735738	-0.425671	C	-2.597732	1.372726	-0.311473
C	-0.975658	-0.290025	-0.257580	H	-0.537747	1.562759	-0.854949
C	-1.469408	1.013053	-0.380938	C	-3.303880	-0.805530	0.402530
C	-1.846754	-1.301889	0.144714	H	-1.787609	-2.314409	0.439695
C	-2.792837	1.292324	-0.089840	C	-3.598836	0.522914	0.134219
H	-0.810969	1.801928	-0.719871	H	-2.827167	2.403192	-0.546272
C	-3.169248	-1.017260	0.438921	H	-4.081880	-1.477098	0.738934
H	-1.472232	-2.313353	0.227014	H	-4.608124	0.890867	0.258207
C	-3.646698	0.279634	0.324181	C	3.791677	-0.010931	-0.082614
H	-3.161997	2.304158	-0.190986	D	4.857588	-0.128446	-0.198949
H	-3.831636	-1.811933	0.754638	C	0.362612	-0.963800	-0.330577
H	-4.681378	0.499959	0.548501	D	0.414786	-2.005363	-0.633346
p1				**p2**			
C	-0.423660	1.120232	2.839667	C	3.565691	0.728428	0.000000
C	-0.423520	1.119515	1.454556	C	3.539427	-0.721386	0.000000
C	0.000000	0.000000	0.740862	C	4.636070	-1.474159	0.000000
C	0.423520	-1.119515	1.454556	D	2.615433	2.593988	0.000000
C	0.423660	-1.120232	2.839667	C	2.482676	1.519147	0.000000
C	0.000000	0.000000	3.537903	D	4.541666	1.200214	0.000000
D	-0.763056	1.996651	3.375196	C	1.143563	1.053842	0.000000
D	-0.776231	1.990494	0.917854	D	2.562081	-1.190745	0.000000
D	0.776231	-1.990494	0.917854	C	0.000000	0.677226	0.000000
D	0.763056	-1.996651	3.375196	D	4.580334	-2.553658	0.000000
D	0.000000	0.000000	4.619331	D	5.624726	-1.031005	0.000000
C	0.000000	0.000000	-0.740862	C	-1.352499	0.225500	0.000000
C	-0.423520	-1.119515	-1.454556	C	-2.405821	1.142830	0.000000
C	0.423520	1.119515	-1.454556	C	-1.642004	-1.140946	0.000000
C	-0.423660	-1.120232	-2.839667	C	-3.716399	0.700122	0.000000
H	-0.776231	-1.990494	-0.917854	H	-2.184240	2.200824	0.000000

C	0.423660	1.120232	-2.839667
H	0.776231	1.990494	-0.917854
C	0.000000	0.000000	-3.537903
H	-0.763056	-1.996651	-3.375196
H	0.763056	1.996651	-3.375196
H	0.000000	0.000000	-4.619331

C	-2.955101	-1.576345	0.000000
H	-0.828622	-1.853020	0.000000
C	-3.995379	-0.658792	0.000000
H	-4.524246	1.419064	0.000000
H	-3.167565	-2.636692	0.000000
H	-5.020911	-1.001775	0.000000

p10

C	1.564511	-0.378907	-0.086112
C	1.843535	0.979970	0.390750
C	3.179201	1.132025	0.440248
C	2.873636	-1.007352	-0.297993
D	1.101983	1.698393	0.696181
D	3.705868	2.014282	0.771102
D	3.010771	-2.015825	-0.655567
C	-0.957272	-0.441056	-0.161689
C	-1.261060	0.876933	-0.506693
C	-1.989529	-1.265135	0.290712
C	-2.549854	1.362531	-0.366729
H	-0.487978	1.510850	-0.916599
C	-3.275377	-0.776593	0.439243
H	-1.772586	-2.295871	0.541131
C	-3.558728	0.541684	0.114381
H	-2.769927	2.384173	-0.645155
H	-4.059306	-1.426493	0.803420
H	-4.564692	0.923609	0.222215
C	3.825247	-0.106724	-0.001094
D	4.892151	-0.255577	-0.063776
C	0.390956	-0.998625	-0.287726
D	0.432121	-2.050055	-0.556735

vdW(i1)

C	-2.487581	-0.270770	0.003178
C	-1.793564	-1.026550	-1.031145
C	-1.190758	-0.468424	-2.075614
D	-3.087891	-1.901340	1.194740
D	-2.497834	0.809126	-0.109297
D	-1.779965	-2.106151	-0.916252
C	0.156511	2.139829	0.322255
D	-0.685205	-1.064169	-2.822851
D	-1.188634	0.606557	-2.212080
D	-3.585192	-0.227394	1.799724
C	-3.081784	-0.826733	1.054047
C	0.897113	0.960916	0.324181
C	1.852396	0.715445	-0.685814
C	0.669189	-0.023442	1.308785
C	2.545179	-0.473297	-0.708498
H	2.016457	1.473593	-1.437987
C	-0.635996	3.126907	0.224943
C	1.365989	-1.210058	1.272961
H	-0.074837	0.166397	2.068094
C	2.300486	-1.436275	0.266837
H	3.273460	-0.662447	-1.484283
H	1.183922	-1.967543	2.021993
H	2.842635	-2.371933	0.241509

tsi1vdW

C	-2.361482	-0.633647	-0.172768
C	-1.423594	-1.745346	-0.112333
C	-0.674622	-2.141438	-1.136349
H	-3.007922	-0.692397	1.830328
H	-2.448911	-0.122113	-1.126131
H	-1.339848	-2.256766	0.841778
C	-0.418187	2.045251	-0.319802

H	0.019454	-2.965339	-1.046732				
H	-0.736112	-1.648675	-2.099155				
H	-3.737503	0.642765	0.778948				
C	-3.075266	-0.206848	0.863662				
C	0.598947	1.132386	-0.047965				
C	1.449543	0.679546	-1.077515				
C	0.770087	0.623297	1.256104				
C	2.43731	-0.241685	-0.806025				
H	1.307649	1.069558	-2.075187				
C	-1.397337	2.815946	-0.571412				
C	1.75564	-0.302566	1.513698				
H	0.104259	0.965889	2.034843				
C	2.589793	-0.733247	0.485937				
H	3.089019	-0.586292	-1.596352				
H	1.881938	-0.69604	2.512419				
H	3.362982	-1.460495	0.693842				
i28				**i29**			
C	-3.64913	0.533346	-0.492974	C	3.534025	-0.662731	-0.557062
D	-3.100907	-1.490222	-0.786189	D	3.063262	1.367877	-1.186953
D	-4.723433	0.384914	-0.512163	D	4.595935	-0.617033	-0.778691
C	-0.228054	-0.341175	-0.050068	C	0.285538	0.522773	0.203448
C	-2.871897	-0.69337	-0.070542	C	2.866242	0.651962	-0.396315
C	1.188121	-0.150076	-0.016125	C	-1.053354	0.23379	0.097033
C	2.033778	-0.97777	-0.756426	C	-1.964048	1.163771	-0.470277
C	1.743777	0.869603	0.758562	C	-1.570756	-1.006188	0.557123
C	3.403963	-0.787393	-0.720553	C	-3.302622	0.859928	-0.568195
H	1.605649	-1.767604	-1.357591	H	-1.58757	2.112977	-0.824823
C	-1.418455	-0.496286	-0.084028	C	1.535028	0.758946	0.249507
C	3.114756	1.055077	0.789543	C	-2.913418	-1.287417	0.447961
H	1.090459	1.510637	1.333835	H	-0.892118	-1.724254	0.996149
C	3.948473	0.228336	0.051218	C	-3.79136	-0.36277	-0.113142
H	4.04964	-1.434634	-1.298272	H	-3.980741	1.581092	-1.004586
H	3.534193	1.848298	1.393243	H	-3.288053	-2.238029	0.803359
H	5.019532	0.375168	0.077183	H	-4.844485	-0.592096	-0.194382
C	-3.290399	-1.154902	1.295783	C	2.711011	1.264689	0.992995
D	-3.230713	-2.201021	1.556814	D	2.827824	2.335801	1.094977
D	-3.423837	-0.423396	2.079856	D	3.053642	0.672957	1.832349
C	-3.137483	1.71087	-0.805364	C	2.942121	-1.840249	-0.436919

D	-2.068885	1.884223	-0.792529	D	1.881779	-1.917902	-0.231563
D	-3.776402	2.536084	-1.088349	D	3.500079	-2.760405	-0.542785
tsi28i29				**tsi1i29**			
C	3.772347	-0.465776	-0.294073	C	-3.169982	0.71229	-0.917223
D	3.19341	1.522327	-0.881885	D	-2.703306	-1.345638	-1.424159
D	4.827606	-0.271089	-0.134475	D	-3.115957	0.973556	-1.968148
C	0.259422	0.330109	-0.160487	C	-0.209678	-0.637776	0.446571
C	2.897349	0.741491	-0.18227	C	-2.785659	-0.643571	-0.608213
C	-1.129923	0.120905	-0.085359	C	1.120532	-0.26603	0.220737
C	-2.029985	1.09833	-0.539558	C	2.05335	-1.186305	-0.292916
C	-1.645484	-1.074727	0.440941	C	1.557232	1.039901	0.513326
C	-3.392264	0.882966	-0.464444	C	3.363113	-0.807778	-0.507401
H	-1.642727	2.021209	-0.948134	H	1.729553	-2.192931	-0.517805
C	1.465518	0.559443	-0.113565	C	-1.426029	-0.87159	0.469875
C	-3.009998	-1.277677	0.509213	C	2.871023	1.402288	0.295507
H	-0.960135	-1.832834	0.793697	H	0.847525	1.754063	0.906834
C	-3.890959	-0.303156	0.058469	C	3.781584	0.484948	-0.215231
H	-4.072713	1.646244	-0.817201	H	4.067161	-1.526142	-0.905363
H	-3.391343	-2.203612	0.918178	H	3.190385	2.410285	0.523658
H	-4.958176	-0.466975	0.113937	H	4.809317	0.774982	-0.383914
C	2.614213	1.263421	1.189318	C	-2.795333	-1.224744	0.769374
D	2.454797	2.31705	1.350323	D	-3.007623	-2.286065	0.841689
D	2.669031	0.588901	2.028602	D	-3.284019	-0.645304	1.545776
C	3.347518	-1.691858	-0.544818	C	-3.547441	1.65749	-0.048844
D	2.296578	-1.899293	-0.703753	D	-3.610378	1.476822	1.016555
D	4.037151	-2.522766	-0.599494	D	-3.798929	2.651632	-0.388499
tsi2p13				**phenylacetylene**			
C	0.101434	-1.460891	0.753932	C	0.000000	0.000000	2.015547
C	1.139741	-2.041497	0.982014	C	0.000000	0.000000	3.213755
C	2.786023	-1.254322	-0.557276	C	0.000000	0.000000	0.585581
C	3.011488	0.032445	-0.70307	C	0.000000	1.204314	-0.119421
C	2.411087	1.098914	0.092845	C	0.000000	-1.204314	-0.119421
C	2.649022	2.390094	-0.109692	C	0.000000	1.200407	-1.503092
D	1.859991	-2.700056	1.403917	H	0.000000	2.136697	0.427380
D	3.707226	0.353881	-1.481575	C	0.000000	-1.200407	-1.503092
D	1.739334	0.786726	0.882657	H	0.000000	-2.136697	0.427380
D	3.316425	2.725438	-0.894619	C	0.000000	0.000000	-2.197833
C	-1.019504	-0.681069	0.361153	H	0.000000	2.138144	-2.041662

C	-1.78874	-1.054553	-0.744519	H	0.000000	-2.138144	-2.041662
C	-1.358914	0.476245	1.068008	H	0.000000	0.000000	-3.279220
C	-2.869849	-0.284275	-1.131594	D	0.000000	0.000000	4.275628
H	-1.525395	-1.947652	-1.293302				
C	-2.441026	1.241117	0.672872				
H	-0.767124	0.765248	1.925418				
C	-3.199229	0.864343	-0.426258				
H	-3.457786	-0.580132	-1.989602				
H	-2.694205	2.135702	1.225086				
H	-4.044802	1.4647	-0.732544				
D	2.18299	3.151549	0.499868				
D	3.15415	-2.114704	-1.095801				
p13							
C	-1.888814	-0.192403	0.000026				
C	-0.688411	0.330657	-0.000303				
C	0.562491	-0.424617	0.000232				
C	1.762344	0.144871	-0.000012				
D	-0.593457	1.419878	0.001434				
D	0.473221	-1.504492	0.000252				
D	1.875716	1.222231	-0.000461				
D	2.666794	-0.44682	-0.000462				
D	-2.907933	0.15816	-0.000418				
C	-1.888814	-0.192403	0.000026				
C	-0.688411	0.330657	-0.000303				
C	0.562491	-0.424617	0.000232				
C	1.762344	0.144871	-0.000012				
D	-0.593457	1.419878	0.001434				
D	0.473221	-1.504492	0.000252				
D	1.875716	1.222231	-0.000461				
D	2.666794	-0.44682	-0.000462				
D	-2.907933	0.15816	-0.000418				

(b)

Atom	X	Y	Z	Atom	X	Y	Z
phenylethynyl				**Isoprene**			
C	0.000000	0.000000	2.063239	C	0.000000	0.525818	0.000000
C	0.000000	0.000000	3.335500	H	-1.663021	1.821120	0.000000
C	0.000000	0.000000	0.669896	C	-0.584876	1.722862	0.000000
C	0.000000	1.216831	-0.046161	C	-0.825145	-0.686586	0.000000
C	0.000000	-1.216831	-0.046161	H	-0.006327	2.637143	0.000000
C	0.000000	1.210125	-1.423103	C	-0.369048	-1.934462	0.000000
H	0.000000	2.143623	0.509225	H	-1.897584	-0.520810	0.000000
C	0.000000	-1.210125	-1.423103	H	-1.047892	-2.775807	0.000000
H	0.000000	-2.143623	0.509225	H	0.689154	-2.161359	0.000000
C	0.000000	0.000000	-2.111120	C	1.493244	0.374837	0.000000
H	0.000000	2.142392	-1.969839	H	1.828042	-0.180338	0.878386
H	0.000000	-2.142392	-1.969839	H	1.828042	-0.180338	-0.878386
H	0.000000	0.000000	-3.192694	H	1.984536	1.345575	0.000000
i5				**i7**			
C	-2.77966	0.294927	-0.241365	C	-0.295647	0.317431	0.000037
H	-2.221856	-1.023065	1.352836	C	-0.844078	1.510937	0.000160
C	-1.954315	-0.832335	0.307158	C	-1.234859	-0.875699	-0.000037
C	-4.16771	0.333492	-0.171885	C	-2.698559	-0.524410	-0.000149
C	0.660936	-0.385466	0.148921	C	-3.144372	0.725295	-0.000124
H	-2.1899	-1.764433	-0.221053	C	-2.248070	1.939851	-0.000021
C	-4.869056	1.390611	-0.704551	H	-1.023407	-1.506840	0.871203
H	-5.94803	1.432145	-0.657795	H	-1.023236	-1.506856	-0.871221
H	-4.355435	2.211543	-1.186305	H	-2.461885	2.564736	-0.873123
C	-0.517969	-0.59532	0.223291	H	-2.462158	2.564819	0.872947
C	2.066763	-0.13622	0.063924	C	1.165029	0.084172	0.000066
C	2.926735	-1.099982	-0.464887	C	1.698719	-1.202387	0.000511
C	2.597923	1.075447	0.508791	C	2.053202	1.163314	-0.00037
C	4.286395	-0.854826	-0.545105	C	3.071887	-1.405527	0.000541
H	2.518129	-2.039151	-0.81072	H	1.044765	-2.063109	0.000844
C	3.958352	1.314955	0.425177	C	3.419069	0.962341	-0.000333
H	1.933936	1.823351	0.919155	H	1.653055	2.16919	-0.000751
C	4.806347	0.351889	-0.101161	C	3.937754	-0.326872	0.000125
H	4.943047	-1.609281	-0.956515	H	3.461987	-2.41454	0.000895
H	4.358264	2.257672	0.772997	H	4.086011	1.814136	-0.000675
H	5.869137	0.54117	-0.16514	H	5.007612	-0.484744	0.000147
H	-2.254503	1.107891	-0.724837	H	-4.212236	0.914952	-0.000184
C	-4.908282	-0.79863	0.495534	C	-3.627879	-1.701677	-0.000269

H	-4.685087	-1.753409	0.015858	H	-4.671566	-1.392002	-0.00032
H	-4.622109	-0.891534	1.544957	H	-3.456006	-2.330135	-0.8776
H	-5.984338	-0.644158	0.453516	H	-3.456119	-2.330227	0.877018
i6				**i8**			
C	-0.109424	1.003074	-0.385485	C	-0.322940	0.346360	-0.063819
C	0.921634	1.685872	-0.787079	C	-0.857894	1.607920	-0.182945
C	2.290908	1.684969	-0.244573	C	-1.251437	-0.833998	0.009682
C	3.084057	0.707199	0.208044	C	-2.713469	-0.512499	0.072885
C	2.938498	-0.751880	0.251255	C	-3.143653	0.764255	-0.028930
C	3.881271	-1.452884	0.885075	C	-2.232285	1.839920	-0.178494
H	0.753280	2.430045	-1.569874	H	-0.200559	2.459187	-0.294724
H	2.721013	2.681225	-0.217544	H	-0.982585	-1.466459	0.867793
H	3.841590	-2.532789	0.938409	H	-1.088296	-1.492060	-0.859440
H	4.716557	-0.966612	1.372403	H	-2.605734	2.848685	-0.280894
C	-1.348374	0.454779	-0.168504	C	1.120575	0.099994	-0.025157
C	-1.767405	-0.711779	-0.864029	C	2.041396	1.127097	0.22944
C	-2.238966	1.014861	0.787068	C	1.638942	-1.185376	-0.226726
C	-3.00152	-1.267544	-0.61566	C	3.400632	0.884848	0.257966
H	-1.102364	-1.151973	-1.593592	H	1.689505	2.128358	0.432716
C	-3.46789	0.440852	1.016702	C	3.002553	-1.427344	-0.198716
H	-1.933097	1.898969	1.328475	H	0.972964	-2.013532	-0.421522
C	-3.86146	-0.701625	0.322752	C	3.893523	-0.39496	0.040424
H	-3.304701	-2.152908	-1.158243	H	4.082465	1.699658	0.46189
H	-4.133769	0.88356	1.74523	H	3.368527	-2.431587	-0.365938
H	-4.828324	-1.146273	0.511647	H	4.957936	-0.583491	0.065316
H	4.041145	1.043594	0.593469	H	-4.206028	0.973802	0.002283
C	1.798749	-1.453579	-0.428943	C	-3.638001	-1.674941	0.226335
H	0.866383	-1.307941	0.115659	H	-3.507786	-2.387435	-0.59356
H	1.646786	-1.069872	-1.437742	H	-3.427501	-2.221198	1.150176
H	1.995039	-2.522906	-0.488038	H	-4.680564	-1.361587	0.244236
i23				**i24**			
C	-3.312606	-0.067507	1.074020	C	2.889515	1.229129	-0.000043
H	-1.649814	0.736356	2.206906	H	0.973161	1.679659	0.878017
C	-1.888470	-0.099415	1.544991	C	1.394818	1.182047	-0.000009
C	-3.430931	0.015853	-0.244694	C	3.401183	-0.026148	-0.000014
C	0.192204	-0.009574	0.132865	C	-0.130798	-0.941365	0.000030
H	-1.651904	-1.013441	2.094745	H	0.973110	1.679646	-0.878015
C	-2.087144	0.056844	-0.923547	C	2.321580	-0.962592	0.000023
C	-1.096215	-0.016352	0.237209	C	1.089638	-0.300066	0.000017

C	1.556381	-0.001899	0.024160	C	-1.474618	-0.413271	0.000017
C	2.292482	-1.212893	-0.111504	C	-2.539811	-1.330675	-0.000022
C	2.291146	1.217340	0.041867	C	-1.806086	0.951556	0.000041
C	3.663037	-1.191935	-0.220695	C	-3.856034	-0.914594	-0.00004
H	1.753043	-2.149694	-0.126941	H	-2.315238	-2.389958	-0.000038
C	3.661726	1.211814	-0.068995	C	-3.125975	1.365076	0.000023
H	1.750791	2.148089	0.144355	H	-1.031601	1.700821	0.000078
C	4.362164	0.013894	-0.201083	C	-4.159797	0.440177	-0.000018
H	4.202569	-2.124115	-0.322945	H	-4.650537	-1.648784	-0.000071
H	4.200314	2.150023	-0.053146	H	-3.349816	2.423622	0.000043
H	5.439511	0.019958	-0.287579	H	-5.189303	0.770661	-0.000033
H	-4.149389	-0.109684	1.758788	H	3.46184	2.144837	-0.000081
C	-4.691846	0.067729	-1.038005	C	4.846375	-0.406099	-0.000005
H	-5.570427	0.029605	-0.395741	H	5.486392	0.474601	-0.000212
H	-4.739306	0.983535	-1.632007	H	5.091236	-1.005423	0.878436
H	-4.742898	-0.76724	-1.740875	H	5.091157	-1.005784	-0.878221
H	-1.956182	0.971579	-1.507927	H	-0.077195	-2.025276	0.000045
H	-1.957871	-0.77837	-1.617173	H	2.436858	-2.037666	0.000044
i9				**i11**			
C	3.171096	-0.248427	0.059236	C	0.203840	-0.019945	0.000143
H	2.355688	-2.197282	-0.212941	C	0.936762	-1.109802	0.000503
C	2.168401	-1.316705	0.413109	C	0.946759	1.305198	-0.000264
C	2.795317	1.013701	-0.374767	C	2.438584	1.162705	-0.000420
C	-0.393292	-0.643944	0.206351	C	3.110380	0.018889	-0.000071
H	2.361566	-1.653527	1.438862	C	2.389329	-1.315242	0.000520
C	3.657581	2.027958	-0.709996	H	0.639204	1.893311	0.871443
H	1.731429	1.207328	-0.453789	H	0.638933	1.892916	-0.872140
H	3.281899	2.984626	-1.041820	H	2.997601	2.092558	-0.000842
H	4.731533	1.911297	-0.656685	H	2.701217	-1.899936	-0.872030
C	0.763648	-0.948772	0.297881	H	2.701312	-1.899224	0.873512
C	-1.770258	-0.272788	0.099565	C	-1.27466	-0.0222	0.000063
C	-2.625439	-0.959832	-0.763293	C	-1.979596	-1.228958	-0.000344
C	-2.276357	0.785034	0.856646	C	-2.006674	1.162841	0.000373
C	-3.956602	-0.595202	-0.863913	C	-3.359965	-1.248291	-0.000391
H	-2.235549	-1.778725	-1.351468	H	-1.424032	-2.158096	-0.000636
C	-3.608265	1.145491	0.750663	C	-3.394489	1.144451	0.000322
H	-1.615567	1.318212	1.525812	H	-1.498044	2.116648	0.000674
C	-4.45193	0.457311	-0.10854	C	-4.077447	-0.058348	-0.000056
H	-4.610177	-1.134902	-1.535612	H	-3.882698	-2.195478	-0.000709

H	-3.989248	1.967005	1.341881	H	-3.940461	2.078376	0.000575
H	-5.492446	0.740512	-0.189392	H	-5.158763	-0.073031	-0.000102
C	4.609366	-0.637116	0.205064	C	4.606107	-0.055949	-0.000214
H	5.145536	-0.539866	-0.742284	H	4.967509	-0.598113	-0.877551
H	5.122626	0.003053	0.9273	H	5.056921	0.935257	-0.000735
H	4.713102	-1.668001	0.542104	H	4.967714	-0.597282	0.877554
i10				**i12**			
C	0.158454	-1.141894	-0.393634	C	0.236826	-0.038454	-0.040259
C	-0.969687	-1.752558	-0.616851	C	0.975346	-1.190107	-0.200917
C	-2.323976	-1.341376	-0.220425	C	0.962745	1.270202	0.095982
C	-2.792583	-0.109731	0.037386	C	2.450412	1.162884	0.157078
C	-1.970800	1.090767	-0.108883	C	3.114679	-0.002075	0.016230
C	-2.318828	2.313174	0.283457	C	2.366114	-1.200972	-0.187222
H	-0.925487	-2.712196	-1.135370	H	0.466870	-2.132018	-0.355765
H	-3.023632	-2.166592	-0.144636	H	0.593665	1.807809	0.979848
H	-1.008196	0.959164	-0.586027	H	0.695157	1.930468	-0.743614
H	-1.657630	3.153663	0.124725	H	3.000466	2.084399	0.306207
H	-3.258302	2.519334	0.779459	H	2.893061	-2.135863	-0.325324
C	1.37832	-0.564046	-0.179331	C	-1.227053	-0.035217	-0.015624
C	1.92366	0.366092	-1.108952	C	-1.969897	-1.21192	0.162097
C	2.136692	-0.856365	0.989171	C	-1.947043	1.158369	-0.15396
C	3.14477	0.953895	-0.8744	C	-3.350653	-1.196211	0.178751
H	1.362285	0.599543	-2.003111	H	-1.461667	-2.153409	0.313385
C	3.3555	-0.2555	1.198443	C	-3.331876	1.173059	-0.137771
H	1.735688	-1.556937	1.707888	H	-1.423171	2.093685	-0.288284
C	3.872366	0.652211	0.275219	C	-4.04415	-0.003044	0.025405
H	3.542619	1.657543	-1.593357	H	-3.89189	-2.121846	0.322428
H	3.917394	-0.491263	2.092292	H	-3.855623	2.112453	-0.254352
H	4.831127	1.11943	0.450157	H	-5.125246	0.007869	0.040817
C	-4.219027	0.069899	0.474087	C	4.613867	-0.080759	0.063689
H	-4.266076	0.499496	1.477232	H	4.94273	-0.738506	0.870288
H	-4.750029	0.751741	-0.192485	H	5.009981	-0.489551	-0.867714
H	-4.748932	-0.880344	0.491502	H	5.059768	0.899989	0.221202
i25							
C	3.395349	-0.902259	-0.000089				
C	2.187316	-1.648396	0.000161				
C	3.130464	0.429483	-0.000206				
C	-0.226962	-1.200388	0.000277				
H	2.116828	-2.726102	0.000275				

C	1.641477	0.624992	0.000021				
C	1.082676	-0.781672	0.000211				
C	-1.459880	-0.446365	0.000180				
C	-2.668087	-1.164491	-0.000443				
C	-1.549644	0.954935	0.000692				
C	-3.892178	-0.526155	-0.000613				
H	-2.630984	-2.246689	-0.000817				
C	-2.777773	1.591735	0.00053				
H	-0.65732	1.559028	0.001277				
C	-3.956441	0.860735	-0.000137				
H	-4.801951	-1.111501	-0.001115				
H	-2.814194	2.673111	0.000946				
H	-4.912951	1.364912	-0.000264				
C	4.095016	1.560394	-0.00044				
H	5.124163	1.204294	-0.000717				
H	3.955725	2.198392	-0.877344				
H	3.956195	2.198356	0.876569				
H	1.316826	1.191454	0.878044				
H	1.316422	1.191458	-0.877843				
H	-0.362654	-2.277134	0.000297				
H	4.385907	-1.334862	-0.000182				
tsi5i7				**tsi5i6**			
C	0.141849	-0.777004	0.269432	C	0.688297	-0.278751	-0.086584
C	1.060337	-1.597685	0.334905	C	-0.523057	-0.455048	0.047364
C	2.517178	-1.739993	0.447596	C	-1.947709	-0.611608	0.017275
C	3.192601	-0.506166	-0.113215	C	-2.855177	0.435522	-0.073467
C	2.636350	0.714452	-0.110278	C	-4.278334	0.279158	-0.030392
C	1.403490	1.004763	0.599543	C	-5.085124	1.354682	-0.127526
H	2.867776	-2.621306	-0.090555	H	-2.289750	-1.639115	0.006719
H	2.780172	-1.901937	1.498646	H	-4.679157	2.352249	-0.232786
H	1.350493	0.803101	1.660594	H	-6.161629	1.256463	-0.107408
H	0.821175	1.858577	0.271509	H	-1.133774	-0.618880	1.190241
C	-1.227649	-0.353898	0.110639	C	2.082431	-0.096783	-0.044425
C	-1.828844	0.508755	1.026685	C	2.633403	1.190085	0.067625
C	-1.973808	-0.813311	-0.975197	C	2.95245	-1.196298	-0.123945
C	-3.146559	0.898293	0.862609	C	4.0034	1.362519	0.10235
H	-1.257142	0.869107	1.870713	H	1.972566	2.043648	0.125687
C	-3.292014	-0.421741	-1.134525	C	4.320276	-1.008686	-0.084636
H	-1.508206	-1.479844	-1.687446	H	2.538748	-2.190801	-0.216042

C	-3.882524	0.435141	-0.218046	C	4.854866	0.268059	0.027931
H	-3.601434	1.565244	1.582321	H	4.411956	2.360267	0.189355
H	-3.859905	-0.786477	-1.979669	H	4.976816	-1.86625	-0.144137
H	-4.91189	0.741158	-0.345172	H	5.926319	0.409037	0.056027
C	3.23926	1.846224	-0.902268	C	-4.858692	-1.102466	0.113897
H	3.510675	2.683528	-0.257146	H	-4.566979	-1.742066	-0.721622
H	4.128812	1.525596	-1.442647	H	-4.508913	-1.582685	1.030064
H	2.515663	2.222343	-1.62933	H	-5.945418	-1.065811	0.1453
H	4.125813	-0.666063	-0.639098	H	-2.462962	1.441643	-0.154197
tsi5i23				**tsi5p4**			
C	-3.401272	0.703200	-0.463594	C	-2.149100	-1.633131	-0.005432
H	-2.121872	2.041383	-1.548814	C	-3.299721	-0.917120	-0.098852
C	-2.211979	1.615677	-0.546794	C	-0.816495	-1.139383	0.002897
C	-3.299840	-0.439714	0.209947	C	-3.511107	0.519239	-0.047174
C	0.246016	0.700179	-0.230864	C	0.331868	-0.781706	-0.005574
H	-2.322781	2.465734	0.134875	C	-4.765353	0.975437	-0.155902
C	-2.046177	-0.706169	0.922135	H	-2.229352	-2.706136	-0.131286
C	-0.957063	0.903493	-0.219973	H	-4.985886	2.033842	-0.122656
C	1.596337	0.283516	-0.125810	C	1.674811	-0.303179	-0.011860
C	2.402419	0.730925	0.928393	H	-5.602305	0.301023	-0.282342
C	2.149348	-0.585945	-1.074362	H	-2.207592	-2.131451	1.952404
C	3.717921	0.317368	1.028218	C	2.749423	-1.192449	-0.075724
H	1.982088	1.403519	1.663034	C	1.929463	1.069062	0.04697
C	3.465576	-0.994827	-0.965742	C	4.048313	-0.716176	-0.081141
H	1.532385	-0.933477	-1.891231	H	2.554093	-2.254651	-0.120159
C	4.255306	-0.546121	0.083772	C	3.230879	1.537908	0.041241
H	4.328594	0.670226	1.848252	H	1.098207	1.758549	0.098095
H	3.878979	-1.667972	-1.704583	C	4.293129	0.648037	-0.02294
H	5.284631	-0.867284	0.164857	H	4.873824	-1.412963	-0.130629
H	-4.310956	0.987642	-0.977616	H	3.417259	2.602142	0.087348
C	-4.388296	-1.474065	0.257964	H	5.309636	1.016861	-0.027171
H	-5.249893	-1.17384	-0.337587	C	-2.357806	1.464523	0.133884
H	-4.020422	-2.428388	-0.125731	H	-1.800005	1.230103	1.040806
H	-4.718087	-1.649909	1.283602	H	-1.656547	1.3897	-0.697096
H	-1.559502	-1.665986	0.79408	H	-2.714838	2.49075	0.198185
H	-1.872931	-0.226748	1.877122	H	-4.206324	-1.504154	-0.187857
tsi7i8				**tsi6i8**			
C	0.331350	0.400275	0.426116	C	-0.137825	-0.648674	-0.140973
C	0.837359	1.663742	0.266358	C	-0.950850	-1.581055	-0.602075

C	1.348659	-0.650593	0.811030	C	-2.379682	-1.696727	-0.358326
C	2.598778	-0.524211	-0.038010	C	-3.198758	-0.699609	0.037535
C	2.975243	0.669434	-0.505547	C	-2.724101	0.617009	0.391787
C	2.158679	1.846355	-0.191561	C	-1.583103	0.742424	1.108257
H	0.945328	-1.658430	0.717508	H	-0.544921	-2.299801	-1.314903
H	1.633244	-0.557086	1.867501	H	-2.833166	-2.627586	-0.676070
H	2.635373	2.815376	-0.088192	H	-1.140350	1.713601	1.292028
H	1.154959	2.193245	-0.933559	H	-1.234085	-0.065932	1.732291
C	-1.077119	0.095090	0.201378	C	1.220035	-0.258582	-0.112720
C	-2.011656	1.139761	0.12406	C	2.197265	-1.098529	0.453273
C	-1.553227	-1.210331	0.028271	C	1.62281	0.999746	-0.595861
C	-3.346156	0.889962	-0.126584	C	3.518843	-0.699838	0.510578
H	-1.665144	2.151155	0.284701	H	1.897557	-2.062213	0.841885
C	-2.892001	-1.457371	-0.224121	C	2.94669	1.385412	-0.535433
H	-0.874347	-2.05005	0.069958	H	0.877725	1.658871	-1.02029
C	-3.797477	-0.411477	-0.304024	C	3.902398	0.540612	0.017335
H	-4.0438	1.71558	-0.174209	H	4.257525	-1.360963	0.943729
H	-3.228678	-2.476458	-0.360733	H	3.239683	2.353231	-0.919809
H	-4.843524	-0.607213	-0.495964	H	4.937494	0.849052	0.0665
H	3.876673	0.781388	-1.094294	C	-3.464424	1.797904	-0.167204
C	3.377636	-1.778115	-0.270985	H	-3.441442	1.797647	-1.259209
H	2.771072	-2.508538	-0.811985	H	-4.515557	1.760568	0.128448
H	4.287222	-1.593601	-0.839848	H	-3.046164	2.738062	0.188323
H	3.65121	-2.240492	0.680841	H	-4.27008	-0.855092	-0.039959
tsi6p4				**tsi8p3**			
C	-0.295511	-0.809522	0.088204	C	-0.352530	0.316090	0.077269
C	0.835921	-1.220330	0.249149	C	-0.870899	1.570588	0.378698
C	2.183798	-1.663615	0.091666	C	-1.251593	-0.737853	-0.153914
C	3.287719	-0.922356	-0.069491	C	-2.638983	-0.520523	-0.190898
C	3.461158	0.530356	-0.105807	C	-3.117332	0.742981	0.105966
C	4.691831	1.009990	-0.299386	C	-2.239540	1.779095	0.401060
H	2.304001	-2.739997	0.111995	H	-0.199159	2.386055	0.610281
H	4.884518	2.073964	-0.332661	H	-0.864549	-1.683519	-0.512716
H	5.540968	0.351613	-0.429841	H	-2.628139	2.759259	0.642380
H	0.675096	-1.880637	2.055237	H	-1.239811	-1.606159	1.556695
C	-1.622435	-0.313801	0.022481	C	1.107023	0.084751	0.023046
C	-1.873812	1.047144	0.227003	C	1.663074	-1.101172	0.500706
C	-2.693302	-1.171864	-0.246802	C	1.961281	1.049169	-0.510762
C	-3.166434	1.533424	0.163087	C	3.030614	-1.314233	0.449066

H	-1.046791	1.710948	0.437303	H	1.019527	-1.851345	0.941459
C	-3.982691	-0.676339	-0.30818	C	3.328192	0.83562	-0.564215
H	-2.500215	-2.223594	-0.404294	H	1.54705	1.965629	-0.909852
C	-4.223516	0.67504	-0.104405	C	3.868819	-0.347347	-0.08382
H	-3.351073	2.586721	0.323745	H	3.443286	-2.237166	0.83368
H	-4.804769	-1.347518	-0.515577	H	3.972703	1.592852	-0.98994
H	-5.233361	1.058512	-0.153421	H	4.936454	-0.514544	-0.125179
C	2.291069	1.45339	0.078453	H	-4.184319	0.925261	0.104444
H	1.550423	1.308395	-0.708125	C	-3.558954	-1.6632	-0.501543
H	1.788425	1.262103	1.026839	H	-3.289898	-2.140466	-1.444728
H	2.620287	2.490804	0.060695	H	-3.493581	-2.424833	0.278741
H	4.20972	-1.480424	-0.187732	H	-4.594604	-1.334821	-0.569223
tsi23i24				**tsi24p11**			
C	-2.843295	1.017790	-0.630135	C	-2.653308	1.206329	0.398637
H	-0.912325	2.061170	-0.681962	H	-0.556294	1.754958	0.583734
C	-1.621876	1.640381	0.031819	C	-1.312426	1.016782	0.381166
C	-3.127342	-0.225176	-0.205951	C	-3.331755	-0.021809	-0.010685
C	-0.007535	-0.349181	0.680493	C	0.093735	-0.987205	-0.323062
H	-1.918137	2.441015	0.716869	H	-0.955151	0.513886	2.411295
C	-2.161718	-0.608908	0.844440	C	-2.389981	-0.945272	-0.293344
C	-1.091543	0.413277	0.704667	C	-1.067632	-0.353262	-0.102649
C	1.387563	-0.234911	0.308812	C	1.449640	-0.449311	-0.192588
C	2.143734	-1.370938	0.022218	C	2.461714	-1.278783	0.294093
C	1.998696	1.020162	0.216083	C	1.780582	0.854737	-0.563405
C	3.467105	-1.256999	-0.368313	C	3.752993	-0.807458	0.449967
H	1.679001	-2.344096	0.106743	H	2.223945	-2.299163	0.566734
C	3.322525	1.129326	-0.17072	C	3.074947	1.323309	-0.41562
H	1.431436	1.907992	0.462348	H	1.025133	1.491137	-1.001764
C	4.060821	-0.007784	-0.467547	C	4.063067	0.498123	0.099169
H	4.0391	-2.147399	-0.591923	H	4.520493	-1.461083	0.841515
H	3.782757	2.106142	-0.236955	H	3.31536	2.334653	-0.71418
H	5.096136	0.080048	-0.767296	H	5.073406	0.866279	0.213585
H	-3.442953	1.56476	-1.346222	H	-3.160611	2.11206	0.696962
C	-4.273024	-1.077009	-0.637701	C	-4.813346	-0.173137	-0.073604
H	-4.908423	-0.560593	-1.355868	H	-5.251319	0.552181	-0.762442
H	-3.913559	-1.999422	-1.09721	H	-5.095891	-1.171059	-0.404614
H	-4.885092	-1.365577	0.219366	H	-5.26463	0.00248	0.905154
H	-1.03239	-1.415552	0.770879	H	0.034883	-2.035061	-0.601996
H	-2.540227	-0.868658	1.832249	H	-2.5587	-1.959523	-0.622432

tsi9i11				tsi9i10			
C	0.090337	0.285004	-0.500691	C	0.527578	-0.479603	-0.075207
C	1.097691	0.839465	-0.952633	C	-0.668020	-0.737475	0.076671
C	2.558261	0.718467	-1.043085	C	-2.076643	-1.001126	0.057986
C	3.096342	-0.062438	0.145715	C	-3.091067	-0.047794	-0.020962
C	2.355375	-1.017031	0.735050	C	-4.449766	-0.497287	0.030693
C	1.100463	-1.516181	0.237351	C	-5.541395	0.283612	-0.032754
H	3.034252	1.700169	-1.072771	H	-2.341700	-2.052042	0.059754
H	2.821223	0.226474	-1.986118	H	-4.594414	-1.569875	0.121424
H	2.694396	-1.401591	1.692876	H	-5.474391	1.359521	-0.123139
H	1.046171	-1.895953	-0.773892	H	-6.532496	-0.144920	0.002781
H	0.434367	-2.005547	0.937393	H	-1.252475	-0.923305	1.226014
C	-1.320546	0.183175	-0.21648	C	1.903926	-0.194693	-0.038523
C	-2.047765	-0.95595	-0.56049	C	2.357235	1.130952	0.062145
C	-1.979291	1.240796	0.41136	C	2.854402	-1.225954	-0.113471
C	-3.40227	-1.032451	-0.28773	C	3.710314	1.406488	0.090572
H	-1.544718	-1.780351	-1.04675	H	1.634538	1.933198	0.117157
C	-3.334628	1.160031	0.68161	C	4.204202	-0.935189	-0.080616
H	-1.416317	2.12317	0.68122	H	2.516884	-2.249553	-0.196885
C	-4.05047	0.024388	0.33431	C	4.641757	0.378923	0.020689
H	-3.954696	-1.920565	-0.56312	H	4.04255	2.432883	0.168938
H	-3.83334	1.987778	1.16738	H	4.923263	-1.741322	-0.136628
H	-5.108797	-0.037419	0.547709	H	5.699615	0.60037	0.043565
C	4.421475	0.381359	0.679465	C	-2.785314	1.412401	-0.118253
H	5.200513	0.287051	-0.082183	H	-3.177896	1.954151	0.746441
H	4.394245	1.43442	0.972556	H	-1.714407	1.594072	-0.178461
tsi9i23				**tsi9p6**			
C	-3.434919	0.068279	-0.060457	C	0.419281	-0.570985	-0.001054
H	-2.55023	-1.471953	-1.271673	C	-0.749081	-0.858857	0.004139
C	-2.367271	-0.425503	-1.003389	C	-2.120124	-1.228470	-0.000959
C	-3.105951	0.150664	1.227504	C	-3.159923	-0.351070	-0.050888
C	0.201059	-0.191618	-0.449501	C	-2.930423	1.081214	0.011476
H	-2.401456	0.13671	-1.940564	C	-3.885356	2.011071	-0.004857
C	-1.80527	-0.322526	1.680462	H	-2.322945	-2.283738	-0.136210
H	-3.797745	0.59348	1.939847	H	-1.894299	1.391689	0.075149
C	-1.014417	-0.304788	-0.419385	H	-3.636725	3.061918	0.042832
C	1.597898	-0.053876	-0.259381	H	-4.936437	1.761287	-0.066203
C	2.420712	-1.182827	-0.157125	H	-2.293998	-1.788031	1.966333
C	2.18257	1.215878	-0.168946	C	1.801952	-0.222249	-0.006223

C	3.782918	-1.041496	0.031909	C	2.782656	-1.215453	-0.056185
H	1.976211	-2.165801	-0.227442	C	2.193591	1.117656	0.039102
C	3.545606	1.347073	0.021143	C	4.122846	-0.872525	-0.06096
H	1.552795	2.091007	-0.247955	H	2.481747	-2.253086	-0.090377
C	4.351547	0.221487	0.122020	C	3.5357	1.453001	0.034247
H	4.405998	-1.922183	0.109990	H	1.436571	1.888383	0.078452
H	3.983055	2.333815	0.091124	C	4.503625	0.460638	-0.015899
H	5.417413	0.328025	0.269686	H	4.873962	-1.649565	-0.099777
C	-4.759276	0.444734	-0.637741	H	3.827698	2.493645	0.069908
H	-5.229902	-0.411785	-1.127834	H	5.55203	0.725523	-0.019569
H	-5.438775	0.808021	0.131629	C	-4.56332	-0.865709	-0.124684
H	-4.64854	1.221658	-1.398457	H	-5.1359	-0.549427	0.749889
H	-1.211094	0.293402	2.344079	H	-5.076652	-0.475633	-1.005514
tsi11i12				**tsi10i12**			
C	-0.231099	-0.057262	0.542292	C	0.071525	-0.394015	0.146054
C	-0.941766	-1.22764	0.526077	C	1.012273	-1.225456	0.552013
C	-1.041646	1.173622	0.889045	C	2.444387	-1.133064	0.321435
C	-2.3566	1.155832	0.146572	C	3.142327	-0.018652	-0.000865
C	-2.971054	0.025539	-0.207303	C	2.457244	1.216868	-0.294516
C	-2.305678	-1.235029	0.174119	C	1.303432	1.262111	-0.993139
H	-0.50126	2.090106	0.658329	H	0.70840	-2.038928	1.212395
H	-1.233112	1.222156	1.968897	H	3.011148	-2.014492	0.598850
H	-2.814599	2.111693	-0.082643	H	2.857787	2.125322	0.145636
H	-2.917468	-2.103426	0.401413	H	0.745447	2.183429	-1.096437
H	-1.42193	-1.811913	-0.584827	H	1.039831	0.468111	-1.676041
C	-4.277061	-0.035564	-0.938416	C	-1.327491	-0.199638	0.115329
H	-5.012071	-0.614754	-0.374979	C	-2.166722	-1.120603	-0.539602
H	-4.68584	0.959347	-1.107391	C	-1.913631	0.94463	0.686986
H	-4.159216	-0.525202	-1.907375	C	-3.53101	-0.910699	-0.597787
C	1.190079	-0.008296	0.217181	H	-1.726416	-1.996911	-0.995381
C	1.937334	-1.196065	0.180531	C	-3.278131	1.142151	0.624098
C	1.856824	1.183698	-0.090929	H	-1.276646	1.665115	1.181809
C	3.275253	-1.190109	-0.160113	C	-4.095056	0.2182	-0.017649
H	1.444251	-2.121071	0.445182	H	-4.16145	-1.632333	-1.099933
C	3.198438	1.186215	-0.433118	H	-3.712328	2.02346	1.076849
H	1.324851	2.1242	-0.084864	H	-5.163012	0.379362	-0.067796
C	3.916782	0.00182	-0.471127	C	4.643204	0.009786	0.072279
H	3.826883	-2.120771	-0.173664	H	4.97671	0.799253	0.75024
H	3.684875	2.122259	-0.673307	H	5.04769	-0.936798	0.426992

tsi10p6				tsi12p5			
C	-0.361840	-0.618597	-0.138733	C	0.254551	-0.013242	0.017435
C	0.781583	-0.994217	-0.304445	C	0.975994	-1.12627	0.436058
C	2.178707	-1.266425	-0.209595	C	0.980535	1.127731	-0.367320
C	3.132264	-0.341060	-0.004948	C	2.379197	1.085015	-0.443611
C	2.801261	1.075273	0.133024	C	3.085724	-0.02915	-0.033472
C	3.681989	2.048391	0.347071	C	2.359614	-1.13128	0.422737
H	2.465495	-2.304226	-0.321703	H	0.44652	-2.001038	0.789840
H	1.750461	1.325310	0.052201	H	0.455645	1.955847	-0.824204
H	3.360652	3.076539	0.438310	H	2.909935	1.954909	-0.808489
H	4.743692	1.860354	0.439177	H	2.890093	-2.01295	0.760804
H	0.510410	-2.047809	-1.913939	H	0.838623	2.132237	1.213733
C	-1.728055	-0.243879	-0.051282	C	-1.223012	-0.01593	0.001433
C	-2.685799	-1.158681	0.397524	C	-1.946773	1.126672	0.340766
C	-2.134138	1.044375	-0.413648	C	-1.929507	-1.163464	-0.358702
C	-4.015945	-0.789668	0.479374	C	-3.33166	1.120274	0.324165
H	-2.373259	-2.154808	0.677241	H	-1.418713	2.020207	0.647099
C	-3.46614	1.404944	-0.326819	C	-3.313842	-1.169823	-0.376168
H	-1.396096	1.751823	-0.765052	H	-1.387795	-2.052993	-0.652037
C	-4.410222	0.491006	0.119226	C	-4.021307	-0.027438	-0.034196
H	-4.749239	-1.504782	0.82615	H	-3.874041	2.014657	0.599774
H	-3.77007	2.403312	-0.610111	H	-3.841914	-2.068141	-0.666368
H	-5.451176	0.776125	0.185268	H	-5.102638	-0.031677	-0.048085
C	4.570924	-0.754543	0.084372	C	4.587772	-0.063805	-0.064299
H	5.164608	-0.26132	-0.687618	H	4.995813	-0.058947	0.947988
H	4.996884	-0.471788	1.048878	H	4.950965	-0.965934	-0.55758
tsi23i25				**tsi25p11′**			
C	-3.017896	-0.724104	-0.774228	C	-2.929912	0.54246	0.115327
C	-1.935258	-1.627925	-0.363934	H	-0.958837	1.437447	0.294787
C	-3.033014	0.379103	-0.003988	C	-1.572436	0.564054	0.154466
C	0.113469	-0.988580	0.037053	C	-3.362741	-0.825966	-0.165954
H	-2.172912	-2.640001	-0.043401	C	0.169334	-1.253456	-0.255492
C	-1.915888	0.377288	1.039926	H	-1.341218	0.406595	2.278432
C	-1.101328	-0.754361	0.500789	C	-2.28273	-1.613768	-0.308741
C	1.420664	-0.380191	0.000422	C	-1.083757	-0.786861	-0.149554
C	2.574381	-1.143758	0.205698	C	1.421683	-0.50175	-0.151319
C	1.563491	0.983059	-0.287706	C	2.528414	-1.112451	0.441283
C	3.825849	-0.557717	0.152688	C	1.56471	0.79478	-0.647476
H	2.472851	-2.200636	0.41231	C	3.726659	-0.434228	0.576254

C	2.817768	1.563808	-0.344767	H	2.437848	-2.125326	0.812741
H	0.678918	1.57744	-0.473983	C	2.766812	1.46957	-0.521020
C	3.95302	0.797253	-0.121913	H	0.738492	1.260919	-1.164813
H	4.708323	-1.159807	0.322498	C	3.848411	0.86209	0.098482
H	2.911672	2.618493	-0.566533	H	4.568883	-0.919216	1.050590
H	4.93298	1.252305	-0.168093	H	2.862513	2.471293	-0.917453
C	-4.027041	1.487725	-0.045855	H	4.786225	1.391534	0.196502
H	-4.535925	1.588501	0.916096	C	-3.858625	1.678021	0.365181
H	-3.536271	2.443759	-0.244037	H	-3.315202	2.605921	0.534238
H	-4.778573	1.321795	-0.816134	H	-4.536174	1.823103	-0.478741
H	-1.368338	1.319077	1.085405	H	-4.478683	1.481638	1.243024
H	-2.33917	0.193777	2.03312	H	0.281862	-2.322933	-0.406318
H	-0.649612	-1.848983	-0.884115	H	-2.264951	-2.671892	-0.518562
H	-3.753254	-0.935312	-1.538259	H	-4.395726	-1.134056	-0.233044
p3				**p4**			
C	-1.259030	-0.745618	0.179981	C	2.618202	0.758555	0.000000
C	-2.635084	-0.562640	0.142409	C	3.438737	-0.302512	0.000000
C	-3.127539	0.702737	-0.159775	C	3.129004	-1.732083	0.000000
C	-0.371907	0.298849	-0.070612	C	1.200767	0.776025	0.000000
C	1.091942	0.073082	-0.025801	C	-1.425026	0.896815	0.000000
C	-0.890847	1.556369	-0.366635	C	4.146303	-2.596749	0.000000
H	-0.219492	2.375199	-0.588380	C	0.00000	0.860294	0.000000
C	-2.260811	1.753081	-0.411205	H	3.079226	1.739751	0.000000
H	-0.864262	-1.723098	0.430067	H	3.979142	-3.665554	0.000000
H	-2.655339	2.730617	-0.654327	H	5.174707	-2.259127	0.000000
C	1.939825	1.008019	0.565079	C	-2.109057	2.114338	0.000000
C	1.654669	-1.078209	-0.573486	C	-2.156144	-0.293709	0.000000
C	3.308292	0.798509	0.607707	C	-3.492313	2.13683	0.000000
H	1.518852	1.898061	1.014021	H	-1.545227	3.036595	0.000000
C	3.022971	-1.28895	-0.531685	C	-3.539162	-0.263464	0.000000
H	1.014376	-1.805027	-1.055909	H	-1.627891	-1.237105	0.000000
C	3.855523	-0.351189	0.059417	C	-4.211021	0.950225	0.000000
H	3.94869	1.532809	1.077623	H	-4.012413	3.084985	0.000000
H	3.440968	-2.185546	-0.969313	H	-4.0954	-1.190891	0.000000
H	4.923939	-0.515233	0.092365	H	-5.292177	0.97135	0.000000
C	-3.571152	-1.69729	0.455459	C	1.705144	-2.208838	0.000000
H	-3.877804	-1.667688	1.502906	H	1.16977	-1.840043	0.875143
H	-4.474535	-1.642652	-0.151514	H	1.16977	-1.840043	-0.875143
H	-3.098982	-2.662563	0.277425	H	1.668585	-3.296788	0.000000

H	-4.197523	0.864611	-0.200103	H	4.499297	-0.077488	0.000000
p11				**p5**			
C	2.653153	1.202643	0.467688	C	0.988166	-1.115058	-0.423034
C	1.323819	1.021372	0.407514	C	2.372328	-1.111551	-0.426529
C	3.342836	-0.019501	0.023358	C	3.090559	0.003398	-0.008798
C	-0.080252	-0.980701	-0.290379	C	0.269562	0.001132	-0.002044
C	2.405931	-0.934229	-0.284440	C	-1.211499	0.000261	-0.000124
C	1.081091	-0.342142	-0.080578	C	0.988377	1.119398	0.413019
C	-1.43767	-0.443559	-0.165269	H	0.45726	1.995605	0.761630
C	-2.456509	-1.278533	0.297526	C	2.372514	1.118686	0.408374
C	-1.763469	0.866026	-0.521898	H	0.456732	-1.989365	-0.775901
C	-3.749573	-0.808642	0.444014	H	2.904796	-1.989934	-0.770183
H	-2.223125	-2.303273	0.557655	H	2.905249	2.001297	0.740623
C	-3.05919	1.333594	-0.382509	C	-1.927611	1.121402	-0.415739
H	-1.001216	1.507887	-0.939954	C	-1.924326	-1.122198	0.417651
C	-4.054463	0.502111	0.108219	C	-3.312732	1.121181	-0.413067
H	-4.522452	-1.46741	0.815991	H	-1.39255	1.994935	-0.764634
H	-3.295235	2.349323	-0.669590	C	-3.309427	-1.124442	0.419491
H	-5.065977	0.869409	0.215033	H	-1.386486	-1.994843	0.764530
H	3.160041	2.094189	0.808176	C	-4.009631	-0.002222	0.004369
C	4.825056	-0.158614	-0.042387	H	-3.849444	1.999426	-0.745950
H	5.257017	0.579099	-0.722187	H	-3.843512	-2.003669	0.754003
H	5.27668	0.008679	0.937946	H	-5.091066	-0.003167	0.006107
H	5.115379	-1.150055	-0.386262	C	4.593546	-0.006194	0.016737
H	-0.021665	-2.029811	-0.564994	H	4.962295	-0.363178	0.980599
H	2.573591	-1.93696	-0.647702	H	4.998578	-0.662629	-0.75271
H	0.562422	1.719974	0.710737	H	4.999193	0.99276	-0.139947
p6				**p11′**			
C	0.000000	0.702676	0.000000	C	-3.379205	-0.820614	-0.140418
C	1.126833	0.277940	0.000000	C	-2.302607	-1.605528	-0.295764
C	2.466342	-0.184206	0.000000	C	-2.937511	0.550656	0.161057
C	2.844873	-1.475430	0.000000	C	0.150106	-1.246640	-0.220348
C	1.854411	-2.548737	0.000000	H	-2.282700	-2.659418	-0.525965
C	2.134144	-3.848935	0.000000	C	-1.590587	0.574565	0.163614
H	3.229684	0.585395	0.000000	C	-1.102972	-0.774803	-0.128975
H	0.818033	-2.232240	0.000000	C	1.405103	-0.497187	-0.124532
H	1.343600	-4.586294	0.000000	C	2.518622	-1.112855	0.450234
H	3.149402	-4.223672	0.000000	C	1.544444	0.802374	-0.614722
C	-1.337536	1.196622	0.000000	C	3.720192	-0.437942	0.573430

C	-2.419022	0.312486	0.00000	H	2.431435	-2.128259	0.81580
C	-1.585364	2.571326	0.00000	C	2.749363	1.474218	-0.49916
C	-3.715595	0.794951	0.00000	H	0.711337	1.273212	-1.11647
H	-2.23075	-0.752047	0.00000	C	3.838221	0.861125	0.10220
C	-2.88454	3.046519	0.00000	H	4.567862	-0.927753	1.03299
H	-0.750375	3.25781	0.00000	H	2.841767	2.478227	-0.89070
C	-3.952889	2.161636	0.00000	H	4.778363	1.38817	0.19075
H	-4.54498	0.100926	0.00000	C	-3.871521	1.679255	0.43307
H	-3.064304	4.112932	0.00000	H	-4.518577	1.452768	1.28331
H	-4.96737	2.536025	0.00000	H	-3.330724	2.598891	0.65033
C	4.299563	-1.837084	0.00000	H	-4.52406	1.860077	-0.42397
H	4.55136	-2.434582	0.878359	H	-0.972558	1.426132	0.396004
H	4.55136	-2.434582	-0.878359	H	0.261494	-2.317935	-0.359027
H	4.927013	-0.94825	0.00000	H	-4.413549	-1.123846	-0.21119
vdW(i5)				**vdW(i9)**			
C	2.200010	0.708985	0.018054	C	1.517587	-0.15654	-1.266654
C	1.801645	-0.485680	0.769975	C	2.266095	-0.135002	-0.005916
C	1.116083	-0.351454	1.904470	C	2.653204	1.030737	0.510776
H	3.226062	-0.200316	-1.592393	H	1.17033	-2.233931	-1.449849
H	1.885850	1.657176	0.442389	H	1.347868	0.813559	-1.722435
C	-1.071792	2.227346	-0.006097	C	-0.80275	2.264503	0.083946
H	0.804094	-1.210526	2.483782	H	3.202598	1.08112	1.441975
H	0.847919	0.626375	2.284120	H	2.422368	1.969497	0.023609
H	3.135975	1.641538	-1.613550	H	0.486379	-1.170443	-2.790589
C	2.886479	0.712690	-1.119989	C	1.035422	-1.242284	-1.862084
C	-1.374324	0.880693	-0.188312	C	-1.266771	0.958673	0.220353
C	-2.144583	0.184577	0.767759	C	-0.840978	0.159688	1.302884
C	-0.875613	0.182963	-1.308848	C	-2.137279	0.404625	-0.742144
C	-2.394711	-1.159565	0.609377	C	-1.265234	-1.145653	1.406284
H	-2.518668	0.726384	1.624464	H	-0.16405	0.588798	2.026669
C	-0.658708	3.403423	0.236181	C	-0.256874	3.393266	-0.117464
C	-1.13223	-1.16131	-1.455355	C	-2.55598	-0.901337	-0.626455
H	-0.27408	0.720322	-2.026839	H	-2.454985	1.023204	-1.569119
C	-1.88634	-1.833002	-0.497712	C	-2.117748	-1.67713	0.442669
H	-2.979215	-1.69317	1.345322	H	-0.934017	-1.759094	2.232252
H	-0.743048	-1.69684	-2.309762	H	-3.218363	-1.326504	-1.367027
H	-2.079438	-2.890808	-0.614929	H	-2.443892	-2.705067	0.526031
C	2.177572	-1.833082	0.226842	C	2.555899	-1.441394	0.673031
H	1.763808	-1.977315	-0.773321	H	1.627903	-1.965455	0.914108

H	3.261606	-1.931819	0.143944	H	3.136437	-2.099963	0.024265
H	1.808221	-2.630507	0.868704	H	3.113868	-1.288637	1.594758
tsi5vdW				**tsi9vdW**			
C	2.206005	0.286190	0.497440	C	-1.423413	-0.723452	1.241370
C	1.640332	-1.065065	0.548697	C	-2.223309	-0.356845	0.069611
C	0.906410	-1.434393	1.597915	C	-2.771738	0.855844	-0.000358
H	1.990108	0.917584	1.353083	H	-0.825087	-2.672660	0.683182
C	-0.380418	2.318403	-0.047174	H	-1.348583	0.039420	2.009508
H	0.464331	-2.419790	1.663745	C	0.307977	2.275051	-0.040508
H	0.728384	-0.756818	2.423082	H	-3.353294	1.167928	-0.857446
H	3.272165	1.812322	-0.470803	H	-2.645542	1.580821	0.793433
C	2.919377	0.791404	-0.503336	H	-0.211930	-2.066133	2.311668
C	-1.071419	1.112640	-0.150870	C	-0.790272	-1.878634	1.417773
C	-1.884490	0.658467	0.907965	C	1.046161	1.099477	-0.160888
C	-0.942496	0.314815	-1.306541	C	0.916749	0.292163	-1.310204
C	-2.544631	-0.546352	0.807438	C	1.912643	0.687453	0.872568
H	-1.973592	1.272842	1.792374	C	1.625424	-0.883494	-1.412882
C	0.311809	3.378751	0.065719	H	0.241467	0.61085	-2.091047
C	-1.600916	-0.890964	-1.392417	C	-0.396919	3.326753	0.076196
H	-0.307079	0.665899	-2.106766	C	2.623911	-0.485972	0.754002
C	-2.401602	-1.321365	-0.338612	H	2.001863	1.309362	1.751667
H	-3.167276	-0.892536	1.620164	C	2.478628	-1.272179	-0.38397
H	-1.494397	-1.505007	-2.275525	H	1.520475	-1.504726	-2.291248
H	-2.916333	-2.269902	-0.410794	H	3.28837	-0.79955	1.546604
C	1.89772	-1.994025	-0.60148	H	3.033507	-2.196611	-0.469979
H	1.53064	-1.56643	-1.536626	C	-2.380997	-1.364977	-1.030614
H	2.967613	-2.170075	-0.727244	H	-1.407696	-1.653624	-1.434612
H	1.406656	-2.952974	-0.447618	H	-2.856772	-2.275689	-0.661682
H	3.164692	0.213849	-1.385537	H	-2.985844	-0.966522	-1.842617
i30				**i31**			
C	-2.437033	0.631258	-0.576385	C	2.437471	-0.877219	0.186241
H	-3.917511	2.245368	-0.175380	H	2.557154	-0.839768	-2.059574
C	-2.892170	1.943125	-0.018981	C	2.217779	-1.427349	-1.216430
C	-3.206660	-0.528742	0.063588	C	3.122832	0.413698	0.444667
C	0.191282	0.288799	-0.307763	C	-0.155835	-0.61018	-0.346548
C	-4.068285	-1.236768	-0.652289	H	2.297924	-2.498821	-1.344542
H	-4.232243	-1.038732	-1.703911	C	3.78841	0.595546	1.580396
C	-0.990998	0.448199	-0.437949	H	4.283131	1.532597	1.798818
C	1.599768	0.093208	-0.157252	H	3.858027	-0.184877	2.327105

C	2.155090	-1.179318	-0.300751
C	2.437411	1.170168	0.136763
C	3.518119	-1.367214	-0.152341
H	1.507927	-2.01444	-0.529639
C	3.799642	0.975681	0.283635
H	2.009489	2.156685	0.247637
C	4.34395	-0.291943	0.139984
H	3.937517	-2.357573	-0.265915
H	4.43921	1.817554	0.511202
H	5.408756	-0.441328	0.255273
H	-2.675432	0.609963	-1.646056
C	-2.946415	-0.776727	1.518073
H	-1.894757	-1.017975	1.682847
H	-3.16449	0.117286	2.106076
H	-3.556201	-1.596149	1.893346
H	-2.246329	2.543621	0.602625
H	-4.638147	-2.042636	-0.208098

i32			
C	3.303910	0.905618	-0.377924
C	2.712630	1.973408	-0.883905
C	2.621329	-0.329719	0.178122
C	-0.042701	-0.166063	0.075098
H	1.634300	2.047772	-0.944028
C	2.974647	-0.478029	1.633146
H	2.929430	0.385549	2.280645
C	1.156873	-0.229243	0.100896
C	-1.468672	-0.081653	0.037450
C	-2.233542	-1.176419	-0.368776
C	-2.115928	1.099088	0.405974
C	-3.61405	-1.088993	-0.404666
H	-1.734485	-2.09162	-0.65496
C	-3.496768	1.180181	0.367095
H	-1.525481	1.947452	0.722877
C	-4.249714	0.08794	-0.037733
H	-4.196538	-1.943576	-0.720903
H	-3.987401	2.10003	0.654737
H	-5.328703	0.15366	-0.06701
H	4.387227	0.856886	-0.328412
C	3.093233	-1.563357	-0.614678

C	1.075894	-0.906739	-0.444944
C	-1.463731	-0.241267	-0.135270
C	-1.927635	1.047969	-0.505880
C	-2.394495	-1.139677	0.448580
C	-3.240327	1.405323	-0.297833
H	-1.232288	1.744687	-0.952925
C	-3.702395	-0.759799	0.646898
H	-2.058193	-2.126041	0.735763
C	-4.139135	0.510412	0.277913
H	-3.57437	2.393305	-0.585336
H	-4.396598	-1.458104	1.094976
H	-5.168339	0.799625	0.437253
H	2.592118	-1.628834	0.951209
C	3.023075	1.486275	-0.600283
H	3.544029	1.193491	-1.514226
H	1.981942	1.675469	-0.867755
H	3.46403	2.415306	-0.24581

i33			
C	2.508974	-0.286573	-0.120691
H	2.56463	-0.092302	-2.359897
C	2.297998	-0.765471	-1.554537
C	2.996943	1.099311	0.046312
C	-0.118053	-0.285731	-0.550284
H	2.476489	-1.81431	-1.755706
C	3.73657	1.544245	1.052226
H	2.697612	1.790196	-0.735874
H	4.046435	2.578862	1.096955
H	4.057269	0.901145	1.861198
C	1.133076	-0.41793	-0.725188
C	-1.444081	-0.100974	-0.232819
C	-2.085679	1.142696	-0.467895
C	-2.216029	-1.151666	0.327386
C	-3.415093	1.313462	-0.154873
H	-1.51194	1.953476	-0.894457
C	-3.544069	-0.957376	0.632465
H	-1.743021	-2.106168	0.511236
C	-4.156647	0.27102	0.396045
H	-3.886029	2.269784	-0.339300
H	-4.115576	-1.76995	1.060800

H	2.810209	-1.472525	-1.661968	H	-5.200231	0.414315	0.638375
H	4.17802	-1.652707	-0.548549	C	2.905637	-1.308029	0.914792
H	2.643906	-2.468746	-0.207582	H	3.991068	-1.417881	0.951561
H	3.047214	-1.463742	2.071134	H	2.5572	-1.010676	1.904209
H	3.294816	2.805014	-1.25658	H	2.468802	-2.278391	0.683275
		tsi30i31				**tsi32i33**	
C	-2.459923	-0.875291	-0.072455	C	2.526426	-0.276398	-0.203069
C	-3.362389	0.262977	0.319119	H	2.168592	0.30802	-2.340099
C	-4.374385	0.042989	1.147078	C	2.193369	-0.515421	-1.644630
C	-2.120752	-1.089213	-1.513101	C	3.195089	1.043324	0.052182
H	-2.158348	-0.269322	-2.210851	C	-0.141307	-0.094175	-0.013322
H	-1.921996	-2.085578	-1.870921	H	2.057218	-1.524651	-1.998464
C	-1.026536	-0.644193	-0.054734	C	4.23433	1.244668	0.844072
H	-4.570617	-0.939825	1.555884	H	2.756681	1.880873	-0.480378
C	1.554862	-0.147368	0.082059	H	4.655399	2.233543	0.961686
C	2.471705	-1.177345	0.346306	H	4.702534	0.44457	1.401748
C	2.048176	1.143912	-0.164409	C	1.072449	-0.190196	-0.163457
C	0.170444	-0.401112	0.068651	C	-1.54604	-0.006845	0.038143
C	3.828657	-0.919401	0.35868	C	-2.194126	1.225355	-0.140920
H	2.101676	-2.17452	0.5395	C	-2.327378	-1.148914	0.273889
C	3.407523	1.388573	-0.148173	C	-3.572212	1.304956	-0.088008
H	1.350297	1.944272	-0.367664	H	-1.600618	2.110847	-0.320683
C	4.305356	0.36159	0.112478	C	-3.704713	-1.055707	0.324793
H	4.522122	-1.724138	0.56254	H	-1.837178	-2.102065	0.414938
H	3.771461	2.38883	-0.340751	C	-4.335426	0.168309	0.144550
H	5.3684	0.558195	0.124299	H	-4.056595	2.261786	-0.229039
H	-5.041223	0.841762	1.444392	H	-4.292758	-1.945192	0.506666
C	-3.064979	1.61462	-0.255923	H	-5.413675	0.236023	0.185762
H	-3.743837	2.36489	0.143723	C	3.113592	-1.466809	0.534481
H	-2.040025	1.913132	-0.029264	H	4.153673	-1.610911	0.241105
H	-3.166417	1.61168	-1.343027	H	3.065666	-1.31537	1.612196
H	-2.738042	-1.793813	0.43868	H	2.556776	-2.370357	0.292341
		tsi5i31				**tsi9i33**	
C	2.502558	-0.802898	0.451032	C	-2.596544	-0.272953	0.044134
H	2.852177	-1.274116	-1.682943	H	-2.840729	-0.49174	2.233153
C	2.387962	-1.651009	-0.777296	C	-2.478899	-1.007977	1.349106
C	2.942162	0.574175	0.464163	C	-2.872082	1.1449	0.065718
C	-0.138943	-0.847128	-0.454757	C	0.081541	-0.534107	0.749217
H	2.545828	-2.715562	-0.640016	H	-2.74976	-2.058939	1.336074

C	3.136807	1.210783	1.628723	C	-3.20407	1.891692	-0.991935
H	3.458440	2.242603	1.658865	H	-2.786712	1.627235	1.034746
H	2.981888	0.711498	2.576171	H	-3.389778	2.950673	-0.885309
C	1.056183	-1.164255	-0.503806	H	-3.305853	1.472451	-1.983990
C	-1.429527	-0.356096	-0.222725	C	-1.133375	-0.690561	0.932288
C	-1.848708	0.8599	-0.794175	C	1.387738	-0.231328	0.348965
C	-2.341345	-1.069138	0.577712	C	2.006855	0.965321	0.757491
C	-3.123518	1.337287	-0.566603	C	2.118505	-1.119837	-0.462754
H	-1.157241	1.416295	-1.411525	C	3.297288	1.255066	0.363289
C	-3.612418	-0.577924	0.796974	H	1.455786	1.654918	1.381469
H	-2.031886	-2.005936	1.019671	C	3.407667	-0.814874	-0.849342
C	-4.013379	0.625089	0.22843	H	1.655123	-2.043669	-0.780016
H	-3.428337	2.27501	-1.011502	C	4.006619	0.370955	-0.440914
H	-4.299703	-1.137442	1.417279	H	3.756765	2.18033	0.684184
H	-5.010653	1.004091	0.403107	H	3.953795	-1.507665	-1.475470
H	2.432286	-1.318345	1.398053	H	5.0173	0.60362	-0.746035
C	3.154115	1.270647	-0.851355	C	-2.751356	-1.057526	-1.222098
H	3.967081	0.808686	-1.415392	H	-3.800341	-1.083504	-1.530813
H	2.255927	1.21799	-1.47013	H	-2.175972	-0.613317	-2.03498
H	3.402498	2.318629	-0.699536	H	-2.408971	-2.083031	-1.091996

(c)

Atom	X	Y	Z	Atom	X	Y	Z
phenylethynyl				**1,3-pentadiene**			
C	0.000000	0.000000	2.063239	C	-2.412988	0.745964	0.000000
C	0.000000	0.000000	3.335500	C	-1.406265	-0.121737	0.000000
C	0.000000	0.000000	0.669896	C	0.000000	0.251327	0.000000
C	0.000000	1.216831	-0.046161	C	1.001864	-0.624254	0.000000
C	0.000000	-1.216831	-0.046161	H	-3.442827	0.417531	0.000000
C	0.000000	1.210125	-1.423103	H	-1.622387	-1.185896	0.000000
H	0.000000	2.143623	0.509225	H	0.222638	1.315124	0.000000
C	0.000000	-1.210125	-1.423103	H	0.762671	-1.684292	0.000000
H	0.000000	-2.143623	0.509225	C	2.451693	-0.270595	0.000000
C	0.000000	0.000000	-2.111120	H	2.954862	-0.685119	0.876410
H	0.000000	2.142392	-1.969839	H	2.954862	-0.685119	-0.876410
H	0.000000	-2.142392	-1.969839	H	2.599580	0.808854	0.000000
H	0.000000	0.000000	-3.192694	H	-2.235227	1.814693	0.000000
i13				**i14**			
C	3.078027	-1.258176	-0.173388	C	-0.147276	-1.579795	-0.221765
C	3.013173	0.095583	0.062294	C	0.894804	-2.355638	-0.313507
C	4.107896	0.925561	0.193023	C	2.297209	-2.039071	-0.005815
H	1.96762	-2.705415	-1.274555	C	2.867663	-0.836498	0.142602
C	1.899803	-2.177878	-0.31642	C	2.233325	0.46036	0.007572
H	1.957356	-2.962879	0.445923	C	2.864768	1.610535	0.240645
H	2.026223	0.541353	0.152489	H	0.72577	-3.382302	-0.642248
H	5.09964	0.493572	0.105101	H	2.934671	-2.909011	0.096002
C	0.594642	-1.533993	-0.228403	H	3.92725	-0.81851	0.377147
C	-0.473799	-0.992433	-0.157701	H	1.194956	0.488858	-0.299889
C	-1.744711	-0.341768	-0.076097	H	3.904113	1.580461	0.557412
C	-2.702322	-0.767924	0.845601	C	-1.237473	-0.76196	-0.117481
C	-2.043171	0.731841	-0.916733	C	-1.641585	0.062486	-1.20574
C	-3.929547	-0.132975	0.922201	C	-1.992811	-0.688489	1.086605
H	-2.473426	-1.598803	1.498129	C	-2.727838	0.897485	-1.083897
C	-3.271879	1.363393	-0.834478	H	-1.0788	0.01993	-2.127881
H	-1.303507	1.062719	-1.632411	C	-3.075451	0.154019	1.181057
C	-4.218185	0.933697	0.083906	H	-1.697549	-1.304171	1.924403
H	-4.663853	-0.472183	1.640088	C	-3.454905	0.953322	0.103795
H	-3.491765	2.194331	-1.490852	H	-3.018967	1.516214	-1.92223
H	-5.177778	1.428417	0.146108	H	-3.636788	0.195777	2.104887

H	4.048652	-1.732534	-0.265349	H	-4.307249	1.612394	0.189196
C	4.021527	2.389454	0.449581	C	2.247892	2.962206	0.106084
H	2.986066	2.721597	0.521815	H	1.207281	2.89469	-0.209541
H	4.529595	2.661199	1.379282	H	2.284215	3.503421	1.054231
H	4.506453	2.96233	-0.346085	H	2.791162	3.568484	-0.622425
i15				**i16**			
C	0.566634	-0.230876	-0.095801	C	0.600724	-0.248227	-0.119385
C	1.216232	-1.372154	-0.082607	C	1.237631	-1.463036	-0.145881
C	1.38649	1.058246	-0.119465	C	1.405225	1.029858	-0.09294
C	2.856817	0.789953	-0.286982	C	2.877311	0.805008	-0.248552
C	3.429323	-0.403447	-0.286561	C	3.436273	-0.422961	-0.269233
C	2.650021	-1.687947	-0.141386	C	2.629412	-1.585481	-0.202517
H	1.065015	1.65172	-0.982493	H	0.642123	-2.366814	-0.164329
H	3.480544	1.671329	-0.390672	H	1.080133	1.67391	-0.921243
H	4.503702	-0.492192	-0.396812	H	3.499011	1.689922	-0.308723
H	2.971793	-2.225559	0.755995	H	4.510402	-0.526145	-0.352198
H	2.865335	-2.354451	-0.982309	H	3.083943	-2.565019	-0.233452
C	-0.914368	-0.158775	-0.080331	C	-0.867343	-0.163422	-0.096505
C	-1.660442	-1.203512	0.467466	C	-1.546421	0.895755	-0.70746
C	-1.603295	0.926855	-0.617494	C	-1.638052	-1.142603	0.540173
C	-3.042847	-1.17078	0.465169	C	-2.929052	0.960635	-0.702695
H	-1.137757	-2.044233	0.904375	H	-0.989373	1.673717	-1.211165
C	-2.989277	0.962128	-0.618582	C	-3.019651	-1.076985	0.54714
H	-1.059393	1.754965	-1.050865	H	-1.1448	-1.952166	1.060551
C	-3.715867	-0.085822	-0.078641	C	-3.674959	-0.025997	-0.077119
H	-3.598771	-1.992365	0.896784	H	-3.426242	1.786697	-1.193311
H	-3.501425	1.814004	-1.045509	H	-3.588069	-1.845487	1.0537
H	-4.796897	-0.056644	-0.07641	H	-4.754926	0.02704	-0.069402
C	1.14432	1.900314	1.140699	C	1.134342	1.827162	1.202912
H	1.45536	1.345163	2.026009	H	0.075985	2.065591	1.299961
H	0.09136	2.156315	1.249915	H	1.438127	1.241741	2.070688
H	1.718683	2.826856	1.099083	H	1.701042	2.758782	1.2013
i17				**i18**			
C	3.320409	0.134033	-0.221069	C	0.098182	-0.899266	-0.447909
C	2.935192	1.327612	0.347238	C	1.326361	-1.268388	-0.660317
C	3.80584	2.328332	0.71893	C	2.55939	-0.68411	-0.085305
C	2.411465	-0.993372	-0.625581	C	2.718301	0.605913	0.240295
H	1.873858	1.484365	0.510043	C	1.764165	1.685968	0.06288

H	4.873699	2.222659	0.577294	C	1.962134	2.919851	0.519326
C	0.991904	-0.686042	-0.46134	H	1.492851	-2.138877	-1.299141
C	-0.175338	-0.449029	-0.312902	H	3.672707	0.895994	0.669588
C	-1.564749	-0.157338	-0.140793	H	0.851814	1.466939	-0.477288
C	-2.370832	-0.985317	0.64191	H	2.85546	3.180755	1.074448
C	-2.132498	0.961767	-0.751951	C	-1.199971	-0.535392	-0.225278
C	-3.714371	-0.698138	0.807517	C	-1.845856	0.422453	-1.056937
H	-1.932917	-1.852106	1.116782	C	-1.946444	-1.091716	0.85104
C	-3.476608	1.243874	-0.581854	C	-3.149171	0.78975	-0.816609
H	-1.509929	1.603809	-1.359305	H	-1.295417	0.853326	-1.881904
C	-4.271126	0.416027	0.197273	C	-3.248546	-0.707415	1.068329
H	-4.329488	-1.346759	1.416204	H	-1.470406	-1.818032	1.494455
H	-3.905777	2.113798	-1.060012	C	-3.863106	0.232758	0.242666
H	-5.32123	0.638478	0.328523	H	-3.622805	1.519212	-1.459852
H	4.376648	-0.04811	-0.391754	H	-3.79975	-1.140994	1.891973
H	3.447944	3.245774	1.162088	H	-4.886929	0.528186	0.423235
C	2.779293	-2.287211	0.125855	H	1.23549	3.703684	0.358004
H	2.613456	-2.161348	1.194939	C	3.673495	-1.674948	0.102708
H	2.172009	-3.120022	-0.225859	H	3.367865	-2.482642	0.771431
H	3.829898	-2.52878	-0.035591	H	3.942747	-2.137036	-0.850469
H	2.580342	-1.182946	-1.692751	H	4.562764	-1.203262	0.516187
i19				**i20**			
C	0.34457	0.23866	-0.107362	C	-0.347407	0.247254	0.000866
C	1.195942	-0.743292	-0.302259	C	-1.2507	-0.788799	0.102368
C	0.920473	1.634737	0.056864	C	-0.85797	1.659083	-0.092762
C	2.414539	1.676664	-0.047669	C	-2.342559	1.771297	-0.196457
C	3.189133	0.622172	-0.24916	C	-3.15304	0.702608	-0.114293
C	2.666481	-0.791868	-0.37935	C	-2.634041	-0.616944	0.062426
H	0.612244	2.048125	1.023245	H	-0.880439	-1.798109	0.230102
H	2.870958	2.654903	0.048989	H	-0.524268	2.23667	0.783351
H	4.265248	0.741941	-0.31381	H	-2.756798	2.762839	-0.325735
C	-1.121751	0.050445	-0.04635	H	-4.226679	0.83412	-0.180751
C	-1.986262	1.120659	0.170783	C	1.100107	0.029461	0.001415
C	-1.678284	-1.221442	-0.205987	C	1.987494	1.093275	0.210768
C	-3.359799	0.928476	0.226522	C	1.663429	-1.236174	-0.221623
H	-1.594478	2.11983	0.299682	C	3.358973	0.899956	0.219939
C	-3.044323	-1.413639	-0.150935	H	1.606094	2.089555	0.382018
H	-1.018354	-2.062735	-0.375215	C	3.030914	-1.427649	-0.213043
C	-3.895254	-0.336767	0.066209	H	1.024303	-2.082233	-0.429708

H	-4.010707	1.77561	0.396542	C	3.891372	-0.36105	0.011554
H	-3.451231	-2.407964	-0.277787	H	4.014184	1.743464	0.392062
H	-4.965342	-0.48689	0.109414	H	3.431058	-2.416494	-0.393377
H	0.486159	2.299921	-0.697335	H	4.961972	-0.512424	0.01559
H	2.961374	-1.177494	-1.361962	H	-0.385935	2.171553	-0.941534
C	3.27899	-1.71241	0.6849	C	-3.575023	-1.773157	0.193067
H	2.920875	-2.734201	0.564273	H	-3.039935	-2.71695	0.287752
H	4.366551	-1.717563	0.603496	H	-4.217991	-1.662176	1.070153
H	3.009974	-1.36786	1.68324	H	-4.234853	-1.84478	-0.675277
i26				**i27**			
C	3.702592	-0.791386	0.423214	C	3.723179	-0.559554	-0.239022
C	3.608147	0.263789	-0.370671	C	3.337485	0.738035	-0.255069
C	2.188687	0.61193	-0.730842	C	1.843642	0.836691	-0.135094
H	2.183195	-1.437219	1.831203	H	2.597165	-2.478409	-0.110646
C	2.364161	-1.386783	0.7558	C	2.580407	-1.398865	-0.141618
H	4.446992	0.839041	-0.739401	H	3.983318	1.601433	-0.308227
C	1.390446	-0.436389	0.063324	C	1.411274	-0.622424	-0.108564
C	0.099787	-0.466678	0.14583	C	0.147645	-1.16115	-0.026358
C	-1.257301	-0.265766	0.081701	C	-1.158745	-0.53693	-0.067485
C	-2.052669	-0.906075	-0.907222	C	-1.410658	0.760457	-0.537304
C	-1.918487	0.573695	1.019619	C	-2.26401	-1.29178	0.356309
C	-3.41333	-0.706022	-0.949957	C	-2.693146	1.277446	-0.555812
H	-1.568236	-1.551536	-1.626608	H	-0.600976	1.365808	-0.913734
C	-3.280449	0.758633	0.957075	C	-3.543793	-0.772019	0.342704
H	-1.329529	1.066737	1.780539	H	-2.101538	-2.302721	0.708571
C	-4.040855	0.124073	-0.023201	C	-3.767277	0.520614	-0.110377
H	-4.000116	-1.199838	-1.713057	H	-2.856634	2.279876	-0.928466
H	-3.763575	1.404937	1.67774	H	-4.372247	-1.377961	0.684292
H	-5.110499	0.274277	-0.064075	H	-4.767785	0.9303	-0.124713
H	4.629168	-1.205615	0.795477	H	4.742206	-0.913388	-0.290756
C	1.796968	2.048769	-0.395176	C	1.430038	1.608591	1.124527
H	0.747813	2.225243	-0.632913	H	0.34794	1.637791	1.237634
H	1.944699	2.245968	0.667261	H	1.851755	1.127407	2.006956
H	2.266818	-2.405641	0.372294	H	1.441794	1.341592	-1.018389
H	2.027504	0.454035	-1.802082	H	1.799847	2.633349	1.084113
H	2.399578	2.758868	-0.963347	H	0.118898	-2.239749	0.092342
tsi13i14				**tsi13i15**			
C	0.552634	-0.911869	-0.066411	C	0.509956	-0.798304	0.029748

C	-0.523752	-1.492212	0.087286	C	1.51779	-1.51107	0.11211
C	-1.827599	-2.08831	0.074959	C	2.984045	-1.459624	0.022502
C	-3.028318	-1.386188	0.039609	C	3.459749	-0.056841	0.327008
C	-3.132874	0.028441	-0.046678	C	2.717536	1.03518	0.104987
C	-4.293039	0.713072	-0.032814	C	1.450019	1.068806	-0.596194
H	-1.83795	-3.169663	0.032287	H	3.447364	-2.160529	0.718004
H	-3.937716	-1.968033	0.120098	H	3.293927	-1.776781	-0.979034
H	-2.203888	0.585417	-0.135032	H	4.40463	0.035307	0.846845
H	-5.222706	0.158522	0.056771	H	3.062936	1.978281	0.521508
H	-1.005503	-1.894473	1.229599	H	1.435801	0.655557	-1.597343
C	-4.404771	2.196049	-0.140714	C	-0.907401	-0.538716	0.064945
H	-4.909513	2.618505	0.731861	C	-1.512667	-0.087275	1.237362
H	-3.424503	2.664467	-0.226138	C	-1.68316	-0.685902	-1.084671
H	-4.996355	2.484535	-1.013295	C	-2.866375	0.201241	1.259886
C	1.805655	-0.274541	-0.033199	H	-0.910414	0.032885	2.127256
C	2.99093	-1.006184	-0.212984	C	-3.03649	-0.394915	-1.057987
C	1.89686	1.112449	0.168965	H	-1.215065	-1.033066	-1.995578
C	4.216268	-0.369589	-0.182451	C	-3.631838	0.050096	0.11311
H	2.932379	-2.073374	-0.375237	H	-3.325645	0.546544	2.176198
C	3.129032	1.736006	0.192649	H	-3.628912	-0.517024	-1.954626
H	0.990782	1.686086	0.306428	H	-4.688867	0.277589	0.132057
C	4.295119	1.002229	0.018975	C	0.53569	2.232255	-0.373333
H	5.119786	-0.948342	-0.319535	H	0.385762	2.421824	0.690445
H	3.181335	2.804957	0.349773	H	-0.440326	2.06795	-0.827415
H	5.25697	1.495289	0.039288	H	0.957682	3.141873	-0.815151
tsi13i27				**tsi13p8**			
C	3.731573	-0.573131	0.379896	C	-2.981844	-1.364942	-0.109241
C	3.501232	0.663009	-0.04862	C	-3.124487	0.062993	-0.016478
C	2.232889	0.973669	-0.705693	C	-4.306419	0.686427	-0.045336
H	2.584875	-2.221459	1.143438	H	-1.804043	-3.107515	-0.224438
C	2.630376	-1.588008	0.254866	C	-1.803419	-2.038043	-0.060408
H	4.235304	1.450135	0.105351	H	-3.890253	-1.94941	-0.197509
C	1.321515	-0.923875	0.064294	H	-2.213879	0.645349	0.080813
C	0.105097	-0.824192	0.119433	C	0.549988	-0.877348	-0.028249
C	-1.264307	-0.466388	0.089741	H	-5.207296	0.08677	-0.142184
C	-2.050278	-0.732165	-1.039555	C	-0.531573	-1.404637	-0.0366
C	-1.859441	0.167967	1.188845	H	-1.803594	-2.651534	1.884176
C	-3.384022	-0.369181	-1.065938	C	1.830996	-0.25095	-0.01596
H	-1.599007	-1.223551	-1.890253	C	1.938125	1.141374	0.011061

C	-3.193552	0.527401	1.152304	C	2.995933	-1.021322	-0.029842
H	-1.259046	0.374937	2.063753	C	3.182386	1.745892	0.023969
C	-3.962069	0.261623	0.027056	H	1.038095	1.740126	0.021777
H	-3.97759	-0.579466	-1.945404	C	4.236781	-0.409894	-0.017093
H	-3.638206	1.018571	2.007293	H	2.915544	-2.099062	-0.04973
H	-5.005598	0.543739	0.002554	C	4.334516	0.973585	0.009864
H	4.668462	-0.867722	0.833498	H	3.253346	2.824802	0.045236
C	1.426682	2.163931	-0.311007	H	5.132193	-1.016211	-0.027665
H	0.390576	2.050825	-0.632593	H	5.305938	1.448537	0.0201
H	1.433298	2.304226	0.770356	C	-4.496408	2.16196	0.045097
H	2.816174	-2.260149	-0.589317	H	-5.009734	2.54316	-0.840631
H	2.124535	0.643797	-1.733113	H	-5.119138	2.42159	0.904176
H	1.812054	3.08215	-0.76929	H	-3.544631	2.682839	0.141181
tsi14i16				**tsi14p8**			
C	-0.453281	-0.717877	-0.113109	C	0.470442	-0.955873	0.119551
C	-1.354661	-1.661104	-0.316355	C	-0.558501	-1.586356	0.258134
C	-2.793132	-1.537943	-0.167084	C	-1.882106	-2.112358	0.168376
C	-3.477459	-0.370432	-0.141901	C	-2.979113	-1.354914	0.027922
C	-2.841759	0.910743	-0.08956	C	-3.005465	0.091011	-0.048245
C	-1.698112	1.13028	0.609768	C	-4.127317	0.794387	-0.196798
H	-1.010787	-2.606142	-0.737404	H	-1.980696	-3.187571	0.225504
H	-3.357006	-2.457709	-0.257253	H	-3.934919	-1.86325	-0.034882
H	-4.55187	-0.406631	-0.282314	H	-2.053417	0.607152	0.018268
H	-3.258741	1.712373	-0.692132	H	-5.071022	0.259823	-0.264454
H	-1.482709	0.472676	1.442537	H	0.029893	-2.786363	1.6821
C	0.934857	-0.461303	-0.115568	C	1.723327	-0.291692	0.048142
C	1.778084	-1.029059	0.858031	C	1.873512	0.995477	0.573631
C	1.501482	0.426592	-1.049809	C	2.823363	-0.916063	-0.547895
C	3.127581	-0.734384	0.877677	C	3.095102	1.639306	0.501692
H	1.353286	-1.7038	1.588679	H	1.025526	1.477875	1.039377
C	2.851935	0.711439	-1.020896	C	4.041731	-0.2652	-0.613861
H	0.860713	0.877804	-1.795292	H	2.708722	-1.911181	-0.95383
C	3.672951	0.135198	-0.058507	C	4.18176	1.012518	-0.091381
H	3.761878	-1.186325	1.62851	H	3.201057	2.634215	0.911995
H	3.271265	1.388059	-1.753407	H	4.886825	-0.757196	-1.075524
H	4.729488	0.36371	-0.037711	H	5.135879	1.518483	-0.145515
C	-0.935538	2.414906	0.5837	C	-4.1998	2.281571	-0.280964
H	0.136663	2.227354	0.508343	H	-4.652079	2.596148	-1.224097
H	-1.23355	3.040021	-0.257596	H	-4.825402	2.686365	0.517675

H	-1.096327	2.976268	1.506716	H	-3.211978	2.734617	-0.206445
tsi15i16				**tsi16p7**			
C	0.535767	-0.165976	0.174659	C	2.845958	0.741515	0.197554
C	1.175975	-1.325679	0.511239	C	3.436636	-0.469059	-0.092517
C	1.431852	1.037336	-0.066211	C	1.447768	0.912191	0.162493
C	2.662018	0.608448	-0.83419	C	0.647497	-0.236152	-0.065915
C	3.160091	-0.626781	-0.785753	C	1.262163	-1.447685	-0.349191
C	2.48157	-1.608644	0.065589	C	2.642791	-1.571473	-0.378746
H	0.899183	1.750329	-0.697945	H	3.462434	1.599109	0.434056
H	3.161841	1.370985	-1.420888	H	4.514303	-0.559229	-0.087997
H	4.054483	-0.901168	-1.328454	H	0.640774	-2.308898	-0.55773
H	3.056943	-2.393127	0.544834	H	3.094787	-2.526148	-0.609708
H	1.466555	-2.318966	-0.342714	H	1.396976	1.542959	-1.563678
C	-0.918489	-0.081726	0.052331	C	0.863409	2.175741	0.750765
C	-1.708672	-1.210386	0.318441	H	0.658999	2.020637	1.812276
C	-1.580501	1.091477	-0.327424	H	1.567862	3.000268	0.657938
C	-3.081909	-1.172925	0.185874	H	-0.06893	2.46736	0.277242
H	-1.218911	-2.115413	0.651031	C	-0.835328	-0.172544	-0.045856
C	-2.959325	1.128537	-0.455679	C	-1.532081	0.653529	-0.92534
H	-1.022292	1.994765	-0.527861	C	-1.559209	-0.972275	0.833992
C	-3.719093	-0.002135	-0.205388	C	-2.91625	0.682207	-0.920322
H	-3.663475	-2.060111	0.398652	H	-0.977813	1.264532	-1.62681
H	-3.441651	2.0504	-0.752294	C	-2.945321	-0.941631	0.84208
H	-4.795492	0.028914	-0.304286	H	-1.027562	-1.615756	1.523032
C	1.816345	1.77995	1.223501	C	-3.627859	-0.113421	-0.034191
H	2.360688	1.114605	1.893324	H	-3.441864	1.32388	-1.614641
H	0.920339	2.12703	1.738694	H	-3.491953	-1.565307	1.53654
H	2.448026	2.642785	1.005968	H	-4.709043	-0.089067	-0.029354
tsi17i26				**tsi17i18**			
C	-3.61905	-0.221965	0.186029	C	-0.217472	0.432014	-0.062938
C	-3.253161	-1.470834	0.457579	C	0.97371	0.705756	0.096822
C	-1.957583	-1.950393	-0.001671	C	2.377051	1.009839	0.086074
C	-2.628441	0.693821	-0.484014	C	3.356125	0.018047	0.022248
H	-3.89863	-2.1242	1.037171	C	3.101743	-1.376554	-0.081242
H	-1.818928	-2.166748	-1.052885	C	4.05218	-2.328968	-0.092686
C	-1.253587	0.156196	-0.313391	H	4.386139	0.347284	0.092201
C	-0.038244	0.249973	-0.229516	H	2.062168	-1.678917	-0.160577
C	1.367399	0.139286	-0.094208	H	5.102938	-2.077704	-0.016846

C	1.97503	0.280593	1.159906	H	3.798401	-3.374988	-0.185436
C	2.175516	-0.113692	-1.209827	H	1.560713	0.891836	1.247741
C	3.346786	0.16815	1.289526	C	2.743083	2.469907	-0.030251
H	1.356226	0.477386	2.024218	H	2.709177	2.769633	-1.07909
C	3.546545	-0.223981	-1.070288	H	2.048083	3.103878	0.51784
H	1.712822	-0.22233	-2.180842	H	3.749251	2.647092	0.346342
C	4.138217	-0.084082	0.177472	C	-1.589276	0.124116	-0.032284
H	3.802458	0.278015	2.264294	C	-2.556385	1.139323	-0.112054
H	4.158384	-0.420875	-1.940206	C	-2.020785	-1.208814	0.06645
H	5.210911	-0.170644	0.282607	C	-3.901345	0.826254	-0.086625
H	-4.588942	0.174455	0.458209	H	-2.235364	2.1684	-0.193622
H	-1.321456	-2.511796	0.670986	C	-3.369219	-1.506854	0.088953
C	-2.722111	2.129523	0.043659	H	-1.28486	-1.998616	0.125238
H	-2.511552	2.15359	1.112619	C	-4.31724	-0.494973	0.013439
H	-2.005086	2.773937	-0.461998	H	-4.633562	1.62015	-0.146889
H	-3.724316	2.527123	-0.121054	H	-3.684733	-2.538557	0.166542
H	-2.835779	0.716516	-1.560666	H	-5.371369	-0.734052	0.031129
tsi17i19				**tsi17p9**			
C	0.250149	-0.206281	-0.298656	C	-0.201886	0.415112	0.028086
C	1.309771	-0.708635	-0.684204	C	0.975714	0.659885	0.04765
C	2.776451	-0.619158	-0.630517	C	2.364003	0.996169	0.046405
C	3.154154	0.816592	-0.317928	C	3.321308	0.029616	-0.036029
C	2.369405	1.663537	0.361659	C	3.080848	-1.388048	0.022349
C	1.134115	1.307789	1.020658	C	4.051614	-2.30213	-0.032443
H	3.187709	-0.860482	-1.6136	H	4.353422	0.352779	-0.116645
H	4.075739	1.176528	-0.758135	H	2.048782	-1.706562	0.11558
H	2.649192	2.712769	0.375739	H	5.092195	-2.015274	-0.123868
H	1.142085	0.541658	1.782785	H	2.470871	1.186274	2.014372
C	-1.186326	-0.143847	-0.16988	C	-1.595721	0.112763	0.00925
C	-1.882239	1.031993	-0.448182	C	-2.030752	-1.213518	-0.035118
C	-1.899745	-1.272976	0.232299	C	-2.542918	1.138545	0.03561
C	-3.260398	1.074722	-0.333711	C	-3.383223	-1.503874	-0.052379
H	-1.331763	1.909243	-0.759208	H	-1.299204	-2.00914	-0.055913
C	-3.278796	-1.225264	0.347892	C	-3.893757	0.840705	0.017736
H	-1.361242	-2.185148	0.448071	H	-2.207977	2.16568	0.071024
C	-3.963045	-0.052883	0.065888	C	-4.31791	-0.479308	-0.026158
H	-3.788741	1.991547	-0.557291	H	-3.709296	-2.534378	-0.086398
H	-3.820725	-2.107858	0.659523	H	-4.61905	1.642544	0.038866
H	-5.039988	-0.017164	0.157425	H	-5.374505	-0.708983	-0.039648

H	0.404309	2.090767	1.187367	C	2.690502	2.450139	-0.196213
C	3.366647	-1.612874	0.383198	H	2.439713	2.712993	-1.225781
H	3.10273	-2.636585	0.118887	H	2.11432	3.097295	0.461687
H	4.452864	-1.527255	0.404524	H	3.750207	2.640218	-0.036417
H	2.986978	-1.404311	1.38283	H	3.833586	-3.359788	0.010659
tsi18i20				**tsi18p9**			
C	-0.234215	-0.139248	-0.050874	C	-0.166299	-0.43581	0.066076
C	-1.286143	-0.872769	-0.358315	C	1.004476	-0.723815	0.210348
C	-2.697719	-0.576144	-0.127024	C	2.402627	-0.992081	0.035849
C	-3.17823	0.675638	0.064893	C	3.293035	0.003446	-0.091499
C	-2.350753	1.838612	0.210749	C	2.991525	1.421262	-0.056921
C	-1.183707	1.819523	0.889929	C	3.912394	2.370815	-0.198696
H	-1.106472	-1.782683	-0.935076	H	4.334389	-0.266667	-0.23272
H	-4.2506	0.821027	-0.015278	H	1.95448	1.697819	0.094296
H	-2.648694	2.737641	-0.318987	H	4.956796	2.126652	-0.351765
H	-1.004161	1.08173	1.657336	H	0.925526	-1.377353	2.050102
C	1.17898	-0.147168	-0.06998	C	-1.551028	-0.129009	0.017933
C	1.901123	-1.118057	0.64874	C	-2.491532	-1.135897	-0.221327
C	1.900423	0.844525	-0.759143	C	-1.992598	1.18383	0.210862
C	3.282648	-1.103731	0.656089	C	-3.839795	-0.832436	-0.264785
H	1.357477	-1.877044	1.194564	H	-2.151387	-2.151107	-0.369375
C	3.280578	0.846276	-0.746662	C	-3.342757	1.477986	0.165209
H	1.355065	1.603259	-1.303648	H	-1.267191	1.963193	0.397658
C	3.980317	-0.12523	-0.040148	C	-4.269474	0.472896	-0.072539
H	3.821547	-1.861355	1.209171	H	-4.559688	-1.618058	-0.448827
H	3.819044	1.611426	-1.289604	H	-3.674415	2.49601	0.31663
H	5.061427	-0.116785	-0.029647	H	-5.324695	0.706419	-0.107366
H	-0.512153	2.667952	0.878321	H	3.65167	3.419292	-0.165975
C	-3.637709	-1.734579	-0.312767	C	2.797345	-2.44044	0.003465
H	-4.67767	-1.421887	-0.23872	H	2.516512	-2.929698	0.937954
H	-3.488644	-2.207962	-1.28588	H	2.279889	-2.962106	-0.803226
H	-3.459718	-2.501209	0.444521	H	3.870598	-2.548873	-0.141244
tsi19i20				**tsi20p3**			
C	-0.341351	0.217102	-0.386314	C	-2.272101	1.708952	-0.475347
C	-1.220342	-0.829777	-0.288231	C	-3.125882	0.657846	-0.225468
C	-0.975427	1.563047	-0.670546	C	-0.887387	1.546434	-0.338859
C	-2.182910	1.745777	0.217000	C	-0.360437	0.271105	-0.065292
C	-2.910390	0.711049	0.632908	C	-1.247152	-0.767676	0.192567

C	-2.534220	-0.647934	0.199326	C	-2.624852	-0.594902	0.132525
H	-0.276288	2.383545	-0.520842	H	-2.66644	2.675303	-0.757672
H	-2.456944	2.754594	0.501435	H	-4.19581	0.799401	-0.312309
H	-3.781005	0.847241	1.262085	H	-0.853432	-1.740936	0.458797
H	-1.656288	-1.290676	0.901864	H	-0.697346	2.348832	1.350476
C	1.093074	0.043194	-0.185606	C	1.101029	0.050842	-0.028005
C	1.642889	-1.248596	-0.174778	C	1.95892	1.022579	0.485666
C	1.966760	1.116966	0.025361	C	1.656068	-1.134062	-0.510867
C	2.989540	-1.452595	0.050484	C	3.327597	0.813216	0.520095
H	0.987330	-2.086668	-0.366481	H	1.546044	1.939002	0.886671
C	3.316853	0.909015	0.251741	C	3.024338	-1.342555	-0.478501
H	1.594363	2.131264	0.033191	H	1.010468	-1.889405	-0.939099
C	3.838237	-0.374698	0.267200	C	3.866256	-0.369567	0.038259
H	3.384579	-2.459869	0.047277	H	3.975222	1.575647	0.931594
H	3.965429	1.758710	0.418815	H	3.43515	-2.265068	-0.866124
H	4.893813	-0.534359	0.439371	H	4.935151	-0.531823	0.063719
H	-1.283599	1.638938	-1.721044	H	-0.224166	2.330533	-0.677235
C	-3.624933	-1.656875	-0.044377	C	-3.558153	-1.726556	0.456505
H	-4.200612	-1.359577	-0.923078	H	-3.061158	-2.691335	0.365622
H	-4.315379	-1.715424	0.797970	H	-3.928174	-1.639828	1.48018
H	-3.202075	-2.641763	-0.235576	H	-4.424969	-1.724258	-0.204296
tsi26i27				**tsi27p11′**			
C	3.340596	-0.642340	0.877669	C	-3.73033	-0.447949	0.115876
C	3.320559	0.540452	0.243601	C	-3.16772	0.831658	-0.279168
C	2.223386	0.659945	-0.815407	C	-1.808432	0.784093	-0.248638
H	0.998342	-1.848759	0.786900	H	-2.796956	-2.338142	0.657769
C	2.294244	-1.517522	0.328040	C	-2.723585	-1.31082	0.336715
H	4.030370	1.340822	0.407335	H	-3.745505	1.693701	-0.578783
C	1.441430	-0.558291	-0.424024	C	-1.453064	-0.609871	0.124795
C	0.232816	-0.897304	-0.017837	C	-0.26344	-1.220998	0.215685
C	-1.136615	-0.446902	0.038819	C	1.078543	-0.628904	0.144581
C	-2.131291	-1.111330	-0.687230	C	1.418086	0.484399	0.909705
C	-1.510929	0.622361	0.861017	C	2.058858	-1.222161	-0.650594
C	-3.449254	-0.697527	-0.617974	C	2.697192	1.012114	0.854948
H	-1.853756	-1.949780	-1.311591	H	0.672903	0.921621	1.561536
C	-2.831753	1.026925	0.932662	C	3.332929	-0.685702	-0.716513
H	-0.753822	1.127966	1.444513	H	1.812009	-2.101903	-1.231277
C	-3.805426	0.372260	0.191505	C	3.654859	0.43501	0.035312
H	-4.204268	-1.213855	-1.195435	H	2.947803	1.873938	1.458411

H	-3.103653	1.858012	1.569488	H	4.078542	-1.146317	-1.350158
H	-4.837234	0.690927	0.248200	H	4.652639	0.849699	-0.009369
H	4.066188	-0.926319	1.626019	H	-4.785061	-0.654498	0.210284
C	1.451054	1.971650	-0.792299	C	-0.901962	1.827604	-0.825769
H	0.627429	1.950165	-1.505364	H	-0.248035	2.281121	-0.084585
H	1.034534	2.154684	0.197860	H	-0.261359	1.397546	-1.597428
H	2.574744	-2.463400	-0.129677	H	-1.697503	1.409308	1.771474
H	2.687106	0.536396	-1.801428	H	-1.496598	2.619367	-1.279661
H	2.101109	2.808872	-1.048072	H	-0.284472	-2.296268	0.370179
p3				**p7**			
C	-0.371760	0.298903	-0.070641	C	0.67316	-0.21917	-0.06282
C	-1.258946	-0.745667	0.180484	C	1.45478	0.90635	0.23008
C	-0.890699	1.556139	-0.366920	C	1.29800	-1.42693	-0.36370
C	-2.634805	-0.562758	0.143046	C	2.83979	0.77865	0.19805
C	-2.260869	1.752882	-0.411208	C	2.67752	-1.53520	-0.39466
C	-3.127401	0.702761	-0.159324	C	3.45303	-0.42295	-0.11469
H	-0.219463	2.375000	-0.588936	H	0.68373	-2.28933	-0.58855
H	-2.655369	2.730436	-0.654306	H	3.44977	1.64187	0.43410
H	-4.197433	0.864587	-0.199247	H	3.14169	-2.48146	-0.63676
C	1.092091	0.073076	-0.025789	H	4.53243	-0.49018	-0.13200
C	1.940055	1.008190	0.564684	C	-0.81264	-0.16910	-0.04791
C	1.654722	-1.078450	-0.573062	C	-1.53369	-0.99152	0.81364
C	3.308525	0.798642	0.607286	C	-1.51474	0.67349	-0.90598
H	1.519175	1.898420	1.013349	C	-2.91967	-0.96762	0.82332
C	3.023032	-1.289236	-0.531293	H	-0.99868	-1.64779	1.48781
H	1.014396	-1.805459	-1.055161	C	-2.89959	0.69685	-0.90021
C	3.855674	-0.351287	0.059386	H	-0.96852	1.30491	-1.59419
H	3.948967	1.533110	1.076880	C	-3.60703	-0.12229	-0.03314
H	3.440922	-2.186039	-0.968600	H	-3.46302	-1.60969	1.50350
H	4.924086	-0.515365	0.092327	H	-3.42826	1.35323	-1.57830
H	-0.864063	-1.722962	0.431016	H	-4.68831	-0.10293	-0.02708
C	-3.572058	-1.696816	0.454755	C	0.84047	2.23038	0.59992
H	-3.086394	-2.662319	0.320051	H	0.51410	2.78150	-0.28353
H	-3.916385	-1.640857	1.489284	H	-0.03379	2.10180	1.23686
H	-4.453799	-1.666827	-0.185088	H	1.56253	2.85241	1.12674
p8				**p9**			
C	-3.289346	-0.327849	0.000000	C	-3.116181	-1.216892	0.000000
C	-2.691649	-1.646486	0.000000	C	-2.358296	-2.452509	0.000000

C	-3.402510	-2.773487	0.000000	C	-2.918048	-3.659501	0.000000
H	-3.163669	1.763085	0.000000	C	-2.591007	0.019408	0.000000
C	-2.613007	0.830735	0.000000	H	-4.197212	-1.309600	0.000000
H	-4.372668	-0.282213	0.000000	H	-1.277889	-2.361664	0.000000
H	-1.607390	-1.695065	0.000000	C	0.000000	0.459472	0.000000
C	0.000000	1.044411	0.000000	H	-3.994439	-3.783082	0.000000
H	-4.486999	-2.703797	0.000000	C	-1.182652	0.234940	0.000000
C	-1.199298	0.936267	0.000000	C	1.404408	0.708462	0.000000
C	1.420544	1.166985	0.000000	C	2.310737	-0.354152	0.000000
C	2.229970	0.028519	0.000000	C	1.892422	2.017105	0.000000
C	2.023225	2.427148	0.000000	C	3.672480	-0.110248	0.000000
C	3.607990	0.150912	0.000000	H	1.935666	-1.368037	0.000000
H	1.766767	-0.948267	0.000000	C	3.255457	2.253542	0.000000
C	3.401819	2.541949	0.000000	H	1.192842	2.841204	0.000000
H	1.399469	3.309967	0.000000	C	4.149002	1.192439	0.000000
C	4.198266	1.406173	0.000000	H	4.365044	-0.940809	0.000000
H	4.224365	-0.737721	0.000000	H	3.622303	3.270858	0.000000
H	3.857078	3.522919	0.000000	H	5.213920	1.380295	0.000000
H	5.275639	1.499014	0.000000	H	-2.319139	-4.559315	0.000000
C	-2.826009	-4.148952	0.000000	C	-3.446267	1.256742	0.000000
H	-3.157814	-4.710172	0.876392	H	-4.504055	0.999735	0.000000
H	-3.157814	-4.710172	-0.876392	H	-3.234682	1.868785	0.878034
H	-1.736934	-4.125528	0.000000	H	-3.234682	1.868785	-0.878034
p12				**vdW(i13)**			
C	3.753792	-0.397965	-0.124093	C	2.382607	-0.458733	0.398522
C	3.163392	0.885937	0.258739	C	1.846104	0.892869	0.349465
C	1.818938	0.803981	0.255448	C	1.377035	1.461294	-0.758465
H	2.851544	-2.30994	-0.635963	H	2.847335	-0.521892	2.453220
C	2.764945	-1.277181	-0.336533	H	2.387966	-1.010148	-0.537177
H	3.730581	1.764154	0.532178	H	1.829450	1.448142	1.283836
C	1.482136	-0.586438	-0.130483	C	-0.416179	-1.676116	-1.582167
C	0.301174	-1.208252	-0.247164	H	1.397998	0.888189	-1.681624
C	-1.04971	-0.630205	-0.161218	H	3.227164	-2.051319	1.488162
C	-1.437588	0.423915	-0.983921	C	2.839708	-1.042225	1.502538
C	-1.986504	-1.176482	0.714957	C	-1.054230	-0.961872	-0.571494
C	-2.720133	0.941675	-0.909928	C	-1.852465	0.159756	-0.884245
H	-0.727505	0.826524	-1.693237	C	-0.870005	-1.319025	0.780628
C	-3.264632	-0.651208	0.798151	C	-2.430212	0.899576	0.121520
H	-1.702165	-2.008957	1.34578	H	-1.985576	0.426216	-1.923021

C	-3.634496	0.411464	-0.013246	C	0.306050	-2.210334	-2.479238
H	-3.006855	1.759166	-1.557461	C	-1.450038	-0.568171	1.778130
H	-3.975606	-1.075002	1.494284	H	-0.246282	-2.169585	1.011626
H	-4.634928	0.817654	0.046731	C	-2.225172	0.540102	1.451273
H	4.812743	-0.587561	-0.209393	H	-3.036044	1.761999	-0.118003
C	0.878747	1.888109	0.671386	H	-1.296881	-0.834526	2.814217
H	0.342992	2.320468	-0.173971	H	-2.674533	1.129490	2.239117
H	0.123974	1.519457	1.36702	C	0.809707	2.838602	-0.841517
H	1.431989	2.68907	1.160666	H	1.376661	3.453646	-1.543582
H	0.332878	-2.279131	-0.429207	H	-0.219937	2.812616	-1.206215
				H	0.815216	3.332828	0.129743
vdW(i17)				**tsi13vdW**			
C	0.941026	1.684619	-0.607519	C	2.276771	0.735331	0.044183
C	1.989412	1.093573	0.202105	C	1.172249	1.67315	0.169721
C	2.924533	0.266874	-0.274493	C	0.365126	2.010397	-0.833266
H	-0.061594	2.737403	0.917772	C	3.063007	0.366298	1.050476
H	0.951159	1.436224	-1.664442	H	2.930405	0.772748	2.046508
C	0.33679	-1.705444	-0.264343	H	3.857799	-0.351916	0.908311
H	2.911664	0.024466	-1.332757	H	2.439455	0.304881	-0.93918
H	-0.78594	2.882462	-0.775003	C	1.782749	-2.71673	-1.279687
C	-0.017839	2.475745	-0.132514	H	1.005669	2.102831	1.154281
C	-0.883028	-1.054344	-0.069306	H	0.543508	1.570011	-1.810395
C	-1.317063	-0.72429	1.229353	C	-0.333235	-1.505567	-0.213827
C	-1.67753	-0.681697	-1.171387	C	-1.380445	-1.035282	-1.034407
C	-2.498474	-0.039337	1.412351	C	-0.37682	-1.243278	1.171245
H	-0.700294	-1.009691	2.069374	C	0.745576	-2.190219	-0.767939
C	1.426608	-2.326372	-0.454246	C	-2.431261	-0.33625	-0.484014
C	-2.861853	-0.004676	-0.976336	H	-1.336909	-1.236792	-2.09512
H	-1.336508	-0.935653	-2.164779	C	-1.426717	-0.532491	1.707827
C	-3.270933	0.319672	0.312457	H	0.438973	-1.591424	1.787547
H	-2.825662	0.218879	2.409693	C	-2.45305	-0.080716	0.883606
H	-3.469528	0.278819	-1.824124	H	-3.234743	0.019799	-1.113324
H	-4.198326	0.856002	0.461412	H	-1.454003	-0.324005	2.767957
H	1.99051	1.343738	1.259627	H	-3.275561	0.477298	1.310272
C	4.013275	-0.351062	0.534002	C	-0.780655	2.960313	-0.728494
H	3.963145	-0.040302	1.577183	H	-0.639179	3.819447	-1.387959
H	4.992085	-0.073438	0.136759	H	-1.71351	2.479584	-1.031801
H	3.939726	-1.438485	0.48854	H	-0.901672	3.327808	0.290359
tsi17vdW							

C	-0.812916	1.815819	0.227812				
C	-1.955591	1.065793	-0.2635				
C	-2.834447	0.451622	0.529683				
H	0.007373	2.377735	-1.629431				
H	-0.700236	1.870538	1.306529				
C	-0.352357	-1.792138	-0.251307				
H	-2.688902	0.517981	1.605039				
H	0.926946	2.949805	-0.133235				
C	0.086534	2.412488	-0.5496				
C	0.84405	-1.09599	-0.07777				
C	1.599145	-0.682274	-1.193228				
C	1.301313	-0.772822	1.215537				
C	2.770433	0.021853	-1.015902				
H	1.238726	-0.927579	-2.181841				
C	-1.42244	-2.456961	-0.413095				
C	2.470483	-0.063681	1.380786				
H	0.713889	-1.088842	2.065616				
C	3.205794	0.331692	0.267759				
H	3.347916	0.336812	-1.873537				
H	2.81741	0.185114	2.373822				
H	4.124215	0.886927	0.402434				
H	-2.080764	1.009175	-1.341041				
C	-4.020132	-0.323262	0.066979				
H	-4.100886	-0.316882	-1.019051				
H	-4.939243	0.08914	0.489449				
H	-3.945671	-1.362754	0.390319				
i34				**i35**			
C	2.179582	1.018897	0.367674	C	0.394153	0.792956	-0.214368
C	3.023459	-0.063522	-0.282683	C	-0.797022	1.233273	-0.260406
C	4.001213	-0.712307	0.330729	C	-2.211142	1.101526	0.225479
H	3.437542	2.809179	-0.055058	C	-2.988209	-0.091612	-0.151588
H	2.458539	1.056472	1.426463	C	-3.833179	-0.723106	0.65222
H	2.79202	-0.271258	-1.322444	C	-1.8206	2.129819	-0.82608
C	-0.407381	0.406977	0.187305	H	-2.137687	1.948883	-1.845858
H	4.20567	-0.484034	1.373472	H	-1.802425	3.170072	-0.528428
H	1.848395	2.7485	-1.030976	H	-2.398167	1.490616	1.219711
C	2.483936	2.344011	-0.257734	H	-2.827105	-0.464336	-1.160029
C	-1.793111	0.06977	0.083173	H	-3.976841	-0.342976	1.659846
C	-2.199947	-1.264955	0.119296	C	1.647877	0.242734	-0.08567

C	-2.757268	1.069258	-0.056532	C	2.053179	-0.850716	-0.895034
C	-3.541376	-1.589508	0.01764	C	2.581456	0.756793	0.851884
H	-1.454527	-2.040305	0.227741	C	3.313198	-1.388556	-0.763702
C	0.755924	0.686676	0.281311	H	1.354474	-1.254382	-1.61434
C	-4.097183	0.73822	-0.157739	C	3.835931	0.202115	0.965368
H	-2.444464	2.103685	-0.083977	H	2.289814	1.590321	1.475358
C	-4.493412	-0.590456	-0.121126	C	4.215493	-0.871504	0.163085
H	-3.844927	-2.627131	0.046977	H	3.602704	-2.222964	-1.388503
H	-4.835486	1.52112	-0.265532	H	4.532819	0.606982	1.687066
H	-5.541081	-0.846553	-0.200304	H	5.20305	-1.300291	0.259017
C	4.862191	-1.757913	-0.301095	C	-4.61763	-1.940089	0.282072
H	5.91456	-1.468037	-0.269509	H	-5.690548	-1.759627	0.376771
H	4.778362	-2.706418	0.233179	H	-4.413397	-2.248271	-0.743085
H	4.585641	-1.926105	-1.341355	H	-4.377717	-2.77583	0.942915
i36				**i37**			
C	2.343335	-0.00179	-0.286159	C	0.05924	0.270848	-0.151505
C	2.90392	1.197168	0.457286	C	-1.205591	0.387176	-0.179792
C	3.794511	2.033881	-0.04863	C	-2.531981	-0.089663	0.345931
H	2.649082	0.089339	-1.335026	C	-3.011419	-1.428604	-0.032804
H	2.553023	1.31356	1.476635	C	-3.660549	-2.252001	0.777447
C	-0.31682	-0.014748	-0.154716	C	-2.434467	1.022217	-0.690625
H	4.192761	2.852694	0.534886	H	-2.718657	0.731076	-1.696835
H	4.151532	1.933041	-1.066758	H	-2.770805	0.229424	1.354998
H	2.403384	-1.762397	1.074505	H	-2.794486	-1.736846	-1.051159
C	2.932567	-1.264943	0.273971	H	-3.884894	-1.978497	1.801207
C	-1.744615	-0.018757	-0.075853	C	1.418584	0.083726	-0.060953
C	-2.455911	1.182199	-0.072413	C	2.08698	-0.846136	-0.899588
C	-2.44599	-1.22315	-0.000627	C	2.198741	0.821265	0.867581
C	-3.837627	1.17539	0.004801	C	3.449042	-1.019369	-0.804736
H	-1.914244	2.115873	-0.131014	H	1.507711	-1.416551	-1.612032
C	0.881032	-0.010375	-0.228544	C	3.559584	0.630471	0.944308
C	-3.827727	-1.223239	0.076331	H	1.705627	1.534155	1.513498
H	-1.89676	-2.154266	-0.003846	C	4.198248	-0.287021	0.113266
C	-4.527381	-0.025627	0.07942	H	3.940151	-1.733984	-1.451667
H	-4.378441	2.111962	0.006562	H	4.136831	1.20111	1.659536
H	-4.360787	-2.162472	0.134018	H	5.267545	-0.429834	0.180382
H	-5.607122	-0.028303	0.139584	C	-2.767827	2.441938	-0.311767
C	4.320096	-1.651406	-0.075552	H	-2.263255	3.146632	-0.972678
H	5.045645	-0.903762	0.270386	H	-3.842217	2.617786	-0.378628

H	4.59401	-2.608314	0.364503	H	-2.448096	2.653526	0.708786
H	4.451579	-1.72458	-1.160326	H	-3.98696	-3.227078	0.444017
tsi13i35				**tsi17i37**			
C	0.357399	-1.118527	0.316801	C	0.012753	0.546659	-0.344448
C	-0.791742	-1.579891	0.341809	C	-1.222757	0.624451	-0.386744
C	-2.34716	-1.142863	-0.362689	C	-2.570196	-0.22271	0.370646
C	-2.932595	0.078515	0.116357	C	-2.76588	-1.585603	-0.038112
C	-3.333917	1.089622	-0.664038	C	-2.846554	-2.628594	0.795626
C	-2.030658	-2.295894	0.537107	C	-2.623055	0.935115	-0.578609
H	-2.45201	-2.253606	1.537318	H	-2.994351	0.669005	-1.566166
H	-2.087709	-3.286931	0.099268	H	-2.585665	0.012918	1.426802
H	-2.323681	-1.328081	-1.42729	H	-2.836533	-1.761253	-1.107687
H	-3.030691	0.178595	1.194752	H	-2.772234	-2.500446	1.868225
H	-3.224502	0.990513	-1.739998	C	1.374607	0.275123	-0.169013
C	1.555908	-0.413953	0.155941	C	2.042877	-0.629247	-1.015722
C	1.900782	0.628589	1.037195	C	2.110795	0.907065	0.85077
C	2.450693	-0.73533	-0.882402	C	3.387106	-0.88827	-0.840321
C	3.08611	1.317141	0.876996	H	1.487541	-1.120048	-1.802644
H	1.222353	0.883592	1.839292	C	3.454273	0.636531	1.013929
C	3.631339	-0.036078	-1.030315	H	1.608873	1.606017	1.505202
H	2.199279	-1.536563	-1.56327	C	4.101933	-0.260032	0.172437
C	3.958765	0.99254	-0.154836	H	3.884677	-1.588094	-1.498217
H	3.333879	2.116977	1.561961	H	4.004488	1.128835	1.804551
H	4.305644	-0.29439	-1.835857	H	5.154778	-0.466965	0.304517
H	4.885927	1.53537	-0.275009	C	-3.144427	2.265057	-0.080218
C	-3.931551	2.363214	-0.165777	H	-2.847095	3.069879	-0.751249
H	-4.934052	2.516597	-0.572359	H	-4.232617	2.243762	-0.019867
H	-4.001873	2.371463	0.921853	H	-2.746875	2.485759	0.910165
H	-3.33281	3.223955	-0.473553	H	-2.993841	-3.632643	0.425049
tsi34i35				**tsi36i37**			
C	0.389775	0.377239	0.089138	C	-0.07494	0.1095	0.214276
C	-0.785002	0.722445	0.001122	C	1.147574	-0.003873	0.201728
C	-2.205196	1.02686	-0.006776	C	2.597879	-0.035492	0.285497
C	-3.136468	-0.125962	-0.178457	C	3.319393	1.223234	-0.061011
C	-4.213481	-0.325127	0.564661	C	4.315591	1.724284	0.649027
C	-1.755445	1.74853	-1.236182	C	2.348661	-1.024114	-0.811017
H	-1.80458	1.252997	-2.192619	H	2.376733	-0.647838	-1.82353
H	-1.478009	2.788064	-1.182596	H	2.967996	-0.484066	1.206482
H	-2.505947	1.684115	0.806577	H	2.979179	1.72713	-0.959622

H	-2.883687	-0.82324	-0.972048	H	4.66511	1.242339	1.554049
H	-4.439464	0.383602	1.356697	C	-1.478888	0.140544	0.127709
C	1.759635	0.053584	0.08334	C	-2.12692	1.061693	-0.711487
C	2.221396	-1.094705	-0.579874	C	-2.264409	-0.746213	0.88243
C	2.69324	0.868315	0.743753	C	-3.505717	1.08716	-0.790386
C	3.566524	-1.408756	-0.581071	H	-1.532208	1.750747	-1.29481
H	1.510089	-1.729634	-1.089381	C	-3.642304	-0.709769	0.794115
C	4.035714	0.543007	0.73457	H	-1.776199	-1.457853	1.533606
H	2.347605	1.75363	1.258948	C	-4.272162	0.204287	-0.040666
C	4.481228	-0.594554	0.074043	H	-3.988552	1.802467	-1.442629
H	3.906	-2.296549	-1.097499	H	-4.232066	-1.400483	1.381762
H	4.742277	1.181926	1.247094	H	-5.351051	0.228986	-0.105685
H	5.532982	-0.844953	0.070511	C	2.322507	-2.490383	-0.560802
C	-5.163965	-1.46717	0.405395	H	1.638235	-2.999711	-1.239304
H	-6.17424	-1.107961	0.19937	H	3.315031	-2.934355	-0.698546
H	-4.862635	-2.125649	-0.408629	H	2.004901	-2.70842	0.459893
H	-5.218125	-2.058592	1.3216	H	4.815291	2.635906	0.351861

Table S7 Vibrational frequencies and infrared intensities on the **(a)** phenylethynyl + 1,3-butadiene-d_6, **(b)** phenylethynyl + isoprene, and **(c)** phenylethynyl +1,3-pentadiene adiabatic doublet ground state potential energy surfaces.

(a)

	phenylethynyl		**1,3-Butadiene-d_6**	
Normal modes	Frequency(cm^{-1})	IR Inten	Frequency(cm^{-1})	IR Inten
ν1	112.68	17.3904	142.31	0.2856
ν2	148.66	4.6072	254.19	1.9456
ν3	251.55	26.3028	396.63	7.5858
ν4	393.87	0	453.32	0
ν5	477.42	3.1292	628.27	0
ν6	490.16	18.9612	733.16	0
ν7	511.05	0.7921	751.59	0
ν8	632.48	0.1684	754.64	68.0522
ν9	696.07	46.3153	759.63	1.5888
ν10	787.71	0.2095	807.89	0.293
ν11	799.2	23.247	846.82	0
ν12	870.13	0	943.33	0
ν13	981.96	0.8822	1027.55	6.0711
ν14	1019.66	4.5667	1068.37	1.5878
ν15	1024.97	0	1069.32	0
ν16	1044.22	0.1747	1215.86	0
ν17	1053.58	0.6553	1602.41	15.3095
ν18	1116.24	5.0608	1684	0
ν19	1185.47	81.7314	2297.96	0
ν20	1191.6	3.3766	2298.46	8.8991
ν21	1230.32	21.1034	2348.47	0
ν22	1324.35	7.2501	2349.94	4.0006
ν23	1358.66	7.8198	2419.64	11.1885
ν24	1483.47	12.0342	2419.79	0
ν25	1514.79	1.8218		
ν26	1614.98	0.511		
ν27	1639.86	92.1565		
ν28	2020.99	45.6399		
ν29	3200.68	0.3554		
ν30	3213.21	3.2854		
ν31	3219.82	5.1552		

ν32	3230.21	3.8096		
ν33	3233.27	5.2791		
	i1		**i3**	
ν1	6.38	0.0096	29.63	0.0318
ν2	40.46	0.431	79.5	0.326
ν3	64.02	0.4513	139.16	3.935
ν4	98.33	1.4504	145.27	0.6152
ν5	123.93	0.7464	233.43	1.9021
ν6	175.62	2.7305	301.81	0.0328
ν7	240.1	0.3268	340.99	0.0066
ν8	273.91	1.705	396.44	2.2334
ν9	319.22	1.0538	414.91	0.8252
ν10	394.91	0.0972	418.68	0.152
ν11	405.65	3.483	503.09	8.3091
ν12	417.68	0.0027	535.11	0.8369
ν13	428.17	0.3085	556.56	18.6198
ν14	540.85	0.8767	588.39	4.2815
ν15	556.55	5.8691	639.62	0.0317
ν16	571.71	0.2598	705.49	1.4721
ν17	631.52	4.8696	719.82	32.9323
ν18	642.56	0.2774	750.39	0.9507
ν19	651.52	34.4954	774.69	19.5781
ν20	715.38	2.4359	778.36	0.4143
ν21	720.88	34.2331	787.44	4.3497
ν22	741.15	0.7068	824.57	22.0862
ν23	767.64	6.1895	859.75	1.0149
ν24	792.61	40.601	871.04	0.0054
ν25	820.04	0.3697	873.21	0.2903
ν26	820.68	2.9999	879.38	0.379
ν27	876.99	0.0028	894.6	1.61
ν28	902.47	0.1572	931.39	0.2069
ν29	919.93	6.4778	945.73	0.6329
ν30	944.1	0.9247	954.21	3.1586
ν31	960.49	3.6022	971.16	1.3056
ν32	1014.07	0.0015	1010.12	0.0042
ν33	1028.25	0.1392	1027.95	0.1069
ν34	1033.19	0.0792	1028.44	0.0297
ν35	1053.23	2.8315	1066.68	5.6658
ν36	1055.97	5.8381	1079.83	3.4372

ν37	1064.39	4.4082	1095.38	1.3425
ν38	1096.71	6.2909	1121.69	7.4337
ν39	1113.98	5.5469	1155.09	0.8421
ν40	1189.57	2.6612	1187.47	0.0297
ν41	1189.69	0.0567	1192.1	0.4208
ν42	1213.32	0.0042	1220.17	0.3943
ν43	1316.91	0.5616	1254.19	1.3034
ν44	1317.44	8.3619	1307.6	0.7452
ν45	1330.34	1.5317	1331.46	0.4507
ν46	1361.79	0.2929	1368.09	0.8146
ν47	1427.59	13.7763	1495.65	6.6225
ν48	1493.07	5.3533	1548.35	20.6937
ν49	1547.23	23.7527	1652.64	2.9505
ν50	1648.11	1.5617	1680.58	12.8293
ν51	1680.25	8.4328	1711.61	18.8351
ν52	2196.01	12.0727	1757.52	2.784
ν53	2248.92	3.8197	2198.21	8.3068
ν54	2291.83	5.1802	2204.4	22.1643
ν55	2333.53	12.8911	2255.24	10.1757
ν56	2345.02	2.1641	2260.78	4.8253
ν57	2379.88	0.622	2331.13	2.425
ν58	2428.69	4.9296	2370.77	13.3537
ν59	3192.31	0.8635	3185.07	3.1705
ν60	3200.93	2.9771	3192.62	0.4583
ν61	3210.97	13.4986	3202.4	13.9463
ν62	3217.99	18.361	3212.85	25.993
ν63	3223.74	8.1231	3220.71	11.4545
	i2		**i4**	
ν1	18.9	0.3476	37.42	0.0934
ν2	28.94	0.0445	83.77	0.1701
ν3	58.03	0.4253	149.76	0.9882
ν4	121.19	0.2721	171.13	0.4509
ν5	127.62	0.7388	261.34	0.1391
ν6	159.43	0.3578	318.2	0.1551
ν7	189.15	2.5261	372.23	3.8126
ν8	273.91	1.6556	414.46	3.9152
ν9	331.21	10.8529	418.47	0.2313
ν10	406.61	0.5411	446.01	3.7971
ν11	412.15	0.0026	503.15	6.3525

ν12	455.01	0.727	558.29	24.186
ν13	488.44	8.5663	562.93	2.4808
ν14	513.92	0.3417	597.55	1.4628
ν15	536.82	4.6598	626.55	2.8142
ν16	627.58	7.3274	639.11	0.0778
ν17	632.14	1.1544	711.79	5.6591
ν18	664.93	9.6043	715.78	35.0768
ν19	697.02	35.3781	766.28	15.7398
ν20	734.44	19.4853	772.54	2.0143
ν21	744.53	3.455	786.04	14.9749
ν22	761.82	4.9768	793.15	12.3158
ν23	764.25	25.0058	829.73	8.668
ν24	770.26	38.3626	845.92	0.1611
ν25	791.01	0.2058	854.28	3.717
ν26	841.25	2.1001	863.14	0.2915
ν27	843.43	0.2301	877.29	0.4286
ν28	847.77	0.0001	908.41	0.4449
ν29	920.6	3.1448	909.88	2.1671
ν30	938.41	0.1632	945.12	2.2114
ν31	987.51	5.2779	998.3	4.0047
ν32	1002.58	0.0042	1006.62	0.0843
ν33	1009.71	2.5031	1022.31	0.3919
ν34	1016.98	0.0008	1025.68	0.0141
ν35	1031.33	1.4365	1055.36	0.0529
ν36	1044.08	3.1255	1070.39	4.1637
ν37	1051.16	3.9153	1074.23	2.4058
ν38	1113.16	5.3986	1136.39	5.3561
ν39	1117.01	0.9894	1192.96	0.2179
ν40	1180.91	0.1026	1205.2	13.0356
ν41	1192.12	1.27	1234.45	0.0411
ν42	1216.85	3.4627	1254.04	1.3827
ν43	1260.05	6.7595	1294.79	3.1068
ν44	1302.5	0.1466	1328.85	0.0662
ν45	1355.08	0.0001	1347.65	0.5944
ν46	1474.99	2.3945	1380.95	0.9001
ν47	1503.05	17.1964	1457.56	0.3347
ν48	1598.45	3.3604	1505.61	5.7202
ν49	1618.75	3.7772	1551.77	23.9452
ν50	1621	10.6907	1595.11	2.2867

ν51	1680.28	6.6876	1646.1	3.6597
ν52	1843.38	10.9552	1671.26	13.3801
ν53	2297.78	6.0041	2154.51	11.9013
ν54	2297.98	11.534	2205.83	9.0066
ν55	2326.69	15.125	2345.91	1.9371
ν56	2345.49	5.8637	2358.89	1.0762
ν57	2346.44	10.289	2373.27	17.686
ν58	2420.21	4.0262	2386.44	8.3531
ν59	3192.36	2.0393	3189.46	3.3516
ν60	3199.01	4.2558	3197.71	
ν61	3212.06	8.0509	3211.89	20.0437
ν62	3217.49	17.3383	3219.62	20.9671
ν63	3223.83	10.6622	3225.18	5.8236
	i21		**i22**	
ν1	15.08	0.5373	44.61	0.0193
ν2	34.81	0.0047	75.46	0.6017
ν3	82.17	0	112.28	0.1958
ν4	98.21	1.4385	179.37	0.2567
ν5	178.36	0.0732	236.88	0.1076
ν6	291.22	0.0244	289.45	0.3569
ν7	313.38	0	314.18	1.583
ν8	337.57	5.3885	339.71	7.4528
ν9	413.82	5.3543	422.27	0.2327
ν10	415.65	0	456.41	6.0923
ν11	494.05	2.6846	488.17	6.7056
ν12	512.85	13.4463	518.91	20.0258
ν13	560.12	5.3042	597.26	5.5685
ν14	615.82	4.7037	634.57	0.4366
ν15	634.83	0.151	648.47	1.508
ν16	693.43	33.1753	668.46	5.6019
ν17	699.82	3.4276	690.92	1.3598
ν18	724.79	0	721.14	37.8337
ν19	734.7	9.0582	745.83	10.0083
ν20	763.19	0	760.02	3.9596
ν21	764.96	43.9688	773.74	7.6966
ν22	784.95	0.0984	780.61	2.382
ν23	785.79	2.2039	792.85	28.8698
ν24	841.12	0	810.71	4.2911
ν25	847.13	3.3165	827.99	3.5365

ν26	860.55	9.5163	840.64	0.7162
ν27	893.73	1.0742	872.41	0.1487
ν28	904.53	0.0002	879.98	0.8996
ν29	908.93	3.143	932.56	10.376
ν30	915.53	0	946.56	2.2514
ν31	995.1	0.11	971.3	2.0497
ν32	997.57	1.5942	1010.31	0.003
ν33	999.05	0	1023.12	0.3614
ν34	1011.39	0.0088	1027.27	0.1498
ν35	1046.84	4.7806	1040.86	0.4127
ν36	1073.36	1.7963	1065.38	5.611
ν37	1096.35	0.5974	1079.71	5.5029
ν38	1112.01	5.1682	1124.03	6.148
ν39	1135.4	6.0933	1176.02	0.145
ν40	1141.9	0.6247	1188.37	0.1554
ν41	1177.97	0.326	1214.47	0.1512
ν42	1196.52	2.5306	1235.93	1.0057
ν43	1235.6	0.4005	1275.97	1.8535
ν44	1283.93	2.379	1320.53	0.9727
ν45	1301.86	0.6208	1339.91	0.5571
ν46	1353.05	0.0743	1369.63	0.3975
ν47	1472.63	1.3794	1466.33	1.7519
ν48	1503.12	22.7321	1495.04	6.0871
ν49	1591.41	3.7556	1515.81	3.3229
ν50	1615.18	9.5299	1543.62	19.7636
ν51	1670.04	22.0762	1640.84	1.4464
ν52	1930	0.372	1666.68	10.908
ν53	2218.5	21.9786	2220.85	3.4004
ν54	2221.07	0.6214	2282.14	4.2076
ν55	2282.61	0	2326.17	8.2393
ν56	2284.28	15.0339	2374.84	4.9971
ν57	2358.18	2.0725	2401.34	7.4062
ν58	2407.17	8.6575	2419.67	3.8002
ν59	3189.8	3.9866	3182.77	6.1562
ν60	3195.71	4.1632	3191.64	0.2203
ν61	3210.01	7.4096	3202.52	21.2213
ν62	3214.54	23.2544	3216.15	25.9143
ν63	3222.19	12.9242	3226.08	5.8709
	tsi1i3		**tsi1i2**	

ν1	-665.23	22.9311	-1502.07	606.41
ν2	24.06	0.12	38	0.15
ν3	64.33	0.4478	41.62	0.2108
ν4	88.01	1.3454	67.71	1.3566
ν5	126.56	1.2041	121.23	0.3535
ν6	237.19	1.3119	128.73	0.3941
ν7	244.66	1.0863	183.94	1.2059
ν8	312.4	2.4936	236.19	1.1546
ν9	353.89	0.446	256.29	0.6581
ν10	418.27	0.0677	317.22	1.4135
ν11	421.9	3.0599	414.77	0.0104
ν12	463.58	3.3809	425.72	1.6421
ν13	486.5	27.881	447.86	12.8887
ν14	497.6	22.7422	484.15	7.8035
ν15	527.71	8.4365	512.06	5.1837
ν16	572.22	4.223	517.06	8.1235
ν17	639.64	2.8838	528.99	7.213
ν18	644.16	3.6153	594.26	2.3121
ν19	672.71	1.0467	641.73	0.1364
ν20	722.58	29.7008	684.92	6.8582
ν21	725.92	4.1655	711.78	44.7766
ν22	770.2	1.0547	713.01	17.7333
ν23	788.73	48.2543	734.23	9.3595
ν24	797.93	0.8352	753.45	19.3007
ν25	810.81	3.0342	763.26	3.0437
ν26	861.02	0.5311	777.82	50.2489
ν27	873.19	4.0302	803.85	2.894
ν28	877.67	0.0041	863	0.008
ν29	898.69	0.4082	921.04	0.9585
ν30	929.85	0.2077	936.32	3.8894
ν31	959.79	3.8277	949.37	1.7649
ν32	960.71	2.38	1005.84	0.0024
ν33	1014.79	0.0064	1015.21	4.7689
ν34	1028.68	0.1731	1017.77	3.1164
ν35	1032.61	0.0489	1023.75	0.0839
ν36	1063.84	2.4213	1027.23	2.4947
ν37	1068.07	4.6838	1060.29	1.4927
ν38	1106.48	0.8624	1088.71	3.6545
ν39	1113.84	6.2419	1115.29	5.4899

ν40	1141.03	2.0815	1187.7	0.1804
ν41	1189.7	0.0273	1201.93	35.0864
ν42	1212.26	0.201	1211.22	2.1571
ν43	1256.82	0.3076	1279.14	5.8565
ν44	1278.11	1.5532	1311.99	0.3748
ν45	1317.94	0.4129	1342.61	53.5107
ν46	1360.54	0.7959	1361.84	0.0002
ν47	1492.55	6.1072	1452.41	31.2138
ν48	1543.22	20.6473	1488.55	3.6098
ν49	1598.65	8.006	1526.85	21.2009
ν50	1648.54	2.1093	1539.31	28.8417
ν51	1677.63	8.5908	1628.44	2.9119
ν52	2081.55	0.2807	1658.31	50.112
ν53	2206.95	14.2808	2141.31	18.9578
ν54	2281.52	11.8146	2294.19	5.0954
ν55	2282.7	0.3979	2333.29	15.4309
ν56	2320.63	3.1592	2336.34	0.9228
ν57	2366.81	8.1595	2351.02	5.9618
ν58	2406.3	3.0735	2424.11	4.1387
ν59	3191.31	1.2389	3191.87	7.0429
ν60	3199.38	2.8563	3198.61	2.7837
ν61	3209.45	13.7901	3210.91	6.3002
ν62	3216.66	18.0606	3216.01	20.6946
ν63	3223.03	9.5676	3223.51	18.3137
	tsi1p2		**tsi3i4**	
ν1	-571.56	11.503	-1257.47	16.3036
ν2	11.57	0.1117	35.5	0.2118
ν3	41.05	0.3042	64.88	1.3183
ν4	72.32	1.4656	125.52	0.7371
ν5	113.65	0.0383	200.25	1.2677
ν6	121.84	0.4605	238.26	2.9621
ν7	180.12	0.6857	325.75	1.5471
ν8	196.01	4.4197	367.13	0.8503
ν9	257.26	6.4523	418.25	0.3802
ν10	260.93	4.5018	424.78	3.4922
ν11	349.25	3.1794	439.19	18.3402
ν12	359.8	3.4118	484.01	1.7765
ν13	416.31	0.0082	542.14	28.0585
ν14	423.79	6.8854	571.27	18.5089

ν15	440.03	4.2417	602.19	2.0242
ν16	536.23	9.5504	638.71	0.4846
ν17	547.48	0.8664	679.06	37.2944
ν18	582.37	2.7244	708.3	5.9961
ν19	641.24	0.5824	715.27	38.2809
ν20	658.57	7.5576	740.71	3.3048
ν21	665.73	5.5123	777.64	10.2424
ν22	718.44	33.9237	785.25	22.6683
ν23	738.29	0.9794	815.21	11.1323
ν24	742.65	29.4835	835.66	4.1947
ν25	758.6	1.7374	860.44	1.8458
ν26	784.72	1.673	865.82	15.6307
ν27	791.43	40.7378	868.76	8.4459
ν28	833.8	2.268	885.66	6.5081
ν29	874.19	0.1012	911.37	4.564
ν30	874.3	0.3943	947.02	3.1236
ν31	937.54	0.4827	979.21	2.3062
ν32	958.81	3.3031	987.78	2.5071
ν33	969.79	0.0625	1009.22	0.475
ν34	1012.49	0.0079	1022.71	0.1695
ν35	1027.58	0.2511	1029	0.2601
ν36	1032.72	0.0531	1065.1	5.054
ν37	1058.51	3.5817	1082.92	1.5781
ν38	1064.12	6.0474	1121.78	11.4241
ν39	1096.94	5.5974	1150.73	8.0607
ν40	1114.76	5.5563	1188.26	0.0555
ν41	1190.81	0.0746	1210.76	2.8066
ν42	1212.16	0.5231	1217.41	0.0735
ν43	1237.6	1.788	1275.8	27.8384
ν44	1317.74	0.312	1323.82	3.1033
ν45	1331.61	17.6204	1346.52	20.8976
ν46	1361.82	0.4296	1365.22	3.6345
ν47	1492.76	5.4275	1443.11	61.7216
ν48	1531.69	7.2345	1496	14.7728
ν49	1558.44	32.3709	1538.57	16.8127
ν50	1602.4	1.4834	1567.86	1.1511
ν51	1646.45	1.5515	1639.87	10.7287
ν52	1678.99	9.281	1643.44	3.0129
ν53	2300.2	1.8299	1666.5	5.9133

ν54	2336.68	1.3914	2191.51	10.8557
ν55	2344.97	3.787	2295.96	5.6233
ν56	2358.87	1.7528	2330.86	7.1565
ν57	2367.79	11.9249	2344.27	5.6453
ν58	2421.98	5.1675	2384.19	11.4844
ν59	3193.49	1.3229	3188.16	3.0263
ν60	3202.13	2.4527	3196.17	7.5951
ν61	3211.73	12.2354	3209.43	14.0081
ν62	3218.99	17.0256	3215.35	17.7187
ν63	3224.74	9.9469	3220.99	14.9091
	tsi2i4		**tsi2p2**	
ν1	-355.01	1.934	-593.85	10.1222
ν2	40.39	0.0493	17.46	0.1203
ν3	68.05	0.2733	38.63	0.744
ν4	76.24	0.4571	65.21	2.2995
ν5	179.76	0.8421	76.36	0.786
ν6	213.57	0.0846	110.39	0.0584
ν7	242.9	0.4796	128.33	1.4421
ν8	272.91	0.7245	217.9	0.1858
ν9	376.71	1.2388	260.84	0.9774
ν10	415.09	0.327	276.82	5.8781
ν11	424.53	5.3589	360.08	11.7574
ν12	471.51	11.7846	373.16	3.6384
ν13	495.41	10.448	416.07	0.1295
ν14	528.94	20.9415	422.09	11.1672
ν15	543.58	0.2358	436.53	3.7106
ν16	605.93	18.2049	535.94	5.8993
ν17	636.47	0.7864	554.87	2.4144
ν18	674.95	13.6672	586.92	1.6498
ν19	711.7	32.3609	640.7	0.7705
ν20	716.64	0.6841	661.14	15.2485
ν21	732.54	2.6978	669.32	5.4995
ν22	776.25	7.5871	716.88	33.3215
ν23	781.49	30.0386	732.43	1.4214
ν24	804.7	5.5245	748.27	31.401
ν25	818.56	3.4237	757.64	1.1539
ν26	852	0.4801	790.01	44.7445
ν27	856.74	0.4402	806.36	0.2049
ν28	862.94	0.0476	843.96	1.0471

ν29	895.04	2.6654	873.62	0.0164
ν30	909.9	0.3787	880.14	1.0864
ν31	938.62	2.3792	941.43	1.1558
ν32	991.35	1.7662	958.23	3.1919
ν33	1006.32	0.0251	970.27	0.2358
ν34	1013.05	1.8045	1013.42	0.0039
ν35	1023.34	0.0314	1026.25	0.2391
ν36	1027.93	1.8423	1033.76	0.03
ν37	1058.75	3.5085	1057.78	2.5867
ν38	1107	2.2365	1063.31	5.25
ν39	1113.65	4.7545	1096.11	3.1503
ν40	1185.5	0.0691	1115.44	5.5878
ν41	1200.94	1.5388	1190.98	0.0948
ν42	1235.94	2.844	1211.58	0.7339
ν43	1305.59	0.6313	1234.47	2.5568
ν44	1313.47	2.1636	1317.87	0.4611
ν45	1357.48	0.2869	1328.74	8.3172
ν46	1483.57	4.692	1362.15	0.5146
ν47	1514.17	17.2701	1492.04	5.7123
ν48	1526.49	6.7516	1542.29	22.7945
ν49	1574.04	2.1059	1611.16	3.9639
ν50	1620.66	2.7983	1643.05	1.5909
ν51	1643.84	10.9215	1670.61	3.0674
ν52	1728.73	0.383	1679.23	1.8072
ν53	2274.3	7.3891	2246.94	9.8359
ν54	2300.03	3.2638	2301.43	2.1284
ν55	2331.52	1.1246	2340.32	1.3552
ν56	2344.44	8.249	2361.38	1.2965
ν57	2363.57	15.6651	2374.3	12.0551
ν58	2422.3	3.0256	2419.92	5.6518
ν59	3189.5	3.4247	3194.3	1.3293
ν60	3195.94	2.1882	3202.85	2.5572
ν61	3207.44	7.1278	3212.38	11.2534
ν62	3212.69	21.8797	3219.8	15.1359
ν63	3221.09	14.8027	3225.42	9.9892
	tsi4p1		**tsi1i21**	
ν1	-695.96	1.4225	-555.15	13.4504
ν2	63.25	0.1182	27.26	0.0204
ν3	87.82	1.1276	36.63	0.0391

ν4	120.84	0.2368	48.17	0.6907
ν5	211.25	1.4085	87.28	1.4324
ν6	264.58	0.1208	173.96	0.8944
ν7	279.59	0.367	227.78	0.5762
ν8	314.51	0.328	280.31	3.2593
ν9	364.16	0.5135	319.19	1.6168
ν10	395.12	0.2144	373.85	4.416
ν11	422.56	0.1967	391.81	0.9024
ν12	473.8	10.3204	417.26	0.0059
ν13	534.12	3.6067	471.98	3.3327
ν14	587.29	32.4142	494.5	15.3266
ν15	608.64	0.8522	537.59	2.6682
ν16	614.63	4.9939	552.01	1.9226
ν17	638.64	0.0067	604.57	3.538
ν18	664.45	1.789	641.88	0.0157
ν19	696.76	0.1436	689.8	2.5243
ν20	726.61	39.6652	716.22	32.8135
ν21	736.21	0.1729	722.85	5.0973
ν22	772.37	20.9187	769.92	2.3792
ν23	810.4	5.3243	786.18	8.2631
ν24	817	6.3651	786.71	38.6378
ν25	843.32	2.0725	819.95	6.9161
ν26	853.21	4.9644	853.87	0.8055
ν27	859.31	0.772	859.06	1.3318
ν28	863.62	0.8805	870.32	0.011
ν29	875.78	0.0355	900.19	1.084
ν30	889.39	0.0962	912.33	0.4848
ν31	957.99	1.5874	924.01	1.8219
ν32	974.69	0.2445	949.85	3.644
ν33	1012.08	0.2034	1009.92	0.0054
ν34	1021.19	4.3689	1023.71	0.5826
ν35	1028.7	0.3066	1028.32	0.0543
ν36	1030.96	0.0427	1061.05	3.4652
ν37	1058.16	0.1593	1068.01	2.1847
ν38	1071.25	2.7021	1100.79	0.8757
ν39	1121.55	5.6769	1113.81	5.7385
ν40	1190.07	0.0072	1160.81	0.4954
ν41	1219.75	0.3237	1188.13	0.0003
ν42	1266.3	0.2953	1209.83	0.8778

ν43	1299.51	1.6192	1258.43	1.2615
ν44	1318.14	0.2665	1305.39	15.4035
ν45	1353.65	2.4024	1314.49	0.0274
ν46	1371.05	0.2384	1360.35	0.143
ν47	1433.16	14.7873	1490.22	4.4594
ν48	1494.86	4.8072	1539.1	35.0831
ν49	1550.35	12.7288	1637.29	2.1837
ν50	1587.42	1.7805	1665.41	30.6216
ν51	1620.06	6.4896	1672.52	7.8257
ν52	1654.81	1.6597	2164.26	22.2614
ν53	1681.42	4.6409	2210.31	9.2336
ν54	2352.63	1.1018	2274.86	6.9789
ν55	2358.28	0.2623	2276.77	4.7266
ν56	2367.53	3.0276	2314.92	5.463
ν57	2377.78	10.2278	2378.43	10.935
ν58	2389.83	8.5311	2402.32	3.1966
ν59	3188.14	3.628	3191.33	2.5654
ν60	3193.3	0.0292	3199.22	3.3174
ν61	3202.59	9.3748	3210.41	12.0533
ν62	3210.13	24.0979	3216.79	19.7806
ν63	3220.18	14.3954	3222.98	10.6806
	tsi21i22		**tsi22p3**	
ν1	-1724.5	29.2839	-390.29	40.322
ν2	28.87	0.2058	49.4	0.3259
ν3	60.13	0.7303	77.38	0.3777
ν4	88.19	0.4618	102.01	0.0781
ν5	165.8	0.843	164.1	2.0276
ν6	244.9	0.3155	175.1	3.3718
ν7	319.73	1.5497	210.84	0.8064
ν8	357.35	3.7211	247.88	0.9828
ν9	389.8	7.0151	310.73	0.8745
ν10	417.5	2.3415	340.45	4.3924
ν11	422	3.6151	423.33	1.7405
ν12	522.7	15.9759	465.05	4.3756
ν13	552.52	1.0802	514.33	23.7543
ν14	626.27	23.3967	529.78	12.5316
ν15	641.25	18.6096	599.64	9.7243
ν16	668.42	6.7903	606.77	9.4336
ν17	718.8	23.4906	635.08	0.5418

ν18	723.5	14.5949	670.03	9.3073
ν19	729.39	2.187	696.94	2.0052
ν20	735.5	4.5673	726.22	41.2429
ν21	755.13	5.9728	740.81	0.63
ν22	765.95	7.2466	752.39	10.2081
ν23	792.07	41.1628	758.38	1.2487
ν24	820.4	5.0727	779.17	17.2021
ν25	832.28	20.9242	804.37	4.3261
ν26	843.92	8.9485	811.8	5.572
ν27	873.04	0.3434	816.84	8.0087
ν28	882.71	0.7834	836.55	22.3167
ν29	895.77	1.9643	847.16	6.3894
ν30	930.23	3.3873	881.67	0.1766
ν31	952.25	4.9786	921.47	18.6753
ν32	989.8	1.1238	964.59	2.0395
ν33	1010.04	0.0952	1000.82	8.0617
ν34	1025.77	0.2283	1018.86	2.0787
ν35	1029.55	0.0706	1028.71	0.3512
ν36	1062.81	3.6137	1037.12	0.6415
ν37	1089.37	1.7704	1047.91	0.6245
ν38	1114	7.0632	1069.34	5.9615
ν39	1124.64	1.043	1122.95	6.3767
ν40	1188.92	0.1724	1191.31	0.1078
ν41	1197	0.8485	1218.66	2.3817
ν42	1210.76	0.5126	1238.92	3.8739
ν43	1222.94	1.502	1260.8	5.8781
ν44	1263.98	1.46	1318.16	11.7052
ν45	1287.24	1.4047	1332.47	6.4895
ν46	1319.9	4.2224	1367.84	0.9832
ν47	1361.26	1.0485	1460.21	87.7227
ν48	1491.12	7.9185	1495.69	8.763
ν49	1537.43	14.4428	1546.82	14.3751
ν50	1558.64	3.6462	1554.5	3.2673
ν51	1645.43	3.6151	1649.83	4.4131
ν52	1672.86	10.1096	1678.77	0.4083
ν53	1762.12	23.7866	1711.1	132.0213
ν54	2214.17	12.8432	2331.64	5.5827
ν55	2292.84	8.2113	2381.84	3.3974
ν56	2295.75	6.7365	2390.62	1.7796

ν57	2362.83	2.0793	2420.49	3.9243
ν58	2405.28	9.2686	2433.31	3.6424
ν59	3187.65	2.6352	3187.8	3.0523
ν60	3194.59	0.327	3195.73	0.1858
ν61	3203.5	7.1345	3206.66	14.3321
ν62	3210.58	25.2463	3217.56	20.2378
ν63	3219.77	17.0643	3225.1	6.7937
	p1		**p2**	
ν1	68.09	0	15.29	0.0264
ν2	91.75	0.8104	40.25	0.2927
ν3	122.2	0.1113	75.48	1.6723
ν4	264.44	0.0456	110.64	0.0007
ν5	310.15	0.0005	121.17	0.5556
ν6	353.6	0.7628	209.21	0.0117
ν7	367.97	0.1218	261.58	3.8526
ν8	423.43	0.154	334.84	5.6272
ν9	470.03	14.5968	349.04	1.7417
ν10	532.38	5.111	416.6	0.1068
ν11	573.65	25.2802	418.97	3.5373
ν12	611.47	0.0075	423.36	4.792
ν13	616.39	6.118	544.63	12.4149
ν14	638.59	0.2126	546.1	0.5054
ν15	668.1	6.4831	590.06	0.515
ν16	682.48	0.1087	641	0.6465
ν17	728.02	41.0032	662.02	10.6353
ν18	738.11	0.005	669.15	4.05
ν19	775.63	26.4258	718.77	34.3061
ν20	818.61	5.7999	739.68	0.5552
ν21	823.82	0.2685	746.85	33.7889
ν22	847.56	2.4741	757.29	1.3425
ν23	856.24	5.1834	791.62	41.8814
ν24	864.45	1.645	805.61	0.1061
ν25	869.73	0.1005	843.56	0.7919
ν26	877.4	0.0225	874.65	0.0003
ν27	891.79	0.3248	881.23	0.4343
ν28	958.81	1.8428	940.54	0.8008
ν29	984.59	0.0167	958.73	3.6538
ν30	1012.88	0.2199	970.92	0.2248
ν31	1025.33	4.5435	1012.71	0.0093

ν32	1028.81	0.5096	1027.3	0.1723
ν33	1030.68	0.0638	1032.59	0.0645
ν34	1060.66	0.0991	1057.95	2.961
ν35	1071.98	2.5272	1063.92	5.5807
ν36	1120.89	5.559	1098.25	4.5003
ν37	1189.7	0.0088	1114.57	5.4953
ν38	1219.51	0.2578	1190.58	0.0643
ν39	1269.73	0.2678	1212.14	0.3372
ν40	1303.99	0.6794	1235.34	0.6683
ν41	1325.35	0.0839	1317.44	0.2677
ν42	1364.08	1.3438	1335.63	16.2949
ν43	1380.49	0.8267	1361.7	0.3598
ν44	1439.75	12.3924	1492.58	5.3577
ν45	1495.58	4.8894	1544.71	26.5461
ν46	1551.49	13.2442	1613.75	4.0412
ν47	1614.86	1.3944	1646.2	1.5176
ν48	1648.19	6.859	1672.12	0.9471
ν49	1656.46	1.3246	1684.9	11.4629
ν50	1682.22	6.1961	2300.68	1.7507
ν51	2349.71	1.9235	2333.04	1.5805
ν52	2356.56	0.1038	2343.17	0.7005
ν53	2367.7	4.3981	2358.79	1.3225
ν54	2376.7	14.4321	2369.72	12.87
ν55	2388.32	8.0611	2419.81	5.9624
ν56	3187.21	3.6481	3193.13	1.5077
ν57	3192.25	0.0494	3201.78	2.4315
ν58	3201.67	9.0622	3211.39	12.5355
ν59	3208.98	25.3174	3218.78	17.7071
ν60	3219.34	15.1773	3224.49	10.2096
	p10		**vdW(i1)**	
ν1	50.72	0.2485	10.19	1.4762
ν2	80.19	0.4826	27.02	1.7149
ν3	107.89	0.0442	36.48	0.5682
ν4	195.7	0.6375	53.37	0.2103
ν5	248.16	0.7056	59.42	1.4387
ν6	308.63	0.5814	103.54	3.3202
ν7	339.82	3.2306	127.34	15.9502
ν8	423.88	1.4844	147.43	4.2759
ν9	464.92	6.2685	158.75	0.204

ν10	509.23	25.2888	254.63	1.2453
ν11	519.99	14.6622	283.38	51.9206
ν12	592.8	1.8402	390.65	0.0854
ν13	605.34	10.825	401.75	8.0398
ν14	635.4	0.5446	454.88	0.054
ν15	673.93	10.048	479.77	3.4414
ν16	696.04	1.743	495.47	32.5702
ν17	726.87	41.5027	511.88	0.5575
ν18	746.37	0.6752	628.82	0.3018
ν19	750.27	10.2066	630.88	0.2278
ν20	759.59	1.1374	690.36	50.3051
ν21	784.74	15.7108	737.83	0.5299
ν22	810.06	8.2674	751.26	0.0448
ν23	810.71	1.2616	758.17	74.6233
ν24	820.29	7.3423	761.61	5.0455
ν25	838.46	20.1637	788.96	1.4515
ν26	848.56	6.0202	797.59	31.8735
ν27	882.22	0.1646	811.97	0.2439
ν28	919.67	16.1107	851.96	0.8603
ν29	964.31	2.1518	864.78	1.1387
ν30	1000.85	6.5919	945.78	0.0057
ν31	1019.03	1.7034	977.62	3.4829
ν32	1028.86	0.3106	1019.31	5.6267
ν33	1037.19	0.6172	1020.81	0.9979
ν34	1048.03	0.5949	1028.81	5.4527
ν35	1070.05	5.4337	1041.66	0.1199
ν36	1123.06	6.1187	1053.64	0.4391
ν37	1191.08	0.0914	1068.03	1.3444
ν38	1219.32	1.58	1069.32	0.2103
ν39	1233.44	5.2407	1117.72	4.1109
ν40	1268.43	4.1973	1188.78	72.4313
ν41	1314.63	10.9336	1191.6	7.6914
ν42	1331.55	4.2767	1214.82	0.1122
ν43	1368.5	0.9204	1232.81	21.9023
ν44	1494.86	9.7664	1327.34	4.9528
ν45	1516.56	92.7225	1360.37	7.0008
ν46	1547.97	23.5024	1483.56	11.4869
ν47	1584.23	3.1267	1515.5	2.8156
ν48	1649.98	3.7357	1600.24	11.3248

ν49	1679.1	0.8139	1614.8	0.546
ν50	1711.69	102.1696	1640.28	116.9044
ν51	2329.62	6.6257	1680.84	0.0793
ν52	2378.14	1.1605	1991.01	29.2883
ν53	2387.75	4.0942	2295.46	1.1271
ν54	2422.62	4.8313	2296.43	3.6357
ν55	2434.94	2.2025	2345.83	2.1307
ν56	3187.1	3.4925	2348.39	0.4197
ν57	3195.65	0.2877	2417.25	4.6731
ν58	3206.42	15.5967	2417.99	2.3277
ν59	3217.47	21.0812	3200.05	0.4906
ν60	3225.64	6.131	3213.28	3.7655
ν61			3220.47	6.4621
ν62			3230.71	4.7995
ν63			3237.34	3.0399

tsi1vdW		
ν1	-23.09	1.2835
ν2	33.94	0.842
ν3	44.07	0.3849
ν4	60.55	0.2904
ν5	70.35	0.4433
ν6	93.68	12.2012
ν7	122.94	15.5821
ν8	148.73	4.2185
ν9	178.28	0.6267
ν10	258.75	37.9454
ν11	302.3	1.52
ν12	391.07	0.0838
ν13	477.53	2.6766
ν14	492.3	28.1083
ν15	512.62	0.7884
ν16	525.13	0.1025
ν17	546.2	15.3286
ν18	631.73	0.1974
ν19	693.28	51.072
ν20	788.08	0.3708
ν21	790.51	1.736
ν22	797.31	23.7382
ν23	867.21	1.0179

ν24	907.7	0.0745
ν25	958.21	43.828
ν26	968.47	64.4388
ν27	977.98	0.2379
ν28	1013.24	1.1432
ν29	1019.64	4.0737
ν30	1020.54	1.4323
ν31	1021.44	0.2148
ν32	1042.22	0.1333
ν33	1054.07	0.5607
ν34	1067.51	44.0453
ν35	1115.67	4.3289
ν36	1185.38	71.4355
ν37	1191.28	2.4502
ν38	1229.54	21.4606
ν39	1236.97	0.0358
ν40	1326.39	4.0772
ν41	1327.18	0.6721
ν42	1331.57	2.2776
ν43	1358.32	6.6038
ν44	1425.43	7.9688
ν45	1481.27	0.3166
ν46	1483.93	11.2047
ν47	1514.77	1.9408
ν48	1617.15	0.9592
ν49	1640.84	83.3517
ν50	1681.24	13.8301
ν51	1743.98	2.8115
ν52	2017.03	19.5186
ν53	3149.12	0.8442
ν54	3152.2	13.6536
ν55	3159.71	0.9813
ν56	3165.62	4.055
ν57	3199.17	0.2373
ν58	3211.03	3.5741
ν59	3218.44	5.7683
ν60	3228.44	3.9278
ν61	3232.09	5.1173
ν62	3245.98	6.7786

ν63	3251.64	4.3981		
	i28		**i29**	
ν1	11.11	0.0055	29.46	0.6795
ν2	49.99	0.6379	50.91	0.5326
ν3	64.59	0.8905	59.64	0.1605
ν4	91.82	0.2156	95.85	0.335
ν5	112.93	0.6584	131.52	0.3138
ν6	139.69	0.2923	199.41	0.1703
ν7	167.88	0.8869	256.41	0.1906
ν8	254.08	1.7451	300.3	0.752
ν9	315.66	2.169	331.82	0.6155
ν10	360.33	3.5561	381.54	2.2954
ν11	361.21	0.6388	415.3	0.0064
ν12	417.12	8.0438	487.35	5.3204
ν13	417.6	7.5316	513.41	0.7374
ν14	522.19	13.4558	538.97	4.9409
ν15	531.47	0.7623	546.76	2.5809
ν16	545.08	5.5861	627.23	1.4684
ν17	584.6	18.7229	635.15	0.0041
ν18	590.13	3.5088	674.42	3.5057
ν19	643.61	0.0785	696.17	32.2314
ν20	673.34	0.9665	724.36	1.3392
ν21	720.4	34.4418	743	25.9765
ν22	738.98	0.1798	765.58	46.3462
ν23	748.7	23.8028	791.01	0.5237
ν24	787.81	5.4824	803.95	4.7303
ν25	792.01	39.7127	817.36	8.0337
ν26	845.65	1.4803	844.77	0.0908
ν27	869.57	0.3509	863.14	5.7215
ν28	876.23	0.0018	879.21	9.703
ν29	913.11	0.723	900.83	17.5957
ν30	945.7	0.4671	912.23	3.5066
ν31	959.69	3.4202	933.91	9.9388
ν32	1013.57	0.0026	946.48	22.8635
ν33	1025.39	4.6524	1000.93	0.0035
ν34	1028	0.1581	1003.32	3.0205
ν35	1032.68	0.0891	1013.47	0.0054
ν36	1045.68	0.3027	1024.12	1.8178
ν37	1063.76	3.0558	1049.22	5.3617
ν38	1094.51	7.0974	1072.98	6.2977

ν39	1114.21	5.7499	1113.48	5.1015
ν40	1171.34	0.5343	1122.35	4.6575
ν41	1190.7	0.0376	1180.32	0.3871
ν42	1193.06	1.6449	1192.67	10.5437
ν43	1213.01	0.0321	1232.99	9.2867
ν44	1304.03	6.5196	1304.85	0.7555
ν45	1317.43	0.2623	1355.3	0.0495
ν46	1361.82	0.3464	1367.59	4.123
ν47	1493.11	5.3534	1476.03	1.6466
ν48	1546.66	24.6169	1510.89	33.8692
ν49	1647.89	1.7042	1596.1	3.8262
ν50	1662.74	12.8401	1620.03	10.3928
ν51	1679.65	8.4452	1661.12	18.2825
ν52	2228.26	5.7355	1984.37	25.5241
ν53	2288.11	6.278	2271.55	6.0214
ν54	2300.16	3.3711	2296.35	5.8456
ν55	2357.44	5.7555	2319.83	6.6216
ν56	2364.7	0.2016	2347.87	8.078
ν57	2421.03	3.9614	2403.73	2.5843
ν58	2445.57	3.208	2419.57	5.1552
ν59	3192.35	0.8993	3190.27	4.4563
ν60	3201.04	2.9881	3196.22	3.7302
ν61	3211.09	13.311	3209.95	8.0243
ν62	3218.15	18.0203	3214.96	21.5777
ν63	3223.87	8.3589	3222.51	12.4039

	tsi28i29		**tsi1i29**	
Normal modes	Frequency(cm^{-1})	IR Inten	Frequency(cm^{-1})	IR Inten
ν1	-659.75	43.8299	-665.78	16.3969
ν2	41.47	0.0614	35.08	0.2396
ν3	47.1	0.4501	45.6	0.1239
ν4	62.47	1.1476	60.92	0.7434
ν5	101.14	0.2127	94.94	0.9226
ν6	133.93	0.2661	149.41	0.6269
ν7	203.11	0.1375	219.1	0.4766
ν8	264.79	0.6607	251.77	0.2556
ν9	299.78	0.2073	304.81	4.1925
ν10	340.43	1.6343	365.42	2.5715
ν11	355.62	1.6711	385.35	4.5588
ν12	416.1	0.0675	415.62	0.0072

ν13	422.45	1.3069	470.32	4.893
ν14	509.88	7.801	511.26	6.8717
ν15	520.55	1.6362	525.93	4.5774
ν16	542.21	5.7554	550.33	1.3866
ν17	556.81	6.2877	624.78	0.0842
ν18	603.7	5.9521	640.29	0.0095
ν19	641.7	0.1076	699.5	16.3136
ν20	682.99	2.2352	707.68	15.3025
ν21	712.36	27.0819	708.9	30.1584
ν22	714.24	6.8336	713.05	6.4456
ν23	745.94	24.306	776.44	45.7537
ν24	778.88	45.7307	795.03	2.978
ν25	792.31	6.0651	803.74	0.5969
ν26	836.89	3.0736	829.91	1.1553
ν27	862.52	1.9226	860.96	0.0308
ν28	864.39	0.0535	866.64	1.3987
ν29	898.08	2.5419	903.08	5.3904
ν30	938.13	3.5441	933.77	3.5693
ν31	954.94	3.7007	969.55	9.0407
ν32	1006.62	0.0019	995.42	0.3826
ν33	1016.24	1.4109	1005.66	0.0126
ν34	1020.95	0.7519	1017.71	4.0009
ν35	1023.45	0.0813	1021.66	0.0215
ν36	1026.86	3.032	1026.93	1.9408
ν37	1059.16	2.2477	1057.73	3.4496
ν38	1093.61	8.6114	1083.86	2.632
ν39	1114.5	5.7194	1114.52	5.7019
ν40	1134.66	3.9332	1146	5.1728
ν41	1187.25	0.0886	1186.04	0.1175
ν42	1206.31	6.7526	1205.26	7.769
ν43	1234.23	10.3875	1284.47	58.5834
ν44	1312.36	0.1493	1311.65	0.2804
ν45	1354.23	16.9988	1349.88	0.0933
ν46	1360.79	0.0824	1359.85	0.0172
ν47	1488.29	3.5121	1486.14	3.2728
ν48	1534.89	47.6309	1529.46	50.2461
ν49	1628.12	2.9418	1562.12	52.3914
ν50	1654.1	33.9778	1621.17	3.1169
ν51	1665.3	13.4486	1646	24.3597
ν52	2105.74	5.8413	2049.68	0.5879
ν53	2277.81	6.4837	2263.68	9.7136

ν54	2299.39	4.9072	2301.93	7.4896
ν55	2302.34	1.8412	2347.76	3.4407
ν56	2356.55	6.6325	2369.74	0.6111
ν57	2420.88	3.9686	2375.53	3.9771
ν58	2467.99	0.9191	2421.58	4.5973
ν59	3190.84	3.8866	3191.06	4.3566
ν60	3198.05	3.1952	3198.31	3.8583
ν61	3209.99	10.0881	3210.71	10.0274
ν62	3215.67	21.2108	3216.52	19.9996
ν63	3222.56	11.8979	3222.97	12.4334
	tsi2p13		**phenylacetylene**	
ν1	-350.22	1.8063	142.92	1.9037
ν2	8.55	0.0066	160.85	1.3527
ν3	28.1	0.1398	372.4	4.2595
ν4	36.13	0.0781	416.39	0
ν5	83.18	0.8354	476.12	0.2766
ν6	106.96	0.3743	544.54	5.9699
ν7	151.09	1.0876	560.2	3.5801
ν8	163.78	1.2552	642.29	0.6642
ν9	195.27	0.5872	679.36	48.9001
ν10	280.87	4.5789	712.67	39.0525
ν11	377.49	10.8647	719.95	32.8806
ν12	415.32	1.2916	783.04	2.64
ν13	417.26	20.6053	792.81	44.6391
ν14	470.52	2.392	876.79	0
ν15	479.6	11.4155	962.18	4.2375
ν16	500.61	16.2594	1014.34	0
ν17	513.37	13.4609	1028.61	0.0413
ν18	548.08	0.9814	1034.16	0.0917
ν19	582.78	3.5396	1063.69	4.2256
ν20	599.54	3.6704	1114.95	5.3244
ν21	643.36	0.1171	1191.08	0.1004
ν22	669.43	7.8059	1212.42	0.0066
ν23	716.78	35.2078	1235.54	0.7992
ν24	739.36	26.5581	1318.57	0.6276
ν25	751.74	4.9906	1362.58	0.3023
ν26	755.12	2.9881	1493.57	5.7146
ν27	780.27	2.3367	1543.52	16.7339
ν28	788.62	47.8907	1649.01	1.337
ν29	829.48	0.9634	1679.5	1.9439

ν30	872.62	0.1338	2244.95	7.0929
ν31	939.66	7.5502	3193.8	0.1726
ν32	955.78	5.9183	3203.3	3.2224
ν33	995.46	24.9293	3212.68	12.5455
ν34	1012.12	0.0272	3220.53	15.9511
ν35	1025.92	0.0364	3225.45	5.3923
ν36	1032.25	0.1148	3483	89.5538
ν37	1052.57	3.3858		
ν38	1062.47	3.4009		
ν39	1115.81	5.3827		
ν40	1176.65	10.143		
ν41	1190.63	0.0516		
ν42	1209.61	0.1838		
ν43	1230.36	1.3149		
ν44	1318.5	0.1784		
ν45	1362.67	0.3784		
ν46	1492.68	5.5316		
ν47	1539.22	17.4094		
ν48	1595.51	8.5612		
ν49	1643.61	1.6777		
ν50	1662.92	5.9405		
ν51	1672.31	4.5166		
ν52	2007.71	1.7504		
ν53	2257.92	5.2102		
ν54	2301.13	2.5099		
ν55	2370.11	0.8383		
ν56	2406.87	0.0987		
ν57	2417.79	5.9143		
ν58	2656.66	40.4517		
ν59	3193.7	1.0787		
ν60	3201.97	2.3767		
ν61	3211.46	12.2081		
ν62	3218.84	15.6119		
ν63	3224.89	7.6528		
	p13			
ν1	149.02	0.0015		
ν2	258.41	6.1799		
ν3	416.97	28.8531		
ν4	450.91	4.2926		
ν5	579.54	6.1826		

ν6	634.65	6.1806
ν7	737.33	1.5349
ν8	743.2	31.8631
ν9	752.15	0.6931
ν10	828.38	1.6593
ν11	937.83	0.3845
ν12	993.97	0.7011
ν13	1050.79	4.5163
ν14	1172.71	0.1776
ν15	1596.91	6.9276
ν16	1660.22	3.2588
ν17	2250.26	4.9306
ν18	2301.43	2.8841
ν19	2362.57	1.7046
ν20	2420.51	5.2149
ν21	2434	0.8111

(b)

	phenylethynyl		Isoprene	
Normal modes	Frequency(cm^{-1})	IR Inten	Frequency(cm^{-1})	IR Inten
ν1	112.68	17.3904	157.73	0.0718
ν2	148.66	4.6072	212.04	0.34
ν3	251.55	26.3028	290.81	0.9831
ν4	393.87	0	413.55	10.0847
ν5	477.42	3.1292	436.72	1.6471
ν6	490.16	18.9612	542.61	0.0721
ν7	511.05	0.7921	655.13	0.0622
ν8	632.48	0.1684	800.3	0.698
ν9	696.07	46.3153	801.74	0.1664
ν10	787.71	0.2095	949.35	41.9046
ν11	799.2	23.247	963.12	46.2652
ν12	870.13	0	973.41	0.9322
ν13	981.96	0.8822	1018.4	0.2518
ν14	1019.66	4.5667	1045.41	14.1313
ν15	1024.97	0	1077.76	0.0217
ν16	1044.22	0.1747	1098.44	4.1308
ν17	1053.58	0.6553	1337.33	0.0529
ν18	1116.24	5.0608	1344.3	0.8391
ν19	1185.47	81.7314	1419.13	8.1952
ν20	1191.6	3.3766	1444.59	3.9412
ν21	1230.32	21.1034	1467.12	2.6248
ν22	1324.35	7.2501	1487.57	8.7643
ν23	1358.66	7.8198	1509.9	6.9906
ν24	1483.47	12.0342	1692.02	30.8796
ν25	1514.79	1.8218	1742.03	1.9879
ν26	1614.98	0.511	3046.84	19.0487
ν27	1639.86	92.1565	3106.14	14.8944
ν28	2020.99	45.6399	3142.83	17.1483
ν29	3200.68	0.3554	3154.54	3.4585
ν30	3213.21	3.2854	3158.73	13.2046
ν31	3219.82	5.1552	3169.62	4.2806
ν32	3230.21	3.8096	3241.64	10.9805
ν33	3233.27	5.2791	3249.59	12.0803
	i5		**i7**	

ν1	7.08	0.0474	29.29	0.0254
ν2	19.93	0.0237	80.45	0.232
ν3	42.05	0.479	131.19	0.5287
ν4	91.61	2.2701	146.67	2.8583
ν5	131.64	0.6042	173.11	1.266
ν6	160.26	0.0416	239.14	0.12
ν7	190.08	2.494	267.6	6.748
ν8	200.99	0.156	281.41	0.035
ν9	267.24	2.8944	335.84	0.4229
ν10	331.32	2.2126	418.54	0.0001
ν11	401	0.1018	431.35	1.2056
ν12	417.53	0.0021	444.36	2.1505
ν13	435.31	1.0361	468.51	1.9693
ν14	485.16	10.688	497.81	1.0981
ν15	503.33	1.5179	572.69	8.0512
ν16	538.19	3.7393	589.73	5.7033
ν17	554.73	5.289	639.76	0.0362
ν18	576.44	0.8018	705.4	1.5452
ν19	581.57	4.3518	720.87	32.4971
ν20	643.57	0.0084	786.09	46.0853
ν21	693.5	3.1966	809.68	0.1437
ν22	720.83	34.9683	819.97	1.1725
ν23	744.17	2.2773	872.57	0.0612
ν24	792.33	39.3148	903.22	0.862
ν25	809.13	46.9027	942.36	0.0825
ν26	867.67	0.5899	961.31	0.953
ν27	876.93	0.0001	971.55	10.3245
ν28	918.92	3.2043	983.11	1.2526
ν29	959.72	3.7188	998.34	2.2772
ν30	987.09	1.6729	1010.53	0.0178
ν31	1009.29	2.0961	1028.26	0.071
ν32	1013.77	0.0006	1029.07	0.0473
ν33	1026.86	0.7747	1068.73	4.1677
ν34	1028.64	0.5379	1071.13	4.4458
ν35	1032.52	0.0724	1074.84	1.1334
ν36	1062.25	0.1998	1088.24	1.7795
ν37	1066.91	4.2024	1129.87	4.5253
ν38	1113.93	5.6364	1177.22	2.3554
ν39	1130.26	21.1556	1190.43	0.1415

ν40	1190.2	0.0281	1209.23	0.3152
ν41	1212.7	0.2244	1222.78	0.5402
ν42	1226.52	0.3099	1242.85	0.4488
ν43	1264.15	6.668	1287.49	0.1785
ν44	1290.14	1.1593	1312.43	1.615
ν45	1317.01	0.2093	1329.9	0.556
ν46	1339.23	27.6842	1351.1	5.4832
ν47	1361.69	0.269	1372.32	1.1091
ν48	1393.3	1.4163	1404.2	0.873
ν49	1431.53	3.1376	1424.93	4.7139
ν50	1448.35	8.5392	1477.57	3.674
ν51	1468.14	5.701	1479.89	1.9619
ν52	1492.84	5.0332	1486.75	9.1039
ν53	1497.23	9.8996	1496.16	7.1651
ν54	1505.45	18.9003	1497.97	12.0007
ν55	1534.93	8.7431	1550.29	20.3118
ν56	1547.64	27.0307	1653.19	3.058
ν57	1648.03	1.5958	1681.35	13.3368
ν58	1680.23	10.9146	1752.98	15.7566
ν59	2380.7	6.8552	1780.2	0.7831
ν60	3006.46	18.0124	3009.86	27.542
ν61	3030.48	7.1398	3026.56	39.705
ν62	3047.34	18.5969	3035.51	36.3494
ν63	3105.9	15.4374	3035.62	13.8108
ν64	3142.76	21.2172	3049.35	9.9582
ν65	3159.58	9.1681	3090.58	19.6754
ν66	3191.87	0.9527	3135.29	19.6793
ν67	3197.52	7.2681	3166.95	30.8076
ν68	3200.68	3.07	3184.55	3.3228
ν69	3210.77	14.3205	3192.2	0.4179
ν70	3217.93	18.9978	3202.06	14.0205
ν71	3223.59	8.4642	3212.95	26.8665
ν72	3256.1	10.715	3220.7	11.3609

	i6		**i8**	
ν1	30.11	0.2534	32	0.1009
ν2	40.87	0.1503	84	0.1803
ν3	51.8	0.4781	143.5	0.1114
ν4	84.09	0.3673	146.93	0.2138
ν5	146.91	0.434	172.41	0.9652

ν6	183.73	0.5103	231.17	0.7726
ν7	223.24	0.3328	292.28	1.0886
ν8	241.59	0.9431	328.31	4.1015
ν9	261.19	2.4757	342.28	1.037
ν10	341.2	1.0715	418.23	0.0249
ν11	408.28	6.4331	434.87	0.2088
ν12	415.78	0.4343	473.65	0.8744
ν13	446.62	4.7683	509.46	0.0829
ν14	483.14	4.4737	536.04	3.7429
ν15	506.39	18.3323	562.71	1.4007
ν16	516.38	2.6964	610.47	1.3816
ν17	587.27	4.5579	638.92	0.0784
ν18	632.48	0.3209	714.31	21.9178
ν19	693.66	8.7959	723.45	6.4561
ν20	695.96	32.6109	741.15	74.2962
ν21	717.68	2.7874	789.83	19.3012
ν22	766.93	46.6356	838.54	2.1543
ν23	782.28	16.5223	861.77	0.1077
ν24	803.31	5.4851	897.44	0.2243
ν25	838.94	16.601	929.44	0.8329
ν26	845.2	0.3824	932.84	0.07
ν27	874.99	5.316	951.19	0.6464
ν28	915.8	4.0501	957.13	9.288
ν29	946.96	41.1988	1005.63	0.1141
ν30	951.76	3.9217	1008.66	0.3785
ν31	994.59	0.9581	1021.18	1.4337
ν32	1002.22	0.0373	1025.18	0.0312
ν33	1015.47	0.0215	1027.47	0.5848
ν34	1018.76	0.0661	1061.69	1.7577
ν35	1030.56	2.9687	1068	8.3281
ν36	1048.17	2.5944	1084.29	3.7459
ν37	1052.76	9.6055	1123.65	4.1786
ν38	1078.61	1.2151	1138.88	4.9948
ν39	1114.15	4.8931	1190.23	0.6228
ν40	1153.54	17.7394	1203.68	1.2984
ν41	1179.63	0.2206	1222.5	0.2352
ν42	1216.53	5.8298	1231.86	1.3947
ν43	1277.02	2.3784	1282.87	15.7324
ν44	1302.95	0.5328	1302.77	2.5917

ν45	1352.17	7.38	1327.2	1.2984
ν46	1355.13	0.4465	1344.51	0.4827
ν47	1377.83	1.756	1373.21	1.125
ν48	1414.61	0.3423	1404	1.0057
ν49	1440.38	7.3402	1422.39	0.7705
ν50	1471.7	1.3973	1450.18	5.0323
ν51	1474.51	2.6919	1456.41	10.1036
ν52	1486.51	8.0192	1483.23	9.1133
ν53	1504.87	32.3035	1490.63	6.3562
ν54	1507.18	15.5103	1497.73	8.6088
ν55	1595.31	3.7948	1542.19	16.3033
ν56	1618.3	3.4551	1553.19	11.366
ν57	1686.63	12.775	1644.16	4.6878
ν58	1727.5	5.7495	1655.54	26.8789
ν59	1886.16	5.7021	1671.62	10.0619
ν60	3053	20.4302	2940.81	25.803
ν61	3059.14	12.414	2980.91	21.3078
ν62	3130.83	8.3656	3026.01	46.8701
ν63	3139.28	20.0091	3076.4	20.4368
ν64	3144.19	3.1171	3133.16	18.1464
ν65	3155.63	6.4749	3180.84	21.9482
ν66	3168.29	36.8685	3188.61	5.7241
ν67	3191.61	3.055	3195.69	7.6917
ν68	3197.78	4.5107	3200.9	11.8496
ν69	3212.03	7.7001	3212.43	9.3983
ν70	3216.78	18.1925	3217.7	11.8704
ν71	3223.5	11.6785	3222.04	32.4875
ν72	3242.19	11.2392	3224.73	7.3817
	i23		**i24**	
ν1	24.03	0.5087	37.34	0.1626
ν2	26.45	0.0107	69.59	0.3865
ν3	81.55	0.0045	117.89	0.0599
ν4	101.97	1.2624	124.63	0.1619
ν5	173.96	0.073	166.48	0.0523
ν6	179.13	0.5888	235.52	0.2121
ν7	238.09	2.9021	283.24	4.4193
ν8	272.53	0.0981	299.63	0.8348
ν9	313.31	0.1478	303.78	0.0965
ν10	382.16	5.9349	380.45	0.3377

ν11	415.68	0.0001	419.77	0.1102
ν12	435.03	2.0432	466.08	1.8211
ν13	446.38	7.9693	519.65	16.785
ν14	501.32	0.907	566.08	7.7286
ν15	565.28	0.0004	604.61	2.6077
ν16	585.45	1.5454	634.27	0.0994
ν17	635.4	0.0067	649.52	12.5799
ν18	660.29	4.8409	710.8	42.6894
ν19	693.33	33.1231	723.73	0.0652
ν20	764.8	44.4302	743.9	7.8021
ν21	786.37	0.6019	770.6	27.6889
ν22	817.09	12.1673	804.64	0.7188
ν23	840.73	0.0062	836.4	0.558
ν24	880.02	6.5501	853.98	4.7365
ν25	901.09	2.45	868.69	24.7193
ν26	908.58	3.1399	907.75	2.8047
ν27	923.59	0.2728	936.79	1.946
ν28	969.95	3.2536	944.38	6.0986
ν29	993.85	8.9163	968.32	18.5124
ν30	999.07	0.0156	980.26	4.6135
ν31	999.85	1.135	1003.26	0.2223
ν32	1011.18	0.0139	1020.37	0.9286
ν33	1044.57	8.1996	1022.25	0.0227
ν34	1046.94	4.9381	1033.22	7.0133
ν35	1069.83	0.2245	1065.99	5.0282
ν36	1106.81	2.3019	1070.07	1.6627
ν37	1112.08	5.2185	1124.93	5.7154
ν38	1173.45	0.0926	1167.63	0.6076
ν39	1178.1	0.348	1169.36	0.037
ν40	1185.34	0.6134	1188.62	0.6291
ν41	1194.75	0.7266	1206.89	1.1327
ν42	1201.4	8.5685	1226.16	0.0379
ν43	1249.64	0.2023	1242.1	2.2094
ν44	1296.48	3.4766	1279.56	4.6387
ν45	1301.81	0.6618	1316.74	0.3786
ν46	1333.46	8.6263	1350.52	1.1681
ν47	1353.26	0.0836	1360.14	1.0691
ν48	1363.25	0.7266	1378.22	1.2508
ν49	1425.66	4.3638	1412.6	0.2328

ν50	1472.84	1.2772	1425.08	0.9938
ν51	1476.58	4.0846	1453.82	6.1054
ν52	1485.21	1.6584	1477.22	1.5425
ν53	1486.19	8.7317	1490.7	7.1769
ν54	1495.76	10.3325	1499.31	13.4176
ν55	1503.51	24.6016	1532.72	2.7977
ν56	1591.12	3.775	1541.64	26.436
ν57	1615.77	10.5194	1630.67	29.976
ν58	1759.29	10.1232	1638.41	1.7242
ν59	1932.62	0.5823	1663.06	11.033
ν60	3036.86	21.8151	3045.29	6.9043
ν61	3041.4	55.2633	3049.05	38.3856
ν62	3048.06	21.5349	3079.92	5.9741
ν63	3071.36	13.1094	3109.97	14.7896
ν64	3077.43	12.7192	3136.61	16.5138
ν65	3092.55	17.7573	3156.77	11.8274
ν66	3132.33	24.0286	3183.91	7.1953
ν67	3189.4	4.6941	3193.09	0.0918
ν68	3195.06	4.1946	3203.53	24.7402
ν69	3201.18	23.9706	3212.14	11.4721
ν70	3209.84	6.7019	3217.91	25.3838
ν71	3213.97	23.5128	3227.28	6.6983
ν72	3222.13	13.9168	3257.81	4.1333

	i9		**i11**	
ν1	7.74	0.0296	28.33	0.0428
ν2	39.5	0.5027	58.33	0.1613
ν3	41.36	0.6089	127.54	0.5294
ν4	58.2	0.0271	138.21	2.4117
ν5	108.46	2.0126	178.87	1.5319
ν6	131.98	0.4995	243.6	5.7433
ν7	204.92	1.794	278.09	1.2718
ν8	263.84	0.8278	280.78	0.026
ν9	286.61	2.2559	322.25	0.7664
ν10	300.25	0.8363	417.93	0.0269
ν11	340.73	2.4678	431.03	1.4912
ν12	356.66	1.3038	432.4	0.104
ν13	417.52	0.0058	452.24	3.833
ν14	419.42	0.1299	539.46	1.3615
ν15	503.66	1.8702	566.66	5.2427

ν16	548.63	1.123	591.77	0.813
ν17	559.29	5.5916	640.89	0.0605
ν18	587.25	1.551	708.71	4.5964
ν19	620.2	2.8821	719.92	33.9942
ν20	643.04	0.0355	763.43	0.279
ν21	720.58	34.7623	785.18	44.9245
ν22	749.89	2.7898	826.21	0.871
ν23	786.56	0.9074	871.58	0.0482
ν24	792.23	39.006	916.47	1.238
ν25	808.63	44.5865	946.27	0.008
ν26	876.07	0.0036	959.65	8.8461
ν27	886.14	0.5685	970.05	3.6147
ν28	959.92	3.5351	980.32	1.7076
ν29	984.72	1.1543	988.65	3.0387
ν30	1002.04	10.0491	1009.6	0.0192
ν31	1013.35	0.0153	1028.03	0.0611
ν32	1017.67	0.9408	1028.04	0.0483
ν33	1027.95	0.1347	1067.08	4.9415
ν34	1029.64	0.2783	1071.46	9.102
ν35	1032.69	0.0772	1076.91	0.8288
ν36	1055.42	0.4848	1100.17	0.0389
ν37	1067.66	3.9764	1129.5	5.9983
ν38	1113.87	5.5785	1180.06	7.6344
ν39	1189.99	0.0431	1189.2	0.0615
ν40	1212.19	0.6434	1215.62	0.8283
ν41	1216.3	14.0137	1219.13	0.584
ν42	1235.1	0.5484	1227.43	0.2953
ν43	1248.42	4.7963	1283.99	1.3934
ν44	1283.69	0.2298	1318.79	2.1678
ν45	1317.13	0.236	1339.12	0.3745
ν46	1327.95	8.0716	1357.81	0.4735
ν47	1361.48	0.3079	1374.31	2.1019
ν48	1400	4.4541	1376.44	0.8255
ν49	1423.06	3.458	1423.73	3.016
ν50	1457.16	32.5999	1474.88	1.7287
ν51	1478.23	5.9934	1481.21	2.2041
ν52	1488.14	7.7102	1484.63	8.7972
ν53	1492.92	5.2908	1495.75	9.3202
ν54	1511.89	16.9434	1498.4	5.5509

ν55	1538.98	1.3827	1547.41	21.7583
ν56	1547.11	23.9158	1652.52	3.2235
ν57	1648.01	1.6003	1680.71	13.5724
ν58	1680.16	9.1987	1756.11	11.2491
ν59	2379.89	1.2842	1785.2	1.5049
ν60	3007.95	23.9811	3018.29	4.5308
ν61	3029.77	6.9671	3019.39	66.7421
ν62	3030.58	29.152	3035.41	44.4679
ν63	3083.86	14.64	3042.26	15.1406
ν64	3124.05	18.0615	3044.17	9.169
ν65	3165.61	12.5068	3090.9	19.7227
ν66	3175.81	1.6735	3132.76	17.7269
ν67	3192.28	0.9311	3163.75	27.4993
ν68	3200.89	2.9972	3185.46	3.1716
ν69	3211.02	13.575	3192.69	0.4754
ν70	3217.97	18.242	3202.46	13.1594
ν71	3223.76	8.4254	3212.06	26.1989
ν72	3259.67	9.4824	3220.08	13.2794
	i10		**i12**	
ν1	19.27	0.2022	34.25	0.0873
ν2	32.48	0.1382	65	0.2501
ν3	61.79	0.3118	132.43	0.1263
ν4	98.51	0.4467	143.77	0.5271
ν5	143.1	0.2257	168	0.3877
ν6	169.09	0.2292	251	3.3135
ν7	220.15	0.5417	290.7	0.5578
ν8	230.58	0.3297	303.42	0.3941
ν9	290.96	1.7108	334.79	0.2817
ν10	325.79	4.122	417.29	0.7921
ν11	335.68	1.0343	420.23	4.3871
ν12	413.42	0.576	455.96	6.0466
ν13	424.86	3.1404	541.57	1.1391
ν14	478.4	2.5539	559.1	0.4344
ν15	488.97	4.8747	578.66	2.8963
ν16	526.03	2.792	610.92	0.0568
ν17	530.86	3.3389	640.97	0.1
ν18	631.69	0.3211	713.21	29.4522
ν19	687.98	6.4612	717.28	8.2245
ν20	694.03	39.5352	756.29	63.1177

ν21	737.7	4.944	787.29	7.1596
ν22	741.93	2.0789	792.07	8.5767
ν23	764.27	44.5506	802.75	0.2539
ν24	803.31	10.4682	861.16	0.0644
ν25	831.98	12.2352	931.32	0.2193
ν26	843.68	2.1029	954.09	1.4983
ν27	910.04	3.6423	956.41	7.0121
ν28	916.18	1.2492	968.89	0.2344
ν29	963.96	44.2451	990.33	14.1327
ν30	978.45	4.1383	1001.74	5.7491
ν31	997.25	0.6241	1005.76	0.2329
ν32	1000.87	0.0213	1021.04	0.4799
ν33	1013.2	0.0025	1024.8	0.0477
ν34	1038.86	1.3655	1071.5	2.6263
ν35	1044.44	12.3396	1072.7	4.2137
ν36	1048.18	2.7789	1093.1	5.9942
ν37	1074.97	2.468	1128.96	4.1211
ν38	1098.47	3.1664	1149.59	6.4088
ν39	1113.56	4.8297	1192.12	0.7087
ν40	1167.71	15.0062	1207.05	5.1717
ν41	1179.47	0.3436	1218.54	0.532
ν42	1218.12	4.8391	1236.52	0.1049
ν43	1255.09	1.8042	1287.82	5.3223
ν44	1301.68	0.672	1302.06	3.7734
ν45	1344.4	0.2831	1330.23	1.798
ν46	1354.67	0.0728	1345.42	0.2035
ν47	1367.42	5.4583	1382.51	0.5153
ν48	1399.22	2.8395	1383.65	5.1169
ν49	1424.33	1.4984	1423.43	2.3509
ν50	1467.5	7.2176	1439.23	1.1298
ν51	1472.34	1.4905	1454.91	6.2727
ν52	1487.49	9.3762	1489.45	6.8124
ν53	1502.91	16.9686	1493	11.2903
ν54	1509.26	5.856	1501.96	4.092
ν55	1591.27	3.8984	1549.18	18.1652
ν56	1614.78	5.6524	1557.91	8.2066
ν57	1680.98	16.3303	1645.5	3.7652
ν58	1724.62	2.6859	1665.41	35.4408
ν59	1886.59	4.3943	1674.93	0.3893

ν60	3044.62	35.0098	2954.71	23.457
ν61	3069.28	22.1733	2991.51	19.2861
ν62	3103.19	15.4185	3045.92	37.3099
ν63	3140.61	13.3294	3106.54	16.67
ν64	3163.94	5.8445	3135.91	16.2824
ν65	3167.08	38.6276	3178.74	20.5252
ν66	3191.2	3.144	3187.56	11.7373
ν67	3196.91	1.91	3189.95	0.2785
ν68	3197.85	5.4287	3197.23	11.6454
ν69	3210.41	8.2819	3205.94	3.9973
ν70	3216.15	17.4616	3213.68	20.3323
ν71	3223.45	12.4541	3221.64	28.3882
ν72	3250.4	10.038	3225.64	4.1537

i25		
ν1	32.75	0.1613
ν2	89.26	0.1501
ν3	107.09	0.0197
ν4	146.03	0.3372
ν5	162.06	0.0883
ν6	240.22	0.378
ν7	247.11	0.4344
ν8	317.99	0.7993
ν9	332.69	3.099
ν10	365.83	0.3503
ν11	420.6	0.0312
ν12	433.92	11.3541
ν13	521.94	13.2003
ν14	545.87	0.1609
ν15	588.81	5.9079
ν16	634.9	2.7915
ν17	644.46	1.9265
ν18	712.49	34.6165
ν19	754.11	4.9343
ν20	767.48	34.5403
ν21	793.28	0.0115
ν22	847.35	1.299
ν23	853.17	9.1949
ν24	869.85	27.9105
ν25	892.8	0.0751

ν26	892.92	0.4996
ν27	912.69	0.4034
ν28	937.2	2.1035
ν29	944.86	10.8731
ν30	1001.76	1.4616
ν31	1003.44	0.1549
ν32	1018.8	0.0287
ν33	1022.21	0.0284
ν34	1032.46	7.8707
ν35	1051.73	1.1716
ν36	1064.23	4.7729
ν37	1120.8	3.1749
ν38	1171.82	8.4707
ν39	1180.23	0.0131
ν40	1187.85	0.6739
ν41	1214.32	3.1056
ν42	1219.98	3.4208
ν43	1251.29	0.5709
ν44	1295.37	0.7946
ν45	1332.55	0.3356
ν46	1347.59	2.1399
ν47	1360.94	1.2937
ν48	1385.54	6.2044
ν49	1417.36	0.6474
ν50	1425.05	3.3713
ν51	1450.16	6.4662
ν52	1475.96	1.4994
ν53	1483.48	8.1071
ν54	1493	10.4979
ν55	1535.05	3.8843
ν56	1541.05	30.2484
ν57	1603.85	24.5334
ν58	1639.06	1.7026
ν59	1664.01	16.2714
ν60	3029.25	44.0939
ν61	3041.72	12.9683
ν62	3076.99	0.9624
ν63	3079.96	23.6854
ν64	3130.75	18.9547

ν65	3156.06	12.6877		
ν66	3183.3	7.5928		
ν67	3192.29	0.1208		
ν68	3202.87	25.4983		
ν69	3212.45	19.5128		
ν70	3217.5	25.0357		
ν71	3230.7	12.5733		
ν72	3257	4.3882		
	tsi5i7		**tsi5i6**	
ν1	-643.73	20.7754	-1886.54	854.1453
ν2	14.66	0.1504	38.71	0.125
ν3	54.03	0.3295	41.59	0.5005
ν4	91.94	0.5459	45.42	0.3288
ν5	109.81	0.8769	119.84	0.2692
ν6	168.94	1.0994	134.09	0.4996
ν7	219.06	2.3948	185.1	2.4434
ν8	234.1	0.5169	208.73	0.1555
ν9	299.97	4.3193	215.4	0.2074
ν10	315.09	2.5838	259.7	0.9148
ν11	382.83	0.9123	341.14	3.5266
ν12	417.96	0.0438	415	0.0066
ν13	432.3	3.0916	440.62	4.9108
ν14	469.56	7.8172	453.97	4.3066
ν15	490.84	3.5501	492.58	17.7613
ν16	514.42	22.7874	511.69	1.1828
ν17	545.88	9.7979	535.06	19.8228
ν18	627.63	1.3889	546.91	2.4114
ν19	646.87	2.3114	575.93	3.4839
ν20	682.4	22.6563	640.49	0.3356
ν21	720.94	30.7338	675.11	1.4775
ν22	730.63	0.5593	704.2	17.4604
ν23	787.72	19.2278	712.95	34.4063
ν24	788.78	30.4521	753.77	6.6933
ν25	858.54	0.943	777.52	47.8215
ν26	866.65	6.6414	828.82	5.4962
ν27	875.14	0.2243	863.08	0.0144
ν28	953.31	1.9335	868.35	0.4134
ν29	956.9	2.2557	886.55	50.2423
ν30	982.02	1.682	935.9	3.79

ν31	987.29	4.4358	998.85	1.0995
ν32	1012.43	0.0064	1005.57	0.0156
ν33	1018.98	0.3786	1012.57	7.5061
ν34	1028.86	0.0793	1020.89	19.3898
ν35	1031.24	0.0488	1023.28	0.662
ν36	1066.43	5.5158	1034.25	9.659
ν37	1073.74	0.4379	1050.52	3.3899
ν38	1108.76	0.4582	1066.57	1.3427
ν39	1115.22	6.4049	1069.91	0.246
ν40	1188.64	0.0244	1115.59	5.4417
ν41	1204.91	1.708	1187.58	0.1788
ν42	1212.96	0.0979	1210.21	5.498
ν43	1223.84	3.6597	1255.81	21.7496
ν44	1272.17	2.9408	1290.05	0.1781
ν45	1317.2	0.3418	1312.38	0.405
ν46	1323.94	1.4821	1322.64	39.7197
ν47	1361.3	0.6937	1356.56	12.0354
ν48	1366.32	1.5058	1362.31	0.099
ν49	1418.15	2.2995	1415.12	9.2959
ν50	1472.82	2.6937	1444.2	2.5063
ν51	1485.05	7.2559	1488.75	3.5516
ν52	1489.09	6.2837	1494.53	8.7464
ν53	1492.43	5.2331	1507.96	7.9298
ν54	1501.67	7.0203	1524.35	60.9203
ν55	1543.59	23.7057	1545.14	12.7269
ν56	1648.33	2.5856	1618.01	14.0967
ν57	1666.97	4.2263	1629	2.9109
ν58	1677.86	11.4068	1656.79	45.538
ν59	2093.92	0.5538	1786.26	70.6952
ν60	3028.48	26.5395	2161.98	31.5888
ν61	3040.71	32.7229	3045.31	22.9446
ν62	3091.75	14.376	3103.9	16.1948
ν63	3101.38	18.502	3143.51	19.7243
ν64	3131.73	10.6466	3157.85	9.263
ν65	3135.35	18.7738	3184.86	3.484
ν66	3182.79	18.6847	3191.77	6.1303
ν67	3191.06	1.3028	3192.48	3.9981
ν68	3199.26	3.3613	3198.86	2.8569
ν69	3209.76	15.1653	3210.74	7.8971

ν70	3216.87	17.7595	3216.33	20.8839
ν71	3222.93	8.7067	3223.34	17.6081
ν72	3225.03	5.5702	3248.48	10.421
	tsi5i23		**tsi5p4**	
ν1	-553.38	10.8601	-769.03	18.7375
ν2	24.53	0.0364	20.94	0.1597
ν3	38.4	0.1565	40.1	0.2474
ν4	48.5	0.4133	47.88	0.0974
ν5	88.6	0.9045	90.91	1.2093
ν6	166.95	1.2291	138.79	0.2259
ν7	183.89	1.062	207.6	0.9956
ν8	226.11	1.8537	227.24	3.5721
ν9	267.66	3.989	258.47	1.781
ν10	322.19	3.8676	300.14	0.5002
ν11	345.99	1.6557	337.09	10.4476
ν12	398.35	3.4958	357.52	5.5156
ν13	417.69	0.0176	389.68	16.2062
ν14	420.26	0.6494	416.77	0.0059
ν15	483.34	1.8561	439.93	2.225
ν16	497.23	1.7448	455.72	6.6337
ν17	542.31	2.0536	459.37	9.4233
ν18	558.48	0.0706	551.59	10.4731
ν19	641.51	0.007	556.49	1.7799
ν20	663.72	1.0403	601.48	1.0978
ν21	716.87	32.9422	642.59	0.0368
ν22	732.75	4.46	704.97	2.3982
ν23	778.31	16.1979	712.27	0.3133
ν24	787.3	37.0975	719.27	34.591
ν25	812.06	9.9719	760.66	1.2913
ν26	871	0.0119	791.77	38.4704
ν27	879.69	1.0521	832.29	7.1892
ν28	945.21	2.6041	850.03	8.3184
ν29	950.31	3.7028	875.24	0.0641
ν30	971.2	3.4233	942.09	42.9656
ν31	981.53	6.7758	959.29	3.428
ν32	1010.23	0.0072	971.28	0.1862
ν33	1016.06	1.1076	1007.15	3.7928
ν34	1023.74	0.4699	1013.18	0.004
ν35	1028.47	0.0553	1020.38	2.4122

v36	1062.24	3.0198	1027.73	0.0085
v37	1076.14	4.1544	1033.06	0.0533
v38	1102	0.2462	1057.69	2.6602
v39	1113.95	5.8192	1067.01	11.7608
v40	1188.35	0	1079.65	1.756
v41	1202.62	1.4466	1114.83	5.2004
v42	1209.85	0.4892	1190.73	0.103
v43	1220.02	2.922	1212.6	0.2426
v44	1276.96	4.4013	1239.01	4.2235
v45	1314.64	0.0146	1305.68	1.7528
v46	1353.43	12.9235	1317.91	0.4614
v47	1360.17	4.1709	1351.6	1.9499
v48	1360.98	0.1542	1362.09	0.3145
v49	1417.04	2.4732	1416.61	0.4223
v50	1468.69	1.6683	1441.98	7.7294
v51	1476.46	4.6894	1468.52	5.4036
v52	1484.36	7.9737	1492.8	14.1501
v53	1490.68	4.4206	1492.87	6.3916
v54	1496.78	8.2971	1514.49	26.7576
v55	1540.03	36.4762	1544.52	30.0769
v56	1637.82	2.1902	1592.36	14.9958
v57	1666.81	25.3883	1646.62	1.5059
v58	1732.52	7.8647	1674.53	6.2683
v59	2177.01	21.5659	1679.09	12.2198
v60	3029.79	23.2819	2344.78	5.8729
v61	3039.16	40.085	3059.38	10.8355
v62	3073.26	11.7243	3128.11	8.4337
v63	3099.62	17.5434	3143.28	19.7097
v64	3128.86	21.8078	3158.09	6.9661
v65	3134.97	16.6059	3169.32	1.6421
v66	3189.55	24.4978	3186.57	12.894
v67	3191.11	2.2531	3193.08	1.4063
v68	3198.95	3.4461	3201.59	2.1343
v69	3210.32	12.1502	3210.94	12.0079
v70	3216.55	19.6906	3218.4	17.3649
v71	3222.78	9.977	3224.32	10.8061
v72	3222.94	6.4451	3247.07	9.3901
	tsi7i8		**tsi6i8**	
v1	-1622.21	35.0766	-369.65	4.2695

ν2	35.7	0.2247	37.01	0.0794
ν3	52.5	0.7493	57.65	0.2125
ν4	107.89	0.8836	71.45	0.6599
ν5	182.13	0.6189	117	0.139
ν6	208.45	1.3826	151.37	0.1605
ν7	224.69	0.6478	190.92	0.7931
ν8	299.11	2.4919	234.09	0.5272
ν9	309	1.7948	273.27	0.5948
ν10	377.33	2.1475	360.09	0.2173
ν11	418.15	0.0803	407.81	2.6803
ν12	441.7	2.0598	416.2	0.0915
ν13	461.37	29.4422	448.76	3.1321
ν14	469.94	1.5598	488.11	20.1779
ν15	519.85	4.3316	514.44	3.4775
ν16	584.1	14.985	537.05	13.5858
ν17	621.84	3.0291	580.83	5.0824
ν18	639.18	0.1673	636.59	0.2836
ν19	703.2	28.1142	711.99	35.6295
ν20	715.07	30.8779	731.42	7.1359
ν21	750.83	37.9728	740.39	15.9569
ν22	790.6	33.6392	764.7	20.716
ν23	808.21	4.7933	781.08	28.0465
ν24	866.23	0.3433	828.44	5.0025
ν25	886.11	28.8063	862.69	0.0447
ν26	891.17	7.4147	885.93	2.0629
ν27	909.96	18.4269	915.61	11.8003
ν28	946.1	2.3993	935.88	0.4373
ν29	987.97	0.4307	953.24	20.1089
ν30	1008.19	0.1998	979.58	1.4708
ν31	1019.56	1.0823	1005.91	0.2236
ν32	1028.53	0.4006	1006.24	2.4673
ν33	1029.03	1.7746	1012.26	2.8521
ν34	1062.66	2.9272	1022.82	0.0096
ν35	1070.48	1.6092	1027.76	1.7956
ν36	1071.91	1.0117	1032.54	1.9422
ν37	1117.74	8.859	1058.46	4.7332
ν38	1165.71	1.7706	1067.46	2.9715
ν39	1175.23	12.3701	1113.03	5.2088
ν40	1188.19	0.8315	1171.19	4.5926

ν41	1213.86	0.3211	1185.32	0.0932
ν42	1225.22	0.7597	1213.93	0.1061
ν43	1242.08	27.0976	1239.64	3.4846
ν44	1310.04	9.3761	1289.12	2.047
ν45	1323.41	2.8726	1308.28	0.5413
ν46	1330.72	13.6299	1341.54	4.8217
ν47	1365.77	1.5931	1357.24	0.1958
ν48	1375.31	17.7964	1412.74	2.0249
ν49	1399.45	17.476	1430.75	2.6975
ν50	1420.92	7.4702	1470.11	3.8885
ν51	1465.84	13.5699	1483.7	4.1766
ν52	1485.59	12.2729	1486.74	7.2852
ν53	1486.39	23.7921	1501.35	14.6749
ν54	1491.9	7.675	1520.85	25.7108
ν55	1499.38	19.1477	1577.58	1.7216
ν56	1541.25	18.3744	1620.62	2.649
ν57	1640.87	3.8759	1641.68	6.1419
ν58	1665.47	6.2115	1653.21	24.2267
ν59	1708.94	19.4318	1750.69	0.5552
ν60	2124.64	26.1692	3038.08	36.552
ν61	2993.15	22.2777	3088.54	16.0807
ν62	3035.94	27.2505	3095.28	15.6413
ν63	3091.79	14.1609	3135.5	14.8626
ν64	3104.28	11.6192	3154.56	16.14
ν65	3137.66	19.1882	3159	4.239
ν66	3159.34	12.6196	3189.11	7.7622
ν67	3187.24	3.4885	3189.56	26.0561
ν68	3191.18	28.7224	3195.42	2.1072
ν69	3195.49	8.2584	3207.13	7.3333
ν70	3209.42	15.1417	3212.36	22.6724
ν71	3215.74	20.6459	3220.98	15.5729
ν72	3220.83	13.4126	3248.38	5.1886
	tsi6p4		**tsi8p3**	
ν1	-790.09	6.6522	-708.77	14.5191
ν2	23.74	0.3293	59.9	0.1169
ν3	42.32	0.7406	83.04	0.0042
ν4	46.95	0.0787	93.34	1.3551
ν5	83.45	3.3811	126.62	0.3755
ν6	88.41	1.22	210.46	1.4862

ν7	148.71	1.905	251.23	0.5093
ν8	230.27	0.3268	291.49	1.1865
ν9	264.42	1.8292	317.69	1.156
ν10	286.97	0.2448	335.44	0.408
ν11	317.29	3.5063	406.15	1.6349
ν12	364.32	4.9061	421.12	0.033
ν13	416.36	0.0761	432.3	2.1466
ν14	421.6	12.936	496.47	6.7062
ν15	439.42	2.9794	529.4	2.5191
ν16	460.43	3.6778	540.9	2.0384
ν17	473.51	30.4634	604.36	4.0996
ν18	552.15	2.7945	635.65	3.9916
ν19	567.56	5.1659	641.19	0.6997
ν20	609.38	4.0171	727.35	33.7825
ν21	642.18	0.0725	734.27	6.3694
ν22	708.45	5.7219	745.29	10.0822
ν23	716.79	30.027	786.6	61.7904
ν24	726.19	9.403	825.41	4.9636
ν25	755.27	0.6542	877.89	0.7902
ν26	790.05	43.6506	882.01	1.1507
ν27	820.45	14.16	938.69	0.246
ν28	837.64	1.1447	958.61	2.2358
ν29	873.77	0.0489	986.2	4.1919
ν30	949.74	41.2056	1009.45	0.6574
ν31	957.54	4.2332	1013.53	0.389
ν32	971.81	0.4073	1015.66	0.4196
ν33	1013.37	0.0058	1027.8	0.1769
ν34	1017.58	1.5921	1031.96	0.2406
ν35	1021.75	0.9181	1032.34	0.1723
ν36	1026.64	0.0707	1062.26	4.0577
ν37	1033.36	0.0366	1072.87	2.5729
ν38	1058.76	2.5627	1088.2	1.1938
ν39	1066.65	11.6716	1120.9	5.4447
ν40	1081.65	1.452	1131.93	4.4615
ν41	1115.82	5.1065	1190.4	0.022
ν42	1190.92	0.1233	1203.43	1.0456
ν43	1212.39	0.3614	1220.47	1.467
ν44	1252.56	2.8033	1224.04	0.1165
ν45	1309.66	0.8233	1303.78	1.8905

ν46	1318.09	0.5118	1327.67	0.8286
ν47	1356.5	1.196	1331.57	0.6564
ν48	1362.62	0.354	1354.34	0.0296
ν49	1417.11	0.0624	1368.64	1.6015
ν50	1440.84	5.613	1421.5	3.2382
ν51	1469.46	1.9705	1444.44	3.5753
ν52	1492.04	5.0545	1490.62	6.7091
ν53	1492.8	10.9615	1495.22	10.6647
ν54	1509.59	30.4327	1507.47	7.8433
ν55	1543.63	27.4695	1535.63	41.1943
ν56	1642.36	1.928	1558.07	0.6983
ν57	1669.13	13.0662	1645.19	19.6708
ν58	1679.99	4.9325	1654.87	17.4173
ν59	1719.25	3.9259	1659.7	5.089
ν60	2246.5	6.2215	1681.17	5.0382
ν61	3057.83	10.8115	3044.63	26.9395
ν62	3125.8	8.7849	3107.03	10.4423
ν63	3141.9	21.0661	3138.8	15.4174
ν64	3157.44	6.5646	3183.89	3.9157
ν65	3166.47	1.4026	3187.36	1.9385
ν66	3187.39	15.922	3188.45	3.7817
ν67	3194.09	1.4648	3192.48	1.31
ν68	3202.6	2.4078	3199.8	20.1443
ν69	3212.06	10.8759	3202.16	0.1833
ν70	3219.53	15.6579	3208.97	20.399
ν71	3225.15	10.8437	3215.53	19.2841
ν72	3245.01	10.2819	3219.49	16.406

	tsi23i24		**tsi24p11**	
ν1	-2342.62	40.9971	-586.89	64.5244
ν2	29.83	0.1192	47.57	0.5563
ν3	51.94	0.7809	55.84	0.8538
ν4	79.55	0.6711	102.63	0.1257
ν5	153.29	0.5039	139.85	0.249
ν6	162.66	0.4091	175.86	0.1128
ν7	222.66	0.0848	214.86	2.0252
ν8	270.32	1.8916	226	1.4986
ν9	302.85	0.3648	256.61	5.9139
ν10	369.12	3.801	282.51	1.3298
ν11	381.74	0.3623	331.01	2.8543

ν12	418.01	0.0334	369.43	0.6117
ν13	454.67	10.9255	384.86	3.3454
ν14	517.26	15.2895	423.45	1.6296
ν15	549.63	4.4074	512.18	10.9699
ν16	604.55	1.6357	598.08	6.675
ν17	634.49	0.4613	598.87	8.2207
ν18	664.4	20.6782	636.59	0.2141
ν19	712.7	10.5501	653.81	8.6301
ν20	721.54	35.2514	681.79	6.8361
ν21	784.4	22.2931	724.13	30.0763
ν22	796.45	27.4603	739.68	22.009
ν23	818.16	17.2377	777.95	2.0136
ν24	873.05	7.1091	801.03	23.6979
ν25	875.48	10.0935	838.09	26.1017
ν26	920.66	2.7131	856.58	11.284
ν27	941.67	7.7343	879.34	0.2145
ν28	952.17	3.9786	929.93	9.9686
ν29	971.15	2.4172	933.6	10.1299
ν30	982.55	27.7402	940.57	20.0949
ν31	1010.43	0.0578	960.54	1.9244
ν32	1025.55	0.1804	972.52	10.4249
ν33	1029.49	0.2026	1015.68	17.1082
ν34	1031.35	5.6112	1017.52	7.0063
ν35	1063.64	3.6881	1028.56	0.2246
ν36	1072.79	3.0953	1034.72	0.3264
ν37	1114.54	9.0233	1065.32	4.4433
ν38	1127.17	2.3893	1069.27	3.0709
ν39	1154.45	11.9203	1106.65	7.5998
ν40	1188.76	0.063	1119.84	9.5635
ν41	1190.92	4.8714	1176.52	2.5546
ν42	1196.6	2.2978	1190.59	0.3684
ν43	1211.67	0.4107	1204.84	5.5664
ν44	1251.41	2.348	1216.54	2.0758
ν45	1291.11	0.7003	1259.05	0.0705
ν46	1302.97	2.2712	1306.48	5.8448
ν47	1320.36	5.3344	1335.3	0.1597
ν48	1346.75	4.1429	1364.4	1.3858
ν49	1361.94	1.1456	1376.98	39.159
ν50	1424.3	3.3432	1413.84	9.824

ν51	1478.86	1.7188	1425.57	1.988
ν52	1486.08	8.4587	1487.34	6.8323
ν53	1491.03	8.5508	1494.19	1.7101
ν54	1495.73	10.1827	1498.47	21.2812
ν55	1537.87	15.0485	1521.13	21.538
ν56	1644.63	3.1898	1547.68	14.5764
ν57	1665.03	5.6435	1650.27	3.0181
ν58	1672.56	8.4077	1668.99	2.4788
ν59	1698.36	15.2452	1679.61	0.9729
ν60	1808.5	17.004	1731.13	81.5645
ν61	3036.21	30.4528	3042.49	36.5498
ν62	3044.83	33.186	3099.45	15.1593
ν63	3093.86	13.3396	3136.05	16.6413
ν64	3104.76	11.3416	3156.87	9.8758
ν65	3106.86	21.5224	3187.67	3.6481
ν66	3133.52	18.8262	3195.33	0.3174
ν67	3187.88	3.0776	3205.72	14.0864
ν68	3194.52	0.4146	3215.59	21.4117
ν69	3199.24	15.1527	3222.82	10.3449
ν70	3203.95	6.7609	3224.54	8.9225
ν71	3210.56	25.7129	3231.54	6.907
ν72	3220.02	17.8593	3273.18	2.4757
	tsi9i11		**tsi9i10**	
ν1	-680.17	24.9161	-1873.04	784.6284
ν2	19.76	0.1717	37.64	0.0982
ν3	50.57	0.4718	40.87	0.2675
ν4	85.2	0.8472	48.06	0.0926
ν5	120.89	1.0779	96.05	0.3217
ν6	181.24	0.519	134.93	0.3892
ν7	219.62	0.5778	142.5	0.714
ν8	252.99	1.4336	214.52	0.1837
ν9	286.31	3.3786	245.38	0.2415
ν10	318.15	1.4158	271.03	1.2185
ν11	370.07	1.9011	332.15	0.2591
ν12	418.14	0.0418	345.14	1.0281
ν13	422.93	4.5873	381.16	10.3006
ν14	486.41	15.5689	415	0.0129
ν15	490.28	3.0621	479.48	4.3134
ν16	507.28	13.2301	516.67	17.5376

ν17	546.13	9.1258	523.24	4.8409
ν18	634.96	1.0133	550.12	6.7519
ν19	641.75	18.1166	611.72	1.4069
ν20	658.88	8.5446	639.69	0.5176
ν21	721.14	33.1081	661.07	4.0399
ν22	736.94	2.0885	712.73	29.3362
ν23	787.44	36.8057	723.34	13.8576
ν24	800.94	13.0489	755.68	10.6695
ν25	817.06	6.9494	777.18	48.1889
ν26	876.04	0.0361	822.14	2.0279
ν27	897.96	3.245	862.11	0.0177
ν28	934.65	7.4322	893.57	48.95
ν29	956.93	2.4312	934.44	3.59
ν30	983.02	3.3316	977.43	4.7902
ν31	1008.7	1.1815	994.76	13.0415
ν32	1013.37	0.0034	1004.88	0.0051
ν33	1028.44	0.1288	1015.03	10.2556
ν34	1031.42	0.0366	1017.93	13.9173
ν35	1059.64	0.1095	1022.91	0.162
ν36	1066.68	4.0233	1042.97	14.4274
ν37	1073.98	2.9404	1052.59	3.3886
ν38	1115.56	6.6729	1063.64	0.9136
ν39	1156.85	3.361	1089.63	9.9455
ν40	1189.65	0.0111	1115.21	5.5518
ν41	1199.99	2.762	1187.49	0.2195
ν42	1213.67	0.2329	1209.68	4.5447
ν43	1221.07	0.5771	1240.21	0.3507
ν44	1273.14	2.7231	1311.05	18.9216
ν45	1317.75	0.3573	1312.53	27.4915
ν46	1322	1.625	1330.41	1.4252
ν47	1362.09	1.0526	1361.72	0.0013
ν48	1362.45	1.3118	1377.79	24.7882
ν49	1421.65	1.2607	1423.33	5.494
ν50	1468.48	4.0017	1452.74	2.7414
ν51	1485.73	5.3238	1474.82	16.178
ν52	1492.05	7.271	1488.43	3.1759
ν53	1492.75	2.3626	1491.49	8.2605
ν54	1500.59	6.4632	1523.22	29.4073
ν55	1544.02	24.5487	1541.31	25.81

ν56	1648.33	2.2685	1619.9	32.1491
ν57	1654.73	1.9767	1628.06	3.0572
ν58	1677.8	11.6816	1656.15	51.2347
ν59	2080.28	1.9095	1793.83	63.8243
ν60	3026.37	12.9062	2158.87	28.9925
ν61	3028.81	56.3234	3035.11	31.7898
ν62	3079.25	18.1316	3087.85	15.1586
ν63	3083.54	17.347	3144.2	7.2892
ν64	3131.02	13.0071	3149.55	18.9166
ν65	3137.2	27.2446	3168.14	7.0863
ν66	3144.53	11.4603	3177.75	3.7315
ν67	3190.7	1.3005	3191.44	7.5424
ν68	3199.15	3.4634	3198.1	2.4838
ν69	3209.55	15.8779	3210.1	6.5477
ν70	3216.95	18.1978	3215.44	21.4916
ν71	3222.87	8.7755	3223.12	18.5718
ν72	3226.99	6.1527	3255.63	10.8507
	tsi9i23		**tsi9p6**	
ν1	-584.53	15.4857	-685.35	34.5419
ν2	30.78	0.044	13.12	0.1009
ν3	36.6	0.0957	42.69	0.4512
ν4	48.63	0.7835	57.39	1.3798
ν5	98.15	1.2373	127.08	0.0852
ν6	170.36	0.449	133.09	0.138
ν7	183.77	0.7961	157.5	0.5134
ν8	236.56	1.757	201.78	0.1475
ν9	266.62	0.6127	247.25	6.3257
ν10	302.05	0.5217	290.45	1.8032
ν11	345.9	3.8182	300.44	10.7274
ν12	393.81	4.529	307.18	1.1721
ν13	399.26	4.8901	337.24	3.663
ν14	417.43	0.0035	384.52	1.3344
ν15	484.02	0.6068	416.43	0.0173
ν16	534.73	2.2601	434.14	17.944
ν17	541.1	2.0005	503.75	1.3693
ν18	564.46	0.0555	515.72	8.9294
ν19	602.53	0.9673	551.5	0.9177
ν20	642.32	0.0013	570.16	9.4236
ν21	716.36	33.2567	630.42	3.0441

ν22	737.19	5.2109	645.56	0.5543
ν23	769.28	15.7541	718.55	34.5479
ν24	786.1	41.4811	733.59	0.628
ν25	814.11	6.4986	766.72	0.0155
ν26	870.12	0.0119	791.14	39.6092
ν27	871.66	0.6072	812.63	1.7305
ν28	932.1	4.3981	873.72	0.0038
ν29	949.17	3.3764	912.62	8.6339
ν30	975.97	2.384	957.91	1.5585
ν31	1006.33	4.9918	962.18	45.5131
ν32	1009.62	0.0057	998.8	0.4165
ν33	1023.69	0.5247	1011.92	0.0207
ν34	1027.85	0.0446	1027.3	0.231
ν35	1051.68	3.1245	1032.18	0.0236
ν36	1062.97	3.3535	1040.58	0.1247
ν37	1073.19	1.1624	1045.43	8.351
ν38	1113.85	5.833	1065.5	1.5155
ν39	1133.16	8.4688	1066.43	1.5269
ν40	1188.35	0.0013	1097.2	15.5162
ν41	1189.39	6.341	1115.04	5.4736
ν42	1209.47	1.7522	1190.85	0.0474
ν43	1221.9	1.2343	1213	0.1629
ν44	1277.19	10.8061	1259.64	6.9451
ν45	1314.72	0.0135	1310.95	12.2253
ν46	1324.13	2.473	1317.89	0.1968
ν47	1360.57	0.1271	1335.56	1.4561
ν48	1375.52	1.7563	1362.32	0.3869
ν49	1424.57	1.624	1380.71	2.6134
ν50	1470.02	4.0388	1424.67	2.9119
ν51	1476.45	1.6389	1462.12	11.0749
ν52	1485.7	7.3032	1486.66	7.806
ν53	1490.3	4.4478	1492.93	5.1225
ν54	1496.67	10.5228	1503.18	5.5359
ν55	1539.43	37.5311	1545.22	29.9064
ν56	1637.24	2.2314	1605.45	8.8136
ν57	1665.72	27.9461	1646.77	1.5439
ν58	1729.61	1.9763	1679.09	8.8274
ν59	2167.62	27.9365	1684.23	11.9524
ν60	3025.27	16.7534	2344.47	1.453

ν61	3032.21	52.5128	3046.14	30.9346
ν62	3064.5	13.7243	3105.11	9.4307
ν63	3084.6	19.0985	3144.45	12.6918
ν64	3129.98	29.1352	3164.96	4.5872
ν65	3133.72	32.5091	3181.26	10.351
ν66	3139.4	11.9102	3186.62	3.232
ν67	3191.11	2.6494	3193.14	1.4051
ν68	3199.2	3.4747	3201.96	2.6671
ν69	3210.34	12.7565	3211.6	12.9809
ν70	3216.86	19.7008	3218.89	17.4233
ν71	3222.91	10.7169	3224.56	10.2137
ν72	3223.71	6.1312	3252.95	7.7426
	tsi11i12		**tsi10i12**	
ν1	-1659.26	23.658	-373.6	2.1005
ν2	34.63	0.1728	40.26	0.0668
ν3	50.26	0.8493	58.03	0.6062
ν4	127.68	0.5989	66.82	0.1335
ν5	157.97	0.0882	139.99	0.0947
ν6	185.47	0.9713	167.53	0.1583
ν7	243.39	0.5044	211.43	0.1687
ν8	256.56	3.8859	230.89	1.1905
ν9	316.44	0.8476	271.75	0.713
ν10	331.26	1.3294	331.09	1.1461
ν11	417.33	0.6784	348.24	5.9344
ν12	429.9	4.592	415.69	0.212
ν13	460.81	6.2293	439.43	0.8222
ν14	502.87	8.6297	480.01	7.2899
ν15	527.06	29.4253	519.53	5.8203
ν16	562.82	3.516	530.05	9.7308
ν17	608.95	9.8566	568.39	3.5889
ν18	639.46	1.1984	636.5	0.2217
ν19	706.2	9.0987	679.87	8.6216
ν20	714.62	32.5692	711.69	36.4158
ν21	747.42	22.1873	738.07	18.1948
ν22	787.05	37.0522	768.61	16.1322
ν23	795.24	12.3953	783.45	21.1452
ν24	844	42.1783	828.57	19.0829
ν25	866.69	1.928	847.09	16.303
ν26	909.58	11.3885	862.84	0.0603
ν27	945.23	4.0891	924.46	0.4315
ν28	950.03	23.6605	937.25	0.585

ν29	976.62	4.5045	960.31	16.3246
ν30	1008.3	0.1954	982.26	0.7555
ν31	1016.08	1.217	996.25	9.5028
ν32	1024.46	0.7451	1006.1	0.0208
ν33	1028.55	0.3477	1014.67	0.2774
ν34	1066.62	4.4116	1022.99	0.0422
ν35	1074.31	3.4555	1045.23	4.9734
ν36	1080.78	0.2528	1058.15	3.6334
ν37	1113.3	11.3255	1081.47	2.6837
ν38	1157.72	0.6613	1111.3	3.8354
ν39	1187.44	1.2077	1115.42	1.7755
ν40	1189.24	9.5219	1184.9	2.5129
ν41	1207.74	2.7366	1186.58	7.2651
ν42	1218.97	1.4182	1210.36	1.787
ν43	1237.76	26.4885	1219.04	1.069
ν44	1305.75	0.4234	1302.45	0.7851
ν45	1321.92	1.7705	1308.5	0.9045
ν46	1341.05	13.5656	1343.01	0.7549
ν47	1348.84	0.2156	1357.26	0.2602
ν48	1367.6	8.4214	1385.99	0.6141
ν49	1404.57	18.5955	1421.73	0.4458
ν50	1426.6	2.4677	1467.99	10.749
ν51	1468.73	17.3485	1483.58	5.1569
ν52	1484	32.372	1486.24	5.3269
ν53	1487.47	10.3811	1502.07	11.0945
ν54	1497.85	24.478	1520.69	23.9107
ν55	1501.21	15.5025	1583.7	3.4132
ν56	1538.88	16.4737	1620.49	2.7564
ν57	1640.5	3.6941	1641.68	19.6097
ν58	1665.21	4.745	1659.19	3.9219
ν59	1720.15	2.3192	1753.96	0.1013
ν60	2126.68	22.2727	3040.39	44.6618
ν61	2995.66	23.637	3085.19	16.6929
ν62	3040.28	36.147	3098.82	16.6792
ν63	3097.83	16.7219	3134.85	16.6866
ν64	3109.68	10.3665	3148.41	17.2268
ν65	3134.64	15.769	3164.81	6.5208
ν66	3145.01	16.8838	3173.22	24.8071
ν67	3170.91	18.6935	3189	3.7979
ν68	3187.53	2.8095	3195.42	2.245
ν69	3195.83	7.7433	3207.03	7.2593
ν70	3208.98	12.9222	3212.27	22.5357
ν71	3215.2	20.9038	3220.75	15.9592

ν72	3220.61	15.0708	3249.44	5.9259
	tsi10p6		**tsi12p5**	
ν1	-765.34	12.9557	-827.33	2.8493
ν2	17.54	0.1122	38.59	0.1985
ν3	39.64	0.9318	69.13	0.2233
ν4	56.41	1.7895	75.41	0.8771
ν5	89.48	2.8518	116.19	0.1789
ν6	126.02	0.1612	196.54	0.1215
ν7	144.77	1.929	290.54	1.9904
ν8	170.47	0.538	293.8	0.3299
ν9	221.36	0.2209	302.84	0.6448
ν10	284.56	1.2679	355.38	0.5241
ν11	303.09	1.3568	405.58	1.5163
ν12	319.85	2.8068	418.52	1.1997
ν13	391.52	1.1128	427.65	1.28
ν14	414.27	5.1167	489.36	1.1737
ν15	416.15	0.0906	526.46	14.1724
ν16	458.25	22.7946	571.12	3.8016
ν17	494.15	5.5854	573.27	2.6787
ν18	519.19	12.3717	637.65	0.0915
ν19	556	1.9423	658.89	0.1685
ν20	579.52	2.6756	724.79	2.507
ν21	637.81	5.0771	727.32	36.6945
ν22	649.55	6.9691	751.47	4.5582
ν23	716.77	33.4856	796.44	47.7157
ν24	742.84	2.486	828.69	0.2356
ν25	760.4	0.8726	856.45	15.5469
ν26	789.82	45.6051	878.6	0.0922
ν27	811.23	3.526	889.62	4.3187
ν28	872.91	0.0676	957.34	1.7407
ν29	879.86	9.0733	997.8	1.2547
ν30	957.02	2.782	1012.94	0.3155
ν31	969.49	45.1026	1013.86	0.5901
ν32	999.77	0.1989	1022.94	5.1751
ν33	1012.72	0.0028	1028.91	0.9474
ν34	1025.54	0.1694	1031.83	0.6627
ν35	1032.9	0.0225	1040.8	5.1617
ν36	1038.42	0.3519	1052.66	0.2846
ν37	1049.82	8.5002	1072.7	5.5003
ν38	1065.25	2.7362	1076.21	2.4743
ν39	1073.6	1.5446	1120.74	4.5541
ν40	1099.42	11.0646	1145.53	5.256
ν41	1115.39	5.48	1190.63	0.0353

ν42	1191.37	0.0645	1215.82	1.6235
ν43	1212.62	0.2262	1224.37	0.0482
ν44	1261.88	2.814	1244.48	1.4455
ν45	1310.98	4.818	1299.59	2.7406
ν46	1317.72	0.2749	1317.82	0.5127
ν47	1339.51	0.4009	1327.76	1.1498
ν48	1362.42	0.4779	1350.32	0.667
ν49	1389.79	0.9424	1368.7	1.4113
ν50	1425.64	1.7899	1423.45	0.4192
ν51	1465.87	11.0601	1438.33	3.1685
ν52	1487.74	8.2479	1491.84	11.7383
ν53	1492.18	5.3136	1494.62	4.6197
ν54	1506.28	3.416	1505.3	4.6591
ν55	1543.44	26.756	1540.47	49.5468
ν56	1642.66	1.8653	1571.22	9.4536
ν57	1668.44	24.4489	1615.69	2.938
ν58	1677.02	3.1919	1655.32	1.5666
ν59	1723.17	2.8924	1672.9	1.7139
ν60	2247.34	8.3409	1680.47	7.7707
ν61	3048.13	34.4286	3050.48	32.6157
ν62	3107.44	12.0402	3113.49	13.8427
ν63	3144.42	14.4009	3137.87	14.2122
ν64	3164.68	5.08	3182.88	13.6343
ν65	3188.8	11.1282	3186.99	4.9917
ν66	3190.02	4.9513	3188.99	8.3374
ν67	3193.91	1.4663	3192.29	2.3262
ν68	3202.46	2.7949	3200.98	5.332
ν69	3212.27	11.3641	3204	8.9733
ν70	3219.36	15.4996	3206.52	1.0886
ν71	3225.12	10.7756	3209.14	27.3085
ν72	3251.5	8.428	3219.26	18.1171
	tsi23i25		**tsi25p11′**	
ν1	-2289.69	49.5285	-493.52	78.1518
ν2	33	0.1385	43.74	0.2881
ν3	48.78	0.4495	75.09	1.4931
ν4	84.84	0.7226	92.03	0.1379
ν5	142.58	1.0035	124.81	0.4554
ν6	172.85	0.2196	168.24	1.1692
ν7	234.95	0.3587	211.02	0.7637
ν8	258.32	0.5492	231.88	5.9247
ν9	326.49	0.5534	243.13	5.8873
ν10	374.61	2.7705	289.16	5.2763
ν11	387.67	4.6101	310.81	0.337

ν12	417.64	0.0054	363.31	3.6919
ν13	468.35	1.8068	404.91	4.4953
ν14	510	4.5575	423.81	1.1853
ν15	534.68	4.7767	518	2.5874
ν16	604.31	7.7768	600.24	7.8124
ν17	635.31	3.5759	618.78	13.0559
ν18	655.46	27.2657	631.63	4.9098
ν19	709.29	12.7323	639.67	0.1698
ν20	718.23	40.1302	665.48	14.5498
ν21	787.28	21.7837	725.23	30.3756
ν22	811.22	6.1298	749.59	28.9444
ν23	834.38	10.4527	763.66	13.163
ν24	858.29	4.1896	803.14	6.3286
ν25	871.39	0.1603	860.12	8.1047
ν26	909.39	28.5895	865	21.6721
ν27	936.21	10.6325	881.84	2.2174
ν28	952.71	3.4375	927.82	0.3184
ν29	959.96	7.5992	929.38	13.1996
ν30	1004.21	5.6824	947.78	31.5354
ν31	1009.55	0.0354	961.05	1.5714
ν32	1023.91	0.365	973.48	12.444
ν33	1027.73	0.0405	1012.76	20.8422
ν34	1054.28	4.3294	1019.24	2.4286
ν35	1055.76	8.2745	1028.81	0.9466
ν36	1062.66	1.6088	1035.93	0.0929
ν37	1112.6	7.2828	1062.7	1.2325
ν38	1132.96	4.8822	1066.68	3.582
ν39	1142.79	17.3943	1107.02	9.8187
ν40	1187.33	0.1088	1120.73	5.4334
ν41	1194.08	0.2752	1165.67	3.1089
ν42	1200.52	1.5064	1191.22	0.0393
ν43	1208.37	0.7972	1213.85	4.553
ν44	1239	1.0681	1219.39	5.6995
ν45	1289.77	5.2254	1257.69	1.8887
ν46	1308.85	1.7484	1303.1	17.4527
ν47	1318.24	2.0456	1335.17	9.9949
ν48	1338.64	3.3726	1367.21	2.2989
ν49	1358.17	0.2897	1387.56	9.1389
ν50	1421.69	1.2859	1411.3	13.2304
ν51	1478.09	3.6673	1422.15	15.7095
ν52	1484.2	9.9794	1484.84	5.8859
ν53	1488.32	3.9604	1490.92	21.2874
ν54	1490.6	9.9542	1498.72	9.2014

ν55	1531.38	17.9276	1543.32	2.863
ν56	1637.29	2.7869	1558.04	30.5087
ν57	1650.27	8.6301	1649.37	42.6669
ν58	1661.38	11.0019	1651.49	5.4437
ν59	1697.54	3.6241	1679.89	1.0083
ν60	1828.62	22.1609	1731.34	81.3026
ν61	3032.51	14.9874	3040.73	27.9241
ν62	3035.55	53.8772	3097.43	12.0614
ν63	3089.13	15.7773	3138.35	12.0624
ν64	3101.02	13.0442	3157.48	10.0702
ν65	3120.66	14.474	3187.55	3.6876
ν66	3134.38	18.2032	3195.36	0.3572
ν67	3187.39	3.4328	3206.02	15.1093
ν68	3194.07	0.6536	3216.56	20.8225
ν69	3204.07	7.4344	3221.77	4.8055
ν70	3210.45	25.7124	3223.91	8.3924
ν71	3211.47	23.413	3247.77	11.2055
ν72	3219.39	16.5914	3262.84	3.1286

	p3		**p4**	
ν1	26.92	0.2226	21.25	0.0458
ν2	60.13	0.069	42.76	0.2221
ν3	91.59	0.7995	45.79	0.1063
ν4	114.13	0.2022	93.59	1.0772
ν5	217.38	1.5718	131.87	0.5009
ν6	257.72	0.0788	213.62	0.1501
ν7	301.04	0.0498	225.72	0
ν8	335.1	0.1982	251.8	2.2667
ν9	403.73	0.6735	335.63	1.0111
ν10	423.19	0.2267	338.96	6.1639
ν11	463.05	3.9617	413.71	0.0007
ν12	522.69	2.9575	426.72	3.2661
ν13	544.44	1.9091	434.68	2.0619
ν14	600.58	3.9704	452.9	9.6984
ν15	637.01	4.033	545.82	11.8899
ν16	642.25	1.597	545.93	1.0964
ν17	728.28	33.1282	592.06	0.0726
ν18	732.89	18.4405	638.89	0.0133
ν19	735.74	2.0571	701.56	4.3019
ν20	786.95	57.9564	708.41	22.3483
ν21	826.01	10.7578	711.78	13.3499
ν22	878.2	0.4872	751.99	0.7712
ν23	885.3	2.6866	779.78	38.0718
ν24	925.12	2.8622	811.33	13.1121

ν25	942.42	2.2623	831.63	0.226
ν26	964.8	1.3596	858.12	0.0433
ν27	1012.95	0.341	926.21	41.9461
ν28	1016.33	1.0304	939.42	3.6476
ν29	1018.35	0.1457	961.92	0.3727
ν30	1026.36	0.3163	989.57	0.0096
ν31	1030.62	0.0365	998.11	0.6268
ν32	1030.84	0.1129	1008.78	0.0725
ν33	1062.97	3.9755	1012.42	0.7232
ν34	1073.2	7.2114	1022.46	0.4064
ν35	1092.02	1.7275	1048.96	0.2836
ν36	1119.3	4.9692	1056.59	10.6124
ν37	1136.74	4.757	1073.91	0.8991
ν38	1190.06	0.0201	1103.41	4.7013
ν39	1206.07	0.1175	1185.19	0.0133
ν40	1219.83	0.4515	1203.26	0.003
ν41	1229.22	0.196	1242.84	7.6447
ν42	1305.03	0.5435	1304.11	1.999
ν43	1327	0.2031	1310.54	0.0545
ν44	1336.23	0.2931	1347.42	3.0973
ν45	1357.71	0.0647	1358.2	0.2701
ν46	1368.85	0.9995	1413.56	0.0897
ν47	1423.22	1.1683	1429.65	4.551
ν48	1462.46	3.1495	1465.08	2.8494
ν49	1493.97	7.7101	1478.15	4.6142
ν50	1497.32	7.7703	1482.27	8.8188
ν51	1512.96	10.478	1499.09	24.7781
ν52	1536.47	33.3039	1528.99	33.7506
ν53	1558.81	0.9362	1607.75	2.2283
ν54	1649.99	8.1734	1625.78	9.1134
ν55	1664.95	3.692	1645.13	3.5758
ν56	1681.74	22.4285	1667.4	10.1573
ν57	1685.78	9.1444	2280.37	1.0679
ν58	3049.66	28.9877	3035.97	9.9977
ν59	3114.07	15.1553	3088.81	10.027
ν60	3136.16	14.033	3108.13	22.4538
ν61	3183.04	5.9383	3123.44	4.696
ν62	3183.77	8.1328	3137.8	5.5778
ν63	3187.23	4.0945	3151.95	20.4553
ν64	3192.21	1.1883	3165.45	2.3747
ν65	3196.54	16.4195	3173.74	5.2105
ν66	3202.09	5.1402	3185.31	16.3185
ν67	3208.85	23.7857	3192.49	18.833

ν68	3212.73	19.8705	3196.69	9.8137
ν69	3219.41	15.3584	3220.69	11.916
	p11		**p5**	
ν1	50.39	0.3201	40.21	0.212
ν2	59.62	0.5667	70.92	0.7583
ν3	105.36	0.1305	71.56	0.0254
ν4	146.94	0.3923	109.3	0.2164
ν5	177.9	0.2811	198	0.0914
ν6	224.99	0.7738	292.9	0.0266
ν7	281.92	0.4219	297.24	0.1799
ν8	294.69	0.5037	357.27	0.3859
ν9	366.28	1.0364	415.51	2.7538
ν10	380	2.9461	420.55	0.4109
ν11	424.37	1.2096	428.6	0.0521
ν12	513.14	14.5239	519.51	14.3608
ν13	598.41	9.1103	566.74	4.3421
ν14	600.2	10.4505	574.23	2.9243
ν15	636.69	0.1816	637.69	0.0353
ν16	651.58	10.1974	663	0.4087
ν17	673.04	7.8269	724.67	1.9737
ν18	724.23	28.6076	728.18	40.0671
ν19	742.52	25.3525	750.28	1.7897
ν20	763.33	0.6124	791.27	50.7523
ν21	800.45	22.5621	830.56	0.0397
ν22	836.86	26.1693	858.93	22.6384
ν23	857.26	11.6861	871.49	0.2369
ν24	880.39	0.155	877.81	0.0646
ν25	924.09	6.7705	955.86	1.7815
ν26	934.56	11.7935	992.53	1.0442
ν27	942.63	24.1442	1008.54	0.5211
ν28	964.72	3.0636	1012.55	0.0975
ν29	973.54	9.5891	1016.93	0.027
ν30	1016.56	12.6612	1028.77	0.1516
ν31	1018.43	11.0367	1030.03	0.0946
ν32	1028.43	0.1553	1036.8	7.4308
ν33	1034.99	0.3585	1057.91	0.3527
ν34	1065.98	4.5037	1073.26	11.4367
ν35	1069.31	2.8585	1079.55	1.4161
ν36	1112.49	3.6263	1118.72	4.5524
ν37	1123.59	12.1581	1154.04	5.8399
ν38	1175.82	3.9114	1189.6	0.0552
ν39	1190.34	0.4375	1217.23	1.1914
ν40	1205.36	5.0654	1226.73	1.5326

ν41	1218.37	2.0506	1251.52	1.193
ν42	1258.84	0.0431	1302.65	1.1088
ν43	1305.81	7.3287	1323.55	0.07
ν44	1335.2	0.1476	1327.98	0.0658
ν45	1366.36	2.7313	1353.57	0.3277
ν46	1375.67	39.215	1367.71	0.6494
ν47	1421.18	13.8832	1423.51	0.2723
ν48	1425.48	0.6326	1451.79	2.2523
ν49	1486.73	6.6155	1492.57	11.1498
ν50	1494.71	5.7987	1497.35	6.2644
ν51	1499.03	15.8985	1506.29	3.7074
ν52	1546.1	5.1334	1542.56	42.0748
ν53	1583.88	52.8158	1577.74	11.6915
ν54	1650.14	3.0704	1637.3	2.1915
ν55	1678.75	2.2816	1659.37	0.8206
ν56	1690.99	2.208	1682	8.8229
ν57	1730.64	67.7199	1694.53	1.9921
ν58	3040.3	38.2521	3047.97	34.2017
ν59	3096.14	16.8939	3112.22	16.2052
ν60	3134.43	17.8785	3135.42	14.371
ν61	3155.63	10.2204	3180.94	18.9724
ν62	3186.69	4.0382	3181.12	12.3309
ν63	3194.86	0.2772	3186.65	2.4457
ν64	3205.44	15.5499	3191.55	1.2848
ν65	3215.84	24.947	3200.68	6.5126
ν66	3219.01	7.6782	3201.18	17.4412
ν67	3223.53	8.3719	3204.25	1.8912
ν68	3230.46	7.9605	3208.56	29.7218
ν69	3265.1	2.8343	3218.95	16.4415
	p6		**p11′**	
ν1	16.62	0.004	44.29	0.1711
ν2	41.85	0.4418	77.05	0.4352
ν3	58	1.5572	89.6	0.1946
ν4	127.78	0.0357	142.5	0.7272
ν5	133.06	0.3011	177.2	1.2215
ν6	165.25	0.0058	216.73	0.7487
ν7	221.69	0.1236	269.99	1.7708
ν8	294.69	1.548	310.07	0.4668
ν9	307.3	0.6676	361.5	3.5915
ν10	322.04	0.1155	398.2	1.0725
ν11	385.87	1.9598	422.14	0.8643
ν12	406.81	8.5279	518.36	4.1243
ν13	417.11	0.0491	600.08	8.4806

ν14	480.75	0.0998	613.89	12.7873
ν15	514.67	6.2609	630.65	5.3636
ν16	550.21	0.4835	639.55	0.0869
ν17	567.29	8.5719	661.24	16.5562
ν18	630.45	4.6837	722.46	30.4484
ν19	644.82	0.9236	746.06	29.6549
ν20	719.17	34.3546	751.25	9.842
ν21	742.57	1.5463	802.34	9.1211
ν22	767.36	0.0825	846.58	28.4522
ν23	791.45	41.2517	860.46	7.5987
ν24	809.38	3.4493	878.27	0.856
ν25	874.38	1.7871	923.98	2.1267
ν26	877.05	7.8968	927.53	13.0004
ν27	957.97	2.6571	948.14	31.4324
ν28	966.87	46.4696	958.31	2.0179
ν29	1000.9	0.3798	971.24	13.0873
ν30	1012.59	0.006	1014.15	9.8043
ν31	1027.01	0.0851	1018.43	13.5283
ν32	1032.19	0.0388	1028.37	0.5894
ν33	1041.62	0.2661	1034.12	0.1928
ν34	1050.05	9.8711	1064.97	4.05
ν35	1066.45	2.6172	1068.35	2.9505
ν36	1074.04	1.4078	1106.48	9.0917
ν37	1101.3	12.2305	1116.21	5.7026
ν38	1114.78	5.2856	1162.19	2.3345
ν39	1190.42	0.0473	1190.54	0.0226
ν40	1213.27	0.0882	1211.58	8.104
ν41	1259.78	5.5592	1214.64	2.1564
ν42	1313.5	12.194	1256.56	1.6983
ν43	1317.27	0.1261	1299.94	16.4037
ν44	1341.18	0.7133	1335.47	10.1992
ν45	1362.11	0.3044	1363.37	2.3158
ν46	1389.16	2.7346	1383.9	9.2912
ν47	1427.06	1.4777	1415.5	11.1709
ν48	1466.17	10.1397	1426.85	19.1648
ν49	1488.63	8.5886	1485.98	6.2804
ν50	1492.7	4.9871	1493.58	17.3639
ν51	1506.94	4.0418	1499.02	10.4273
ν52	1546.37	33.7314	1544.88	3.432
ν53	1646.21	1.8074	1587.74	56.3572
ν54	1670.21	25.2407	1649.76	3.2793
ν55	1683.75	2.2963	1679.12	2.1162
ν56	1723.77	4.1291	1684.94	18.282

ν57	2343.87	1.1349	1729.7	64.5388
ν58	3046.58	38.7073	3040.16	33.719
ν59	3105.43	12.6861	3096.08	15.9816
ν60	3142.16	14.9718	3135.55	13.9857
ν61	3164.32	4.7995	3156.5	10.4827
ν62	3175.21	17.4965	3186.57	4.0635
ν63	3185.54	2.6019	3194.4	0.258
ν64	3192.56	1.6207	3204.98	14.4682
ν65	3201.27	2.6764	3214.82	18.6648
ν66	3211.12	13.0002	3219.51	5.5635
ν67	3218.31	18.3383	3221.99	12.4187
ν68	3224.07	10.7603	3246.19	13.1693
ν69	3251.04	8.7662	3251.69	2.0546

	vdW(i5)		**vdW(i9)**	
ν1	11.55	1.16	5.88	1.0173
ν2	28.65	4.2068	33.84	3.1669
ν3	43.13	0.0656	41.99	0.9683
ν4	64.01	0.0484	51.31	0.6373
ν5	75.01	1.7722	71.69	1.0568
ν6	85.86	2.7013	82.39	3.0619
ν7	131.19	18.0257	127.19	19.5925
ν8	146.81	4.2527	148.44	4.2041
ν9	177.17	0.7694	174.49	0.8945
ν10	232.5	0.3254	226.7	0.6325
ν11	279.76	49.4071	276.03	51.5272
ν12	292.76	0.6754	293.16	0.7904
ν13	393.47	0.127	395.7	0.3663
ν14	419.75	12.4172	416.6	12.3091
ν15	437.14	1.2653	436.95	1.1497
ν16	479.56	3.5657	479.34	2.845
ν17	495.16	31.1299	495.67	31.0126
ν18	511.42	0.5737	512.06	0.5583
ν19	541.45	0.1843	541.67	0.1338
ν20	631.04	0.174	630.91	0.229
ν21	656.69	0.0311	650.53	1.0562
ν22	691.9	50.731	696.22	49.4382
ν23	789.03	1.4778	788.7	1.3908
ν24	797.45	30.4581	797.19	1.5584
ν25	799.68	4.6481	798.56	33.4921
ν26	801.14	1.0921	801.73	0.5543
ν27	865.76	1.5032	870.97	1.148
ν28	948.1	48.476	955.72	16.5918
ν29	961.53	53.3355	956.63	90.6705

ν30	975.21	0.3148	973.77	0.4848
ν31	978.84	1.6062	983.91	2.9371
ν32	1019.66	4.75	1018.17	0.9295
ν33	1019.99	1.5632	1019.59	5.2457
ν34	1021.58	0.2901	1025.19	0.4274
ν35	1041.78	0.1691	1043.45	0.0665
ν36	1053.34	3.6339	1052.79	18.0937
ν37	1053.87	19.8484	1053.78	0.5604
ν38	1077.34	0.4508	1076.26	0.1758
ν39	1098.44	2.4225	1098.63	2.7352
ν40	1116.91	3.7683	1117.32	4.3503
ν41	1188	71.9453	1187.96	67.4685
ν42	1190.46	5.567	1191.13	5.3764
ν43	1231.81	21.7522	1232.04	20.3405
ν44	1326.35	4.9174	1326.79	5.5305
ν45	1342.38	0.4205	1338.21	0.2893
ν46	1343.5	0.4271	1343.29	0.4993
ν47	1359.22	6.6053	1360.08	7.407
ν48	1418.82	12.1538	1417.36	13.3663
ν49	1443.97	4.8391	1445.28	5.0266
ν50	1466.63	2.9256	1467.56	0.9085
ν51	1482.78	11.2111	1483.67	11.6631
ν52	1488.44	8.6051	1488.62	6.7989
ν53	1510.98	5.669	1511.47	5.372
ν54	1514.68	3.0667	1515.36	1.8631
ν55	1614.85	0.7483	1615.23	0.5891
ν56	1639.79	109.7082	1640.65	101.725
ν57	1690.46	22.5392	1690.97	20.3703
ν58	1740.21	2.2897	1740.24	2.772
ν59	1993.45	26.0733	1995.45	25.3676
ν60	3046.08	17.8898	3041.94	19.2858
ν61	3104.9	19.0999	3100.46	18.2895
ν62	3139.44	13.9334	3139.86	15.1421
ν63	3152.98	2.9939	3152.43	3.5745
ν64	3158.88	6.4955	3158.08	4.6923
ν65	3168.45	0.8675	3168.51	2.4453
ν66	3198.89	0.3534	3199.13	0.3647
ν67	3211.63	3.8672	3211.73	4.0905
ν68	3219.11	6.1793	3219.32	6.0984
ν69	3230.02	4.6763	3230.31	4.5362
ν70	3236.37	2.6686	3236.05	3.109
ν71	3240.59	5.7641	3240.82	6.1373
ν72	3248.43	6.892	3247.37	8.5641

	tsi5vdW		tsi9vdW	
ν1	-17.64	0.9989	-25.53	1.4284
ν2	28	0.8567	31.69	0.6796
ν3	44.8	0.1565	47.87	0.5752
ν4	55.44	0.973	67.03	0.036
ν5	74.9	0.5693	78.85	0.2179
ν6	83.74	2.6363	95.94	0.8178
ν7	116.92	23.4713	124.63	22.9512
ν8	148.34	4.1836	147.72	4.3232
ν9	173.96	0.0515	176.42	1.5456
ν10	229.88	0.0388	225.64	0.0857
ν11	261.3	39.3646	258.27	37.5201
ν12	292.8	0.2877	290.21	0.5596
ν13	391.69	0.1291	393.96	0.225
ν14	420.25	15.3158	417.22	13.4937
ν15	436.82	1.3505	436.66	1.3106
ν16	477.67	2.4002	477.14	1.993
ν17	490.57	25.6252	490.4	25.972
ν18	512.82	0.6085	512.64	0.6334
ν19	541.19	0.2419	539.97	0.1711
ν20	632.4	0.1782	632.2	0.1777
ν21	656.8	0.4217	658.69	1.1577
ν22	693.4	51.7369	694.36	51.2987
ν23	788.44	0.3506	788.01	0.2227
ν24	794.84	14.1125	796.26	19.8642
ν25	798.13	13.5241	799	6.6196
ν26	802.18	0.5822	801.67	0.2007
ν27	867.15	1.184	867.77	0.7956
ν28	944.07	47.3965	957.23	45.4111
ν29	968.9	59.8998	962.87	65.5904
ν30	974.12	1.3436	971.85	3.8118
ν31	978.3	0.4104	979.14	1.714
ν32	1019.16	0.3094	1016.57	0.3172
ν33	1020.3	4.8132	1020.24	4.1073
ν34	1021.36	0.1632	1022	0.2135
ν35	1041.6	0.0601	1042.02	0.0234
ν36	1051.64	21.4022	1048.56	17.7397
ν37	1054.67	0.5322	1054.27	0.4258
ν38	1076.65	0.3478	1077.08	0.1536
ν39	1097.83	1.713	1095.92	2.5622
ν40	1115.69	4.0746	1115.88	4.4617
ν41	1185.26	70.0562	1184.82	64.4496
ν42	1191.28	2.5531	1191.17	2.8942

ν43	1229.57	20.7708	1229.33	20.8066
ν44	1326.04	4.1719	1326.31	5.0678
ν45	1338.27	1.1016	1335.43	0.3526
ν46	1343.42	0.2841	1342.78	0.5379
ν47	1358.37	6.4168	1358.58	7.1573
ν48	1418.78	11.4458	1418.31	12.2295
ν49	1443.78	5.94	1443.22	4.9628
ν50	1466.41	4.3473	1466.16	0.6353
ν51	1484.07	10.8239	1483.99	10.9431
ν52	1487.81	9.3952	1488.67	7.1749
ν53	1510.8	4.2206	1511.11	4.218
ν54	1515.21	2.0916	1514.77	1.4481
ν55	1617.42	0.952	1617.33	0.5951
ν56	1641.54	80.3982	1641.5	72.8223
ν57	1689.85	18.9383	1689.01	19.7924
ν58	1738.8	4.7249	1736.85	8.5289
ν59	2017.26	20.5326	2021.62	30.6206
ν60	3047.68	18.2251	3042.82	19.0592
ν61	3107.07	18.2059	3100.61	20.3364
ν62	3139.94	13.2034	3140.67	14.6316
ν63	3154.41	2.6787	3156.83	2.5209
ν64	3160.01	9.2409	3158.88	4.5274
ν65	3168.23	0.5467	3168.42	2.563
ν66	3198.43	0.2759	3198.46	0.3137
ν67	3210.68	3.3696	3210.62	3.6321
ν68	3217.77	5.1727	3218.07	5.5399
ν69	3228.01	3.6925	3228.7	3.9697
ν70	3231.3	5.3675	3231.76	4.2583
ν71	3240.99	7.3822	3245.18	6.2835
ν72	3253.16	4.6457	3247.87	10.0338
	i30		**i31**	
ν1	10.94	0.0063	25.98	0.3187
ν2	42.7	0.2243	42.16	0.2018
ν3	47.86	0.5465	54.7	0.1674
ν4	77.97	1.0421	81.39	1.0051
ν5	135.46	0.1506	129.18	0.6661
ν6	136.02	1.7627	180.01	0.0546
ν7	173.89	0.0672	206.03	0.1
ν8	184.89	0.0405	280.83	0.6027
ν9	227.7	0.8143	328.26	2.2643
ν10	301.46	1.8003	347.63	0.6592
ν11	343.9	1.3281	397.26	7.9364
ν12	402.55	1.061	414.42	0.0082

ν13	417.59	0.0029	433.23	4.7166
ν14	422.48	1.2567	487.53	6.4856
ν15	465.11	17.4256	499.59	0.6018
ν16	499.39	24.8652	540.16	1.5996
ν17	552.02	13.8174	577.07	3.5689
ν18	560.45	4.5756	636.21	0.0133
ν19	596.47	6.4741	670.18	0.4694
ν20	608.23	6.8751	695.7	33.0983
ν21	644.84	0.0751	741.14	0.9284
ν22	720.73	35.5314	760.44	0.308
ν23	723.07	3.131	765.34	44.4015
ν24	761.78	1.9002	825.8	24.2231
ν25	792.3	39.4129	843.3	0.7366
ν26	814.22	2.4898	904.72	6.7421
ν27	876.85	0.0015	912	3.5778
ν28	915.74	0.4509	923.02	34.2676
ν29	946.37	42.3865	937.07	24.2138
ν30	960.04	3.6064	965.46	6.9357
ν31	981.23	0.3103	999.13	0.0214
ν32	1013.88	0.0025	1001.48	8.8615
ν33	1027.82	0.1621	1011.86	0.9343
ν34	1032.83	0.0714	1012.7	0.0073
ν35	1034.73	5.803	1049.26	7.739
ν36	1061.33	4.2282	1061.32	13.9979
ν37	1073.99	0.6947	1070.07	6.3525
ν38	1092.93	0.1592	1078.39	0.5613
ν39	1104.21	1.0208	1100.01	33.5203
ν40	1114.24	5.9442	1113.77	5.4187
ν41	1190.72	0.038	1121.4	5.2356
ν42	1213.22	0.1791	1180.76	0.3431
ν43	1231.49	3.1653	1200.58	1.5036
ν44	1277.31	1.5063	1305.22	0.9254
ν45	1300.9	4.885	1305.78	1.4026
ν46	1317.25	0.2211	1323.93	32.9431
ν47	1342.9	29.5532	1355.51	0.0802
ν48	1362.26	0.3385	1370.82	0.3292
ν49	1417.36	11.5105	1421.05	15.397
ν50	1453.74	0.8252	1457.97	1.9131
ν51	1459	0.5732	1472.91	3.9301
ν52	1481.82	6.9359	1476.67	1.775
ν53	1493.17	5.3555	1490.62	7.6035
ν54	1501.2	13.1862	1506.29	10.4794
ν55	1547.33	26.5024	1512.52	38.9925

ν56	1648	1.7325	1597.45	3.69
ν57	1680.11	10.2169	1620.84	12.8124
ν58	1742.03	27.4086	1730.76	36.0928
ν59	2375.71	1.5506	1981.37	28.0237
ν60	3015.28	10.9456	3047.06	18.3797
ν61	3045.97	15.311	3105.86	11.7356
ν62	3106.79	12.1492	3137.06	16.3092
ν63	3141.66	20.6749	3145.32	19.4252
ν64	3152.05	9.2496	3154.81	6.0895
ν65	3166.51	13.2735	3163.29	8.5489
ν66	3192.36	0.8666	3190.13	4.9655
ν67	3201.13	3.007	3196.03	3.7185
ν68	3211.09	13.8539	3210.15	7.1507
ν69	3218.23	18.1017	3214.71	22.0997
ν70	3223.91	8.3797	3222.52	13.2855
ν71	3236.47	12.8297	3225.35	4.0905
ν72	3285.57	5.3822	3240.31	13.2831
	i32		**i33**	
ν1	12.23	0.0035	27.63	0.4253
ν2	50.17	0.5174	51.33	0.1923
ν3	60.35	0.9334	65	0.2766
ν4	96.77	0.2781	107.8	0.5994
ν5	141.39	0.5853	149.3	0.1347
ν6	155.06	0.8209	181.27	0.0803
ν7	164.45	0.2435	252.92	0.1144
ν8	234.38	0.4615	262.26	0.9323
ν9	267.38	0.0594	289.08	0.4177
ν10	311.68	2.3146	364.51	1.4419
ν11	338.96	0.2237	375.07	0.351
ν12	358.07	0.1426	414.01	1.7728
ν13	391.09	0.706	417.67	3.124
ν14	417.49	0.0001	445.46	3.7314
ν15	457.71	4.7873	486.27	9.6315
ν16	487.7	4.465	513.75	1.2088
ν17	545.03	3.3232	553.26	0.082
ν18	561.52	30.258	635.55	0.0196
ν19	593.08	31.3978	648.19	0.9618
ν20	617.07	3.7523	696.19	32.4566
ν21	644.69	0.176	708.17	3.7085
ν22	667.76	1.234	740.94	3.5086
ν23	711.05	14.8032	765.61	44.0977
ν24	720.57	33.6786	812.03	29.2453
ν25	792.02	39.2033	843.69	0.051

ν26	815.75	0.0467	909.85	17.9238
ν27	876.19	0.0031	912.98	5.2905
ν28	914.51	0.5285	937.62	15.6684
ν29	959.34	3.3017	951.72	37.6309
ν30	968.52	0.2482	979.69	2.9394
ν31	978.21	1.137	992.11	17.0591
ν32	980.34	37.3929	999.48	0.0404
ν33	1013.43	0.0035	1011.13	0.9377
ν34	1027.96	0.1026	1012.85	0.013
ν35	1032.59	0.0661	1041.25	18.9746
ν36	1043.14	11.6974	1049.7	7.8438
ν37	1062.17	4.4875	1062.25	36.921
ν38	1065.07	8.8121	1070.47	10.2191
ν39	1114.17	5.7722	1104.77	12.7218
ν40	1175.16	2.613	1113.25	5.413
ν41	1190.15	0.0424	1179.77	0.3109
ν42	1202.7	3.4692	1189.57	14.2668
ν43	1213.38	0.364	1222.05	5.9984
ν44	1228.43	2.448	1305.3	0.755
ν45	1306.07	7.5171	1313.65	1.7881
ν46	1316.94	0.2381	1330.9	6.3034
ν47	1343.25	7.2233	1355.19	0.0428
ν48	1361.76	0.3601	1364.68	2.6664
ν49	1409.84	6.124	1421.69	5.9153
ν50	1445.72	6.5634	1458.91	3.6075
ν51	1456.96	0.6825	1468.95	4.178
ν52	1492.92	5.0773	1476.69	1.7525
ν53	1497.64	4.8415	1495.27	3.8141
ν54	1503.87	5.1353	1510.47	28.2633
ν55	1546.38	25.681	1515.12	17.5275
ν56	1647.51	1.8658	1597.86	3.7477
ν57	1679.42	10.3711	1621.14	14.0424
ν58	1730.87	13.3647	1722.83	41.9627
ν59	2356.98	0.2889	1978.75	29.1138
ν60	3053.11	25.6041	3047.37	34.6308
ν61	3132.52	22.0984	3118.32	19.1892
ν62	3144.83	14.5868	3127.82	14.3016
ν63	3152.95	8.1152	3135.3	17.6614
ν64	3156.66	13.9848	3154.62	9.1231
ν65	3167.87	12.4577	3168.25	4.2227
ν66	3192.25	1.1558	3190.34	4.7082
ν67	3200.64	2.8664	3196.47	4.2446
ν68	3210.84	13.0879	3210.6	7.6583

ν69	3217.68	18.3247	3215.32	21.4896
ν70	3223.65	9.1521	3217.04	4.472
ν71	3248.68	9.3546	3222.6	13.0171
ν72	3273.98	6.3773	3250.04	10.2276
	tsi30i31		**tsi32i33**	
ν1	-668.21	42.21	-649.85	41.735
ν2	31	0.0339	39.45	0.01
ν3	40.91	0.0579	46.12	0.4623
ν4	45.34	0.3128	54.99	0.7082
ν5	69.61	1.1447	101.48	0.3367
ν6	133.06	0.6122	157.53	0.0379
ν7	178.05	0.2206	194.92	0.4404
ν8	212.93	0.0271	253.97	0.6168
ν9	272.33	0.1407	284.67	0.037
ν10	323.72	2.5314	301.84	0.4458
ν11	347.39	0.6724	352.62	1.5555
ν12	359.19	1.8523	363.01	0.0926
ν13	416.19	0.0085	411.67	1.5536
ν14	440.55	2.4683	417.49	0.3805
ν15	478.74	4.3216	437.94	1.1634
ν16	518.8	4.2082	511.91	5.6245
ν17	541.01	1.5907	524.66	5.3308
ν18	556	4.2948	537	1.2214
ν19	627.05	1.7513	625.82	2.2424
ν20	642.71	0.2004	639.64	3.3463
ν21	658.4	20.2747	648.57	5.0035
ν22	712.78	29.596	677.64	13.3612
ν23	716.54	3.9811	713.09	31.8562
ν24	776.02	4.1534	737.32	6.9236
ν25	779.24	43.0478	779.44	45.8761
ν26	785.71	0.6118	790.13	1.6127
ν27	863.61	0.0075	864.4	0.0026
ν28	937.81	2.8966	923.08	0.5125
ν29	946.54	1.6951	938.89	3.1788
ν30	949.96	43.396	959.32	14.437
ν31	980.45	2.4431	971.16	33.1983
ν32	1005.66	0.0038	993.31	2.414
ν33	1014.52	0.7904	1006.36	0.0012
ν34	1019.54	2.9055	1019.56	1.767
ν35	1023.45	0.0565	1023.7	0.0375
ν36	1060.05	3.8462	1047.4	10.3792
ν37	1067.73	11.1777	1059.57	7.5457
ν38	1082.48	1.5108	1070.24	16.9166

ν39	1114.19	5.9115	1114.24	5.8162
ν40	1130.54	14.3287	1141.32	6.8505
ν41	1186.69	0.0899	1187.07	0.0718
ν42	1206.48	1.8012	1206.69	5.2054
ν43	1214.06	1.6727	1226.76	2.7919
ν44	1295	9.0213	1284.08	0.5785
ν45	1312.07	0.1798	1312.49	0.0978
ν46	1316.17	23.9258	1323.58	23.7213
ν47	1357.94	11.9223	1360.39	0.5716
ν48	1360.26	0.6861	1361.53	7.6278
ν49	1421.86	10.5976	1415.2	6.7814
ν50	1448.18	1.8699	1450.49	5.7219
ν51	1465.49	1.6296	1459.52	4.6405
ν52	1488.17	3.5463	1488.49	3.3508
ν53	1489.97	12.1485	1502.15	4.5666
ν54	1504.67	19.3394	1511.42	4.8081
ν55	1534.76	51.811	1535.49	50.4257
ν56	1628.47	2.8797	1629.29	2.8993
ν57	1655.1	39.9059	1655.97	39.5407
ν58	1745.18	24.7769	1736.62	17.9722
ν59	2108.78	7.6195	2109.75	8.9218
ν60	3049.01	16.3553	3057.45	25.4459
ν61	3108.52	10.652	3137.07	13.0656
ν62	3115.48	8.2976	3143.52	17.3817
ν63	3145.08	21.4124	3159.77	8.3195
ν64	3154.59	9.8489	3172.49	5.6088
ν65	3189.68	6.247	3179.32	6.6043
ν66	3190.87	3.883	3190.85	4.2197
ν67	3197.71	2.9507	3197.98	3.2986
ν68	3210.02	9.6642	3210.25	10.0494
ν69	3215.38	21.7951	3215.76	21.2885
ν70	3222.72	12.976	3222.69	12.7735
ν71	3239.36	12.8255	3250.28	8.8876
ν72	3309.78	1.6254	3301.7	2.0716
	tsi5i31		**tsi9i33**	
ν1	-676.72	7.3676	-649.14	7.5489
ν2	34.04	0.3496	35.18	0.4386
ν3	42.9	0.0796	43.4	0.0109
ν4	53.19	0.3617	60.17	0.6045
ν5	96.97	1.1162	111.58	1.025
ν6	119.4	1.3511	138.52	0.4992
ν7	197.27	0.0606	188.85	0.4334
ν8	225.15	0.6273	193.41	0.0881

ν9	271.89	1.3332	273.07	0.9772
ν10	323.07	2.877	294.51	2.6997
ν11	369.88	4.9259	348.35	3.646
ν12	402.4	7.8618	394.7	2.7215
ν13	415.89	0.0083	399.83	1.013
ν14	430.91	6.3062	416.11	0.0175
ν15	507.12	8.3061	429.34	8.7867
ν16	515.87	0.843	507.91	9.5349
ν17	529.8	5.1897	523.09	1.1044
ν18	555.73	1.0851	552.83	0.0161
ν19	639.45	0.0025	639.49	0.0024
ν20	692.11	5.262	680.74	12.6975
ν21	708.09	10.3521	708.65	29.9756
ν22	709.4	22.0456	714.34	1.5036
ν23	775.31	46.7168	746.71	0.8086
ν24	787.3	1.0218	774.99	46.4881
ν25	832.56	0.2175	858.63	0.0618
ν26	858.77	0.0541	909.56	45.0993
ν27	893.44	42.4449	930.09	3.1668
ν28	930.81	3.2433	941.5	1.1534
ν29	945.65	1.873	960.31	8.5924
ν30	976.65	1.3434	1003.74	0.1104
ν31	1003.47	0.0241	1005.04	9.0723
ν32	1007.84	3.8891	1015.13	1.0256
ν33	1016.96	3.3198	1019.79	0.0292
ν34	1020.11	0.0446	1022.35	12.2597
ν35	1038.67	0.6116	1049.11	5.9373
ν36	1058.47	4.4348	1056.14	0.8706
ν37	1072.12	0.5088	1062.25	4.3192
ν38	1107.24	1.7179	1085.81	21.461
ν39	1113.99	6.031	1113.93	5.8339
ν40	1146.07	9.5118	1165.82	3.3378
ν41	1182.71	7.8453	1184.64	0.1665
ν42	1184.77	0.1513	1204.47	9.0586
ν43	1206.13	4.3358	1253.81	15.1877
ν44	1310.98	0.5555	1310.52	0.4515
ν45	1319.01	5.2474	1326.34	17.2709
ν46	1323.01	49.5976	1347.09	1.5763
ν47	1359.05	0.0155	1351.5	23.2824
ν48	1387.61	5.8654	1358.91	0.0096
ν49	1421.75	18.0312	1423.16	5.3105
ν50	1453.08	3.2358	1456.33	11.2555
ν51	1476.48	5.2197	1475.07	2.5624

ν52	1485.92	2.9263	1485.49	2.8948
ν53	1491.69	5.7809	1488.02	5.3095
ν54	1507.77	7.8855	1508.69	8.7374
ν55	1530.32	51.1655	1529.37	52.9673
ν56	1620.92	3.1543	1619.59	3.2457
ν57	1641.12	48.2181	1640.8	73.072
ν58	1654.03	16.7073	1658.44	24.0051
ν59	2067.92	0.6744	2064.94	0.9784
ν60	3044.74	20.0834	3033.78	42.575
ν61	3103.32	12.01	3101.04	23.0779
ν62	3111.34	23.7786	3103.21	13.9357
ν63	3144.89	16.293	3134.4	12.702
ν64	3158.31	5.3948	3153.65	11.9606
ν65	3182.32	1.8416	3168.78	2.4266
ν66	3190.45	5.0195	3177.73	5.0669
ν67	3197.37	3.3164	3190.43	5.2481
ν68	3208.99	5.2148	3197.29	3.6223
ν69	3209.84	9.5032	3210.11	9.567
ν70	3215.3	22.5422	3215.47	21.8465
ν71	3222.36	13.0623	3222.54	13.2571
ν72	3247.31	11.0425	3254.81	9.6958

(c)

	phenylethynyl		1,3-pentadiene	
Normal modes	Frequency (cm^{-1})	IR Inten	Frequency (cm^{-1})	IR Inten
ν1	112.68	17.3904	131.97	1.0585
ν2	148.66	4.6072	202.05	1.9123
ν3	251.55	26.3028	208.77	0.067
ν4	393.87	0	260.34	2.3828
ν5	477.42	3.1292	462.55	0.5076
ν6	490.16	18.9612	489.42	0.0238
ν7	511.05	0.7921	656.74	2.8089
ν8	632.48	0.1684	864.23	6.4716
ν9	696.07	46.3153	917.57	6.6942
ν10	787.71	0.2095	953.24	36.4845
ν11	799.2	23.247	998.65	10.1544
ν12	870.13	0	1000.04	19.3425
ν13	981.96	0.8822	1057.7	39.1114
ν14	1019.66	4.5667	1076.83	0.9696
ν15	1024.97	0	1109.43	0.0176
ν16	1044.22	0.1747	1216.83	1.4656
ν17	1053.58	0.6553	1307.85	1.4309
ν18	1116.24	5.0608	1334.64	0.4029
ν19	1185.47	81.7314	1351.17	2.7386
ν20	1191.6	3.3766	1421.4	3.0959
ν21	1230.32	21.1034	1461.6	6.4638
ν22	1324.35	7.2501	1484.93	7.3496
ν23	1358.66	7.8198	1498.3	9.3767
ν24	1483.47	12.0342	1700.6	7.1524
ν25	1514.79	1.8218	1763.17	19.7671
ν26	1614.98	0.511	3039.34	32.2637
ν27	1639.86	92.1565	3095.39	17.3961
ν28	2020.99	45.6399	3125.97	7.8623
ν29	3200.68	0.3554	3145.31	1.3733
ν30	3213.21	3.2854	3149.89	6.6579
ν31	3219.82	5.1552	3153.34	40.6994
ν32	3230.21	3.8096	3161.89	12.0446
ν33	3233.27	5.2791	3246.23	12.3311
	i13		**i14**	

ν1	11.89	0.004	17.95	0.0176
ν2	32.28	0.2216	23.79	0.1489
ν3	60.42	0.137	70.17	0.3412
ν4	102.43	1.1776	84.11	0.9855
ν5	109.87	1.0408	118.86	0.5055
ν6	128.34	3.2216	163.88	1.5658
ν7	193.18	0.1349	179.27	0.2199
ν8	202.78	2.4097	205.43	0.0318
ν9	236.6	0.0126	241.03	1.0563
ν10	275.01	2.7282	288.54	0.136
ν11	335.26	1.6687	376.58	7.6596
ν12	396.69	0.1861	412.28	0.1573
ν13	417.78	0.0046	462.76	2.6721
ν14	420.98	0.5386	476.18	0.435
ν15	473.38	0.4944	488.6	5.9686
ν16	547.34	0.8294	513.01	1.2309
ν17	558.41	6.4762	533.96	3.9029
ν18	642.67	0.4525	631.54	0.3841
ν19	655.29	3.9731	692.89	32.7513
ν20	719.98	0.8303	718.93	18.8691
ν21	720.99	34.6378	733.75	11.9092
ν22	743.44	2.954	763.98	42.7519
ν23	762.71	17.4388	795.56	15.3155
ν24	792.44	39.7608	840.3	0.4893
ν25	877.11	0.011	854.18	11.0643
ν26	925.43	1.4905	880.04	2.632
ν27	930.3	5.0788	909.48	4.3101
ν28	946.66	17.6273	940.83	14.6203
ν29	959.92	3.7214	960.9	17.3728
ν30	997.79	25.3548	996.01	1.7587
ν31	1014	0.0099	998.58	13.0422
ν32	1028.2	0.0094	1000.65	2.1987
ν33	1032.72	0.11	1012.7	0.0028
ν34	1035.39	3.1415	1034.48	14.8601
ν35	1037.74	6.1953	1046.82	5.2156
ν36	1067.36	2.7123	1076.56	0.7359
ν37	1113.96	5.4961	1101.02	0.7548
ν38	1132.32	2.2698	1112.86	4.8467
ν39	1190.7	0.0332	1149.12	5.961

ν40	1203.88	0.9998	1174.15	3.7967
ν41	1212.99	0.1648	1178.64	0.3341
ν42	1225.54	0.7149	1216.88	2.1463
ν43	1278.71	3.3622	1271.73	2.5588
ν44	1292.79	0.0107	1301.4	0.6396
ν45	1313.99	6.0969	1328.74	2.1928
ν46	1316.97	0.2266	1352.61	1.5371
ν47	1361.59	0.372	1354.36	0.2345
ν48	1365.51	14.4298	1369.09	1.1505
ν49	1417.88	1.069	1420.9	4.9713
ν50	1456.07	2.8655	1452.66	5.7263
ν51	1467.96	23.1992	1471.95	1.4951
ν52	1480.03	5.7055	1484.73	5.435
ν53	1492.76	5.0145	1497.38	17.797
ν54	1510.68	21.6936	1502.47	16.4498
ν55	1542.26	21.8471	1590.93	3.8268
ν56	1547.24	25.0483	1614.53	5.4484
ν57	1647.96	1.6413	1686.34	3.4519
ν58	1679.95	9.394	1745.37	27.1257
ν59	2378.78	2.6899	1884.47	3.3959
ν60	3016.18	27.0263	3037.99	29.4583
ν61	3023.08	35.591	3075.3	23.876
ν62	3037.12	6.067	3093.99	15.3908
ν63	3070.4	19.2238	3126.26	3.8417
ν64	3120.82	12.529	3147.93	29.4864
ν65	3151.08	0.7692	3155.45	3.8367
ν66	3160.71	16.1623	3186.78	37.9125
ν67	3171.99	42.934	3191.42	1.9574
ν68	3191.85	0.7784	3195.25	13.4293
ν69	3200.73	2.9553	3197.27	5.1486
ν70	3210.62	14.0329	3211.49	7.6214
ν71	3217.89	18.3872	3216.6	17.0556
ν72	3223.57	7.8065	3223.77	11.5995
	i15		**i16**	
ν1	35.42	0.116	47.87	0.1579
ν2	77.71	0.0765	70.53	0.0062
ν3	103.85	1.7464	101.66	0.7383
ν4	144.42	1.3984	146.93	0.3881

ν5	228.79	0.0436	229.54	0.0333
ν6	244.82	0.5453	252.16	0.3015
ν7	257.69	0.117	276.56	0.1162
ν8	294.18	3.3062	321.66	0.1096
ν9	325.67	0.1235	404.32	0.7081
ν10	417.75	1.4447	419.84	0.1757
ν11	420.09	0.1642	422.05	0.4109
ν12	472.96	3.678	482.66	7.2254
ν13	495.12	0.3717	548.49	1.406
ν14	561.24	1.357	574.9	1.268
ν15	598.31	3.733	609.74	1.3745
ν16	638.04	6.2775	639.7	0.1126
ν17	642.26	6.1028	663	1.6185
ν18	714.92	11.2938	705.36	56.3021
ν19	722.33	36.3166	721.68	45.9147
ν20	740.24	14.3041	734.33	7.7148
ν21	796.78	34.6185	791.51	20.0788
ν22	827.53	2.6962	808.05	8.8016
ν23	873.13	0.2736	839.96	1.2521
ν24	911.5	0.2418	870.45	0.2052
ν25	942.96	6.1643	943.95	4.4127
ν26	952.27	1.5542	950.77	2.8199
ν27	968.82	8.882	961.97	1.7601
ν28	989.08	2.6318	996.03	1.6555
ν29	1009.43	0.0275	1002.5	3.4585
ν30	1016.17	1.7459	1009.93	0.1126
ν31	1023.01	0.8266	1024.07	0.4695
ν32	1027.78	0.1221	1026.18	0.7758
ν33	1029.44	0.0508	1031.27	1.2029
ν34	1068.18	4.768	1042.46	2.8657
ν35	1074.42	0.8949	1067.1	3.7879
ν36	1096.42	2.0998	1071.21	2.49
ν37	1116.31	6.2236	1110.21	4.6187
ν38	1154.35	4.6731	1123.19	5.8329
ν39	1188.94	0.063	1136.61	4.0186
ν40	1209.01	0.844	1190.66	0.0791
ν41	1210.38	1.2568	1201.18	0.5395
ν42	1224.27	0.2245	1223.34	0.271
ν43	1280.4	0.4506	1283.71	2.9018

ν44	1317.32	2.9607	1287.44	0.3104
ν45	1323.67	0.4622	1298.3	5.4886
ν46	1340.63	0.6741	1322.51	2.5993
ν47	1357.83	0.4229	1346.83	0.4883
ν48	1375.69	0.5509	1369.7	0.7467
ν49	1408.32	3.9103	1404.06	4.4636
ν50	1421.59	6.378	1427.35	2.4689
ν51	1476.15	4.6572	1440.89	4.4717
ν52	1493.92	3.4176	1493.36	2.9026
ν53	1500.14	7.5425	1499.44	6.4475
ν54	1506.83	3.0852	1506.51	4.9652
ν55	1547.58	18.3471	1540.74	17.0515
ν56	1652.02	2.3871	1552.75	5.0863
ν57	1679.71	11.1669	1633.15	4.5376
ν58	1741.66	15.8358	1647.41	1.6939
ν59	1769.78	0.893	1672.31	12.53
ν60	3024.57	15.7135	2977.9	17.6209
ν61	3030.76	38.3797	3050.53	28.3262
ν62	3049.34	26.5584	3128.46	19.5662
ν63	3054.69	9.5323	3138.52	16.0644
ν64	3123.25	22.6504	3177.25	5.6953
ν65	3137.2	21.8342	3187.19	7.9993
ν66	3159.76	7.933	3188.97	0.3955
ν67	3186.01	35.5415	3195.07	2.0742
ν68	3187.07	1.7227	3199.05	31.1612
ν69	3193.79	0.9004	3206.03	7.0568
ν70	3203.37	11.1183	3211.6	24.4919
ν71	3210.94	27.8004	3220.2	23.4508
ν72	3219.57	13.4782	3221.39	11.1643
	i17		**i18**	
ν1	14.57	0.012	22.52	0.2837
ν2	40.91	0.4063	28.93	0.1258
ν3	66.1	1.121	67.99	0.2814
ν4	74.4	0.5027	98.8	0.7079
ν5	127.77	0.521	150.16	0.5668
ν6	158.41	0.4675	162.69	0.5993
ν7	189.77	0.0634	181.59	0.0721
ν8	232.2	0.1216	210.87	0.7547

ν9	274.62	0.2084	240.62	0.8825
ν10	306.97	0.1743	305.49	0.4039
ν11	369.3	0.8058	312.43	1.481
ν12	417.77	0.081	412.05	0.2199
ν13	418.28	0.3596	446.87	5.8199
ν14	457.23	2.0804	475.3	2.2182
ν15	499.93	4.8499	482.55	6.0006
ν16	551.74	2.9391	526.37	3.3517
ν17	558.88	7.5894	537.58	1.7564
ν18	587.91	0.128	605.64	2.9179
ν19	644.31	0.0607	631.82	0.2328
ν20	664.52	3.8656	683.93	13.5881
ν21	712.04	2.7495	692.78	33.6358
ν22	721.2	33.7664	763.66	44.6819
ν23	773.56	1.2881	784.92	6.3452
ν24	792.63	40.1747	835.05	3.6976
ν25	816.19	48.4488	847.27	4.3385
ν26	861.97	1.5496	879.19	8.3725
ν27	877.48	0.0061	909.8	3.2996
ν28	943.94	1.1992	913.59	0.2894
ν29	960.36	3.5179	957.75	43.7323
ν30	1014.36	0.5381	970.05	3.5523
ν31	1017.22	20.8629	993.94	1.95
ν32	1023.28	5.9288	1000.15	0.0393
ν33	1028.22	0.8571	1012.79	0.0027
ν34	1033.18	0.0445	1041.16	10.1501
ν35	1036.9	5.37	1046.39	5.7696
ν36	1064.96	3.8669	1054.96	6.8357
ν37	1078.96	0.6448	1074.98	9.582
ν38	1114.47	5.8037	1112.82	5.1864
ν39	1148.04	0.2369	1131.05	0.6429
ν40	1191.08	0.0292	1156.48	10.7387
ν41	1201.93	0.8697	1178.11	0.3207
ν42	1213.47	0.1569	1216.11	1.4475
ν43	1282.09	2.1473	1233.43	7.0766
ν44	1297.56	0.491	1301.7	0.5977
ν45	1306.75	2.4587	1322.07	1.4863
ν46	1317.41	0.2341	1341.54	5.5537
ν47	1329.69	10.0069	1353.56	0.11

ν48	1362.4	0.3307	1389.76	4.5779
ν49	1376.86	24.7591	1422.06	5.5505
ν50	1412.65	3.1048	1461.99	11.9975
ν51	1493.18	5.0911	1471.56	1.3462
ν52	1497.64	5.7317	1484.97	7.8511
ν53	1504.46	7.6395	1499.9	10.4602
ν54	1510.61	19.4811	1502.71	13.2541
ν55	1527.65	6.7033	1590.87	3.9675
ν56	1547.57	26.4331	1614.47	4.0021
ν57	1648.05	1.7194	1684.53	3.8576
ν58	1680.26	9.7986	1737.08	12.7798
ν59	2374.25	1.5036	1893.32	8.7524
ν60	3007.27	12.1988	3037.72	31.9151
ν61	3054.8	30.8819	3060.65	31.2991
ν62	3135.08	26.0093	3093.9	16.1385
ν63	3142.4	20.2361	3139.99	14.5804
ν64	3156.48	3.7077	3151.48	3.9392
ν65	3161.81	30.6208	3153.78	26.0564
ν66	3170.21	7.1657	3191.38	2.9679
ν67	3192.15	0.8474	3195.53	4.2283
ν68	3200.86	2.8635	3197.25	4.7127
ν69	3210.78	13.5003	3210.38	7.8559
ν70	3217.89	18.1116	3215.86	17.1744
ν71	3223.67	8.283	3223.51	12.2814
ν72	3259.51	8.5005	3246.35	11.3427
	i19		**i20**	
ν1	26.55	0.0039	33.16	0.0876
ν2	77.06	0.7261	75.32	0.5738
ν3	108.01	2.0294	89.39	0.0554
ν4	133.52	0.6239	144.88	0.5987
ν5	190.02	0.2032	152.59	1.5615
ν6	238.97	0.0423	218.65	0.2097
ν7	280.66	0.0136	296.94	0.2051
ν8	308.54	0.152	312.97	0.1388
ν9	362.16	2.8686	342.29	0.3237
ν10	416.99	1.5877	415.08	1.6763
ν11	418.72	1.0389	418.59	0.0682
ν12	468.69	0.6609	458.02	2.317

ν13	497.51	2.4159	510.01	0.7265
ν14	569.37	4.2605	551.67	0.845
ν15	583.05	2.4319	564.62	18.6675
ν16	604.35	4.532	622.39	2.478
ν17	639.8	0.1191	638.4	0.3512
ν18	711.99	15.1891	700.85	4.7451
ν19	720.01	34.8368	714.63	40.4626
ν20	749.51	32.5543	746.23	26.4921
ν21	791.05	24.9221	788.05	28.1557
ν22	847.23	2.2152	850.42	0.6923
ν23	871.61	0.038	861.58	0.1014
ν24	906.67	1.007	918.95	9.8362
ν25	943.44	0.9647	930.74	0.9882
ν26	944.51	1.7748	934.52	0.2199
ν27	971.13	6.6728	957.65	4.7375
ν28	978.79	6.0555	987.46	25.2307
ν29	1009.84	0.0491	997.43	0.907
ν30	1021.36	0.7835	1003.18	10.3087
ν31	1027.81	0.104	1005.85	2.5822
ν32	1028.64	0.0643	1020.75	0.8797
ν33	1039.72	0.9037	1024.38	0.0791
ν34	1067.31	1.391	1044.8	4.4367
ν35	1068.27	4.4748	1047.74	3.7892
ν36	1098.7	4.3088	1072.52	4.8578
ν37	1117.52	6.3884	1129.81	5.0431
ν38	1151.15	1.5215	1191.64	0.4141
ν39	1189.49	0.0778	1195.7	3.8663
ν40	1207.73	0.7352	1219.78	0.1082
ν41	1217.27	0.3078	1222.07	0.1058
ν42	1233.15	0.8396	1231.7	15.2754
ν43	1280.61	0.2986	1254.24	14.5568
ν44	1314.61	0.5528	1305.35	1.5597
ν45	1327.86	1.3639	1330.27	0.5556
ν46	1344.83	5.7402	1361.14	2.93
ν47	1359.83	0.1593	1384.1	2.0848
ν48	1378.06	2.0114	1420.68	0.3915
ν49	1407.49	3.1408	1433.32	2.8966
ν50	1421.52	2.2925	1443.85	3.6559
ν51	1481.49	4.4989	1461.07	13.7946

ν52	1495.7	7.0779	1484.82	6.0239
ν53	1499.57	6.4927	1493.07	9.8462
ν54	1505.13	3.6364	1499.41	11.26
ν55	1547.47	21.0221	1526.79	2.8327
ν56	1652.6	3.2074	1553.83	23.2059
ν57	1680.36	12.7555	1644.78	5.7078
ν58	1740.47	15.4195	1658.74	6.29
ν59	1768.56	0.7755	1672.67	21.98
ν60	3018.25	17.4019	2953.3	25.7761
ν61	3022.43	33.0603	2993.09	20.6421
ν62	3048.76	8.9065	3030.99	44.7869
ν63	3050.46	38.8564	3083.37	18.1156
ν64	3128.09	26.1109	3129.2	15.6203
ν65	3135.95	21.1306	3173.35	13.2795
ν66	3159.26	9.4418	3187.02	12.769
ν67	3185.11	5.2668	3189.59	4.0016
ν68	3185.59	30.5008	3197.17	4.296
ν69	3192.28	0.4645	3198.92	24.6483
ν70	3202.25	12.6658	3212.68	20.6094
ν71	3212.04	25.6926	3220.49	24.1813
ν72	3219.99	13.2721	3224.67	5.0583
	i26		**i27**	
ν1	24.65	0.6411	46.45	0.1183
ν2	34.55	0.0794	86.62	0.2136
ν3	65.04	0.1902	121.92	0.0331
ν4	101.09	1.0485	165.73	1.105
ν5	171.04	0.3653	212.68	0.1756
ν6	236.97	0.4162	241.02	0.2964
ν7	247.84	0.0932	268.31	1.0211
ν8	268.82	1.1423	299.17	0.2626
ν9	305.89	0.4298	327.66	0.5102
ν10	411.68	6.9918	376.23	0.5957
ν11	415.44	0.33	423.71	0.1166
ν12	453.01	5.5039	511.76	9.2905
ν13	499.16	4.267	550.51	0.1856
ν14	516.29	3.5893	607.67	10.4339
ν15	586.57	1.4773	631.16	1.4054
ν16	626.95	3.1849	638.81	4.1108

ν17	638.25	1.0308	701.04	15.2848
ν18	695.14	33.4808	718.14	38.6198
ν19	715.68	22.3692	728.24	33.9753
ν20	756.59	17.32	769.13	22.4219
ν21	766.95	44.0971	786.1	4.284
ν22	786.93	0.224	803.39	4.9064
ν23	843.65	0.0557	823.15	7.8663
ν24	865.08	1.9392	859.13	14.4663
ν25	909.98	13.6872	870.69	6.9918
ν26	912.98	3.7702	881.37	2.4143
ν27	962.74	4.3496	936.65	2.2792
ν28	974.01	6.5014	949.45	6.7451
ν29	996.94	1.0182	970.52	1.3723
ν30	999.98	0.225	1005.3	0.3851
ν31	1000.52	0.2852	1007.89	0.0197
ν32	1012.98	0.0114	1024.15	0.2413
ν33	1017.79	0.4256	1027.79	1.0781
ν34	1047.91	4.7002	1039.71	2.0683
ν35	1087	5.2711	1064.97	4.5296
ν36	1111.78	5.6683	1087.76	5.9441
ν37	1115.27	1.2939	1107.54	0.849
ν38	1132.18	3.4546	1128.11	12.1892
ν39	1149.67	1.7868	1130.35	4.3518
ν40	1178.3	0.2584	1187.52	0.7049
ν41	1181.44	0.7002	1200.09	2.0172
ν42	1188.53	0.8829	1220.43	0.238
ν43	1251.23	0.1061	1239.99	1.1128
ν44	1291.26	5.5563	1276.48	1.6694
ν45	1302.53	0.5032	1296.63	1.0297
ν46	1325.92	7.5366	1324.68	0.1078
ν47	1340.36	1.9591	1349.62	2.3768
ν48	1353.02	0.0332	1363.17	0.2208
ν49	1384.54	2.3187	1391.95	2.0559
ν50	1414.86	4.3778	1408.42	2.443
ν51	1474.02	1.6468	1430.04	3.8338
ν52	1480.53	5.0858	1479.37	3.8649
ν53	1500.54	14.2998	1502.82	2.7058
ν54	1501.96	6.5334	1508.04	2.8563
ν55	1504.78	12.0528	1531.02	4.8546

ν56	1594.01	3.8482	1542.46	22.5242
ν57	1617.52	7.3298	1565.81	1.7008
ν58	1718.15	18.6494	1640.49	1.3812
ν59	1918.27	0.0554	1664.62	12.997
ν60	3030.37	17.0259	3052.48	6.6306
ν61	3045.06	28.9324	3055.81	30.6688
ν62	3050.02	25.088	3128.89	19.2345
ν63	3083.71	11.0229	3145.32	9.9742
ν64	3120.87	30.0935	3152.95	12.6318
ν65	3127.69	20.8852	3183.65	6.8718
ν66	3189.5	4.1429	3192.81	0.1747
ν67	3195.34	3.9626	3203.35	22.2343
ν68	3195.62	6.0901	3215.29	5.6983
ν69	3209.51	7.1522	3217.72	25.075
ν70	3213.87	22.3578	3225.93	13.2039
ν71	3221.82	22.1063	3239.28	5.8454
ν72	3222.37	20.7057	3242.78	13.7776
	tsi13i14		**tsi13i15**	
ν1	-1890.96	585.3859	-655.03	43.51
ν2	29.22	0.0786	32.77	0.0087
ν3	34.47	0.0681	54.98	0.2745
ν4	60.19	1.1718	70.85	0.6357
ν5	103.45	0.6896	111.34	1.5778
ν6	119.31	0.4519	153.22	0.2617
ν7	168.13	4.1051	228.57	0.3188
ν8	197.01	1.7978	238.57	3.3876
ν9	206.43	0.9378	288.06	4.8256
ν10	249.28	2.5796	303.66	0.1295
ν11	329.04	1.8274	338.02	0.2933
ν12	378.03	2.3763	418.27	0.0139
ν13	403.41	4.5832	443.38	3.6686
ν14	415.06	0.018	465.87	7.1038
ν15	478.5	4.0862	510.23	19.1622
ν16	485.21	4.0227	522.36	9.4623
ν17	520.53	13.4363	560.47	3.4938
ν18	552.39	3.4451	642.26	0.2718
ν19	639.85	0.2818	692.06	28.0952
ν20	677.5	11.5815	717.03	9.4321

ν21	692.69	18.4493	722.23	31.885
ν22	712.31	32.7852	766.05	10.419
ν23	748.44	10.1629	781.84	36.9928
ν24	776.43	46.6362	828.2	1.4188
ν25	789.79	4.4382	875.86	0.04
ν26	839.84	15.8911	894.62	3.5457
ν27	861.42	0.013	926.22	0.9411
ν28	933.44	3.2683	956.08	3.6299
ν29	944.39	16.6073	965.51	3.7306
ν30	975.56	9.436	978.54	2.1875
ν31	992.92	46.1873	1009.67	2.3326
ν32	1004.13	0.1089	1012.66	0.0203
ν33	1016.84	2.1898	1026.05	18.9174
ν34	1021.4	9.9311	1028.67	0.9514
ν35	1021.74	1.7695	1031.75	0.0503
ν36	1059.93	0.259	1065.7	4.5512
ν37	1060.27	3.4319	1112.55	6.5497
ν38	1104.47	2.77	1126.7	4.6378
ν39	1114.71	5.3652	1150.93	2.4918
ν40	1159.54	15.4592	1189.68	0.0215
ν41	1186.81	0.1833	1209.27	0.1179
ν42	1207.73	6.2605	1211.25	0.0452
ν43	1218.67	1.1755	1247.21	0.6634
ν44	1300.6	13.5268	1273.27	2.3554
ν45	1311.39	0.5445	1316.74	0.0662
ν46	1318.36	5.3526	1323.2	0.6904
ν47	1332.84	13.313	1346.86	1.2513
ν48	1361.27	0.0051	1359.93	0.3915
ν49	1418.25	15.3876	1412.96	2.5144
ν50	1428.72	1.4807	1436.14	10.8788
ν51	1482.27	6.2326	1470.86	5.0629
ν52	1487.23	8.5994	1488.74	5.3834
ν53	1489.26	1.6672	1492.6	10.8561
ν54	1509.15	47.8515	1495.19	4.8858
ν55	1537.53	34.6862	1542.96	21.484
ν56	1627.98	2.9549	1648.12	2.0845
ν57	1636.24	13.3432	1656.81	7.3978
ν58	1656.53	46.2729	1676.68	10.4946
ν59	1796.94	93.414	2070.83	2.9736

ν60	2158.76	42.9616	3016.92	32.4753
ν61	3031.78	49.5952	3030.74	24.9478
ν62	3083.73	18.4943	3088.53	14.8719
ν63	3122.46	6.8359	3090.74	14.5736
ν64	3146.73	10.4483	3131.13	14.056
ν65	3153.48	25.6111	3133	9.0324
ν66	3183.85	5.4766	3164	12.8798
ν67	3190.67	6.503	3190.89	1.4546
ν68	3197.48	2.6952	3192.91	19.3101
ν69	3199.99	10.574	3198.78	2.2836
ν70	3209.52	7.6273	3208.74	11.9992
ν71	3214.97	21.5747	3215.2	18.9702
ν72	3222.44	16.4974	3222.26	10.4735
	tsi13i26		**tsi13p8**	
ν1	-546.02	28.0609	-735.88	28.6121
ν2	32.48	0.0189	13.74	0.119
ν3	37.44	0.1052	31.19	0.2638
ν4	44.96	0.3119	72.74	1.3444
ν5	95	1.6553	104.68	0.699
ν6	123.54	0.2586	111.14	0.5468
ν7	152.31	1.1087	159.75	1.4796
ν8	206.33	0.0366	201.57	1.0043
ν9	259.07	0.5629	207.67	1.8176
ν10	294.35	2.4498	238.48	5.813
ν11	359.29	4.3026	308.71	4.4424
ν12	383.65	3.4803	325.13	14.6305
ν13	417.62	0.0151	355.74	2.6179
ν14	471.46	5.6606	399.94	1.738
ν15	498.62	0.7619	412.25	6.9066
ν16	538.11	2.0952	416.86	0.0389
ν17	563.37	0.6107	482.38	9.0361
ν18	634.23	15.7726	535.97	2.557
ν19	642.53	0.0155	549.29	0.8977
ν20	696.76	18.1203	585.87	7.2198
ν21	716.39	31.6706	641.68	0.0934
ν22	751.54	13.0202	680.96	4.8979
ν23	785.22	43.2935	718.9	34.1627
ν24	796.24	4.4423	761.87	0.519

ν25	870.09	0.0388	790.9	16.9126
ν26	900.3	1.9888	792.56	30.6979
ν27	921.48	4.9827	869.72	18.6341
ν28	947.21	3.727	875.17	0.8213
ν29	954.15	4.7271	946.74	21.605
ν30	992.91	2.0667	958.06	2.9176
ν31	1009.54	6.5305	983.56	12.4851
ν32	1009.89	0.2689	991.45	8.9027
ν33	1012.83	1.9435	1012.64	0.0852
ν34	1023.24	1.8369	1026.24	25.8769
ν35	1027.33	0.124	1027.27	0.0631
ν36	1062.46	3.6368	1032.3	0.272
ν37	1109.73	4.0741	1064.6	5.1767
ν38	1113.67	5.8693	1072.11	0.2501
ν39	1151.28	2.579	1106.64	0.8244
ν40	1188.51	0.0142	1114.41	5.5485
ν41	1193.85	1.5444	1165.13	0.2121
ν42	1208.56	1.9379	1190.3	0.0531
ν43	1212.41	2.3256	1212.74	0.105
ν44	1276.27	9.9743	1241.47	4.8725
ν45	1313.67	0.0133	1302.74	4.3848
ν46	1340.26	1.2696	1313.46	1.5886
ν47	1354.55	7.7798	1317.33	0.1751
ν48	1360.38	0.1237	1344.3	1.8909
ν49	1409.91	8.4195	1361.87	0.3565
ν50	1424.04	5.611	1420.07	5.372
ν51	1474.39	5.3704	1447.95	10.0706
ν52	1487.28	8.468	1483.19	7.1753
ν53	1489.94	6.5705	1492.53	6.2632
ν54	1492.96	4.6823	1495.03	23.8424
ν55	1538.23	38.767	1544.94	31.124
ν56	1635.24	2.5856	1590.2	14.0298
ν57	1663.56	34.6127	1646.17	1.5112
ν58	1706.57	14.3525	1678.98	12.2948
ν59	2163.97	43.3785	1706.2	38.5112
ν60	3011.55	39.7817	2344.69	1.0725
ν61	3031.87	21.3439	3039.42	31.7469
ν62	3075.33	11.7412	3095.44	14.1338
ν63	3084.54	12.357	3128.65	4.6363

ν64	3121.89	8.4475	3151.88	24.41
ν65	3131.74	28.7827	3166.8	5.1661
ν66	3154.83	17.2329	3178.29	7.8007
ν67	3190.6	3.0909	3192.63	1.5347
ν68	3198.32	3.3889	3198.58	11.848
ν69	3205.36	25.2245	3201.28	2.6389
ν70	3209.79	11.7941	3211.11	13.227
ν71	3215.92	19.884	3218.44	17.5677
ν72	3222.38	10.7608	3224.14	9.8706
	tsi14i16		**tsi14p8**	
ν1	-385.73	3.1887	-751.75	15.3737
ν2	38.5	0.0168	18.58	0.1662
ν3	69.16	0.3205	32.07	0.4083
ν4	75.76	0.109	70.78	2.5322
ν5	155.77	0.9643	86.69	2.1051
ν6	164.86	0.5749	106.54	0.3696
ν7	213.06	0.119	112.79	3.5975
ν8	227.08	2.9352	177.83	2.0223
ν9	297.71	2.7913	207.4	0.1066
ν10	310.38	1.7622	212.45	0.6653
ν11	359.65	1.4523	271.92	4.2191
ν12	417.27	0.0356	344.13	2.5026
ν13	448.5	1.5745	395.87	1.1196
ν14	491.35	9.4307	416.46	0.0806
ν15	515.66	6.7438	420.76	2.3267
ν16	531.43	0.429	462.85	13.8332
ν17	583.1	5.5261	488.4	23.2901
ν18	636.15	0.3185	527.14	0.5436
ν19	712.9	36.7531	561.89	1.9854
ν20	720.96	39.8159	586.37	2.3198
ν21	761.45	5.513	642	0.2336
ν22	773.12	9.9384	694.14	12.7797
ν23	781.13	26.4428	717.41	33.0843
ν24	864.09	0.0388	754.08	2.5554
ν25	878.65	8.9997	772.33	13.1739
ν26	889.12	6.7829	790.38	47.8589
ν27	924.18	2.241	865.32	11.628
ν28	935.91	0.3017	874.29	0.0835

ν29	958.64	26.8287	946.67	25.0189
ν30	982.41	5.1676	957.76	3.5856
ν31	998.94	0.8678	991.38	7.3685
ν32	1007.09	0.023	998.28	13.1241
ν33	1016.64	0.5881	1013.59	0.0041
ν34	1023.56	0.085	1026.57	0.074
ν35	1051.29	6.4702	1033.2	0.0315
ν36	1058.41	3.3266	1034.79	20.7301
ν37	1093.21	2.3947	1064.15	4.5074
ν38	1112.62	5.0045	1076.44	0.6261
ν39	1138.58	1.1234	1104.46	0.6464
ν40	1171.88	6.2374	1115.07	5.5134
ν41	1184.79	0.082	1165.49	0.3053
ν42	1213.54	0.1851	1190.76	0.0743
ν43	1236.34	1.3671	1212.59	0.2175
ν44	1299.78	1.102	1253.2	2.2839
ν45	1308.09	0.9069	1306.54	3.4147
ν46	1332.93	2.9976	1317.39	0.13
ν47	1342.94	1.9127	1318.83	2.4399
ν48	1357.25	0.1319	1347.73	2.3398
ν49	1422.17	3.0489	1362.14	0.437
ν50	1458.31	2.1787	1420.71	5.498
ν51	1483.25	5.6578	1444.54	2.8024
ν52	1486.24	5.21	1483.85	6.84
ν53	1499.08	9.2774	1491.83	5.8252
ν54	1520.11	26.0324	1496.22	19.2941
ν55	1573.63	7.7087	1543.91	26.9442
ν56	1619.87	2.8759	1642.88	1.8375
ν57	1641.37	15.9498	1668.61	12.2091
ν58	1650.16	5.4971	1677.32	0.772
ν59	1752.83	0.3892	1746.82	41.6368
ν60	3042.9	25.6236	2250.84	11.645
ν61	3093.38	16.3788	3039.83	30.6214
ν62	3105.39	8.8036	3096.07	14.7889
ν63	3129.31	11.2874	3128.68	3.9739
ν64	3147.64	9.9474	3150.3	27.1408
ν65	3168.33	13.5064	3167.97	0.7338
ν66	3172.74	12.5541	3175.3	12.18
ν67	3189.08	4.0692	3193.53	1.3764

ν68	3194.66	31.7351	3202.26	2.7276
ν69	3195.09	1.8511	3207.15	15.0795
ν70	3206.6	6.4323	3211.81	12.3918
ν71	3211.77	22.0074	3219.37	15.4508
ν72	3220.82	15.4016	3224.97	9.7585
	tsi15i16		**tsi16p7**	
ν1	-1704.88	55.8271	-911.82	1.3412
ν2	20.77	0.0765	52.01	0.0515
ν3	57.64	0.7563	85.62	0.706
ν4	116.34	1.2604	109.44	0.278
ν5	163.86	1.3389	146.3	0.3581
ν6	221.13	0.9533	187.14	1.5167
ν7	243.17	0.9495	277.44	0.2179
ν8	251.31	0.0758	298.15	0.2951
ν9	338.71	2.9828	332.34	0.4361
ν10	388.82	6.8326	404.95	2.0063
ν11	417.32	0.3029	422.18	0.3408
ν12	431.03	12.4359	437.78	0.3445
ν13	466.51	5.9474	475.18	5.562
ν14	509.54	5.8866	507.34	1.7751
ν15	555.9	19.0314	545.9	14.5866
ν16	605.59	3.5881	575.73	2.1209
ν17	638.57	0.8147	584.96	0.4234
ν18	659.28	20.9135	634.58	2.8548
ν19	712.82	18.8088	640.39	0.4723
ν20	729.9	5.9865	730.04	2.0765
ν21	731.1	63.415	731.56	40.7793
ν22	796.32	24.4709	765.99	11.6655
ν23	815.98	39.9999	772.6	54.8111
ν24	838.76	23.4339	806.08	13.0978
ν25	865.65	1.5432	828.6	0.3402
ν26	920.92	24.7696	882.69	0.0999
ν27	946.55	1.6986	901.86	0.1643
ν28	980.76	6.3937	960.98	2.2524
ν29	984.94	1.5663	986.24	0.7001
ν30	1008.93	0.6158	1013.7	0.6903
ν31	1011.72	1.9982	1017.09	0.1035
ν32	1022.5	0.8861	1019.76	0.2103

ν33	1025.07	9.6021	1029.06	0.2308
ν34	1028.68	0.0707	1032.94	0.9712
ν35	1067.22	3.9483	1034.6	7.9177
ν36	1090.16	5.1607	1065.64	5.7746
ν37	1107.13	1.1743	1073.02	1.4915
ν38	1116.99	7.0783	1084.29	4.0721
ν39	1168.96	7.6793	1115.13	5.819
ν40	1188.31	0.1748	1157.8	3.2946
ν41	1204.14	2.5647	1189.17	0.0199
ν42	1221.76	0.1749	1191.14	0.069
ν43	1235.58	22.0382	1215.68	0.6517
ν44	1293.08	0.3512	1228.42	1.7102
ν45	1314.51	2.2062	1295.02	1.7262
ν46	1325.74	1.3213	1303.36	0.5153
ν47	1343.38	9.953	1323.5	0.0142
ν48	1373.33	9.1302	1334.05	0.1621
ν49	1399.46	1.9445	1363.89	1.0961
ν50	1408.23	18.8112	1428.18	4.5787
ν51	1417.24	13.3944	1477.53	5.4378
ν52	1484.78	36.6072	1487.52	2.6554
ν53	1496.53	6.614	1501.66	9.6535
ν54	1500.81	11.5184	1504	8.2384
ν55	1506.76	13.5499	1526.08	35.2432
ν56	1541.13	16.1883	1552.65	2.659
ν57	1642.45	4.1218	1618.62	0.5328
ν58	1668.02	4.9888	1651.65	2.4174
ν59	1686.99	6.0665	1659.95	1.52
ν60	2116.78	22.3518	1681.47	5.0826
ν61	3044.17	33.3082	3056.63	19.3296
ν62	3065.12	9.8775	3128.2	12.9984
ν63	3120.91	22.2716	3170.45	11.3253
ν64	3133.39	16.3293	3183.89	2.5169
ν65	3163.88	8.585	3187.5	4.7677
ν66	3172.56	10.6194	3189.35	0.721
ν67	3187.37	3.2347	3193.43	2.134
ν68	3195.21	6.9244	3198.88	4.9883
ν69	3207.08	26.9051	3205.52	17.9886
ν70	3207.67	9.9367	3207.82	22.4924
ν71	3213.7	24.6759	3218.83	27.8542

ν72	3220.29	15.238	3219.34	8.8048
	tsi17i26		**tsi17i18**	
ν1	-585.1	14.362	-1889.06	781.312
ν2	27.93	0.0052	34.27	0.053
ν3	48.06	0.528	41.14	0.1294
ν4	51.48	0.1513	57.33	1.5059
ν5	74.52	0.8552	120.45	0.3575
ν6	171.58	0.9018	138.19	0.5328
ν7	196.86	0.3502	161.33	0.2135
ν8	236.58	0.3038	190.54	1.4869
ν9	263.93	0.3407	207.38	0.615
ν10	316.22	2.12	236.41	0.4195
ν11	358.5	4.435	295.82	1.8412
ν12	401.19	2.0816	376.63	3.4711
ν13	417.44	0.0003	414.44	0.2981
ν14	487.09	0.5348	419.91	1.5676
ν15	498.75	0.8644	468.28	10.1128
ν16	538.16	1.2447	511.24	6.8469
ν17	543.21	1.1689	535.12	1.4459
ν18	589.4	1.2233	602.83	15.021
ν19	642.98	0.0642	627.68	8.9505
ν20	677.52	30.8564	642.46	0.4427
ν21	701.67	10.6433	653.79	12.9416
ν22	716.58	31.8387	698.59	10.1558
ν23	753.42	4.4811	712.83	30.8494
ν24	786.13	46.422	777.47	48.5381
ν25	801.55	3.4673	796.45	2.2158
ν26	871.14	0.0055	832.76	19.8622
ν27	878.99	1.2364	862.62	0.1442
ν28	950.14	3.429	886.7	2.7319
ν29	957.72	0.9269	897.31	50.8029
ν30	960.91	1.2339	934.99	3.5849
ν31	1010.57	0.0055	974.02	1.0653
ν32	1023.7	0.376	1004.96	0.0219
ν33	1028.61	0.1909	1018.11	4.0091
ν34	1029.02	5.5167	1022.96	0.0156
ν35	1044.51	1.8464	1030.34	16.8769
ν36	1063.12	3.5036	1055.36	8.0184

v37	1070.93	5.1146	1060.36	1.1442
v38	1109.91	3.297	1079.87	10.238
v39	1114.03	6.1391	1115.29	5.7875
v40	1134.62	7.3828	1143.1	3.0427
v41	1188.74	0.0003	1187.59	0.1845
v42	1197.5	0.5983	1209.24	6.5613
v43	1209.7	0.8455	1229.98	15.1185
v44	1273.36	5.5741	1264.02	23.2244
v45	1313.91	2.2055	1311.9	0.4544
v46	1315.03	0.3792	1319	4.7505
v47	1336.02	12.3623	1361.87	0.0084
v48	1360.74	0.1765	1382.48	5.652
v49	1393.63	5.1	1424.82	1.7058
v50	1416.44	3.3778	1434.87	5.1502
v51	1475.85	2.1214	1488.5	3.2644
v52	1490.47	4.2001	1491.95	12.0779
v53	1498.9	7.2449	1498.41	1.0766
v54	1505.02	3.3029	1519.68	52.3872
v55	1539.45	35.0275	1538.26	23.7148
v56	1637.34	2.2709	1611.19	10.846
v57	1665.86	25.0347	1628.49	3.2472
v58	1694.8	9.8296	1656.66	46.6898
v59	2159.64	15.8188	1799.49	46.9478
v60	3011.72	13.4388	2155.83	34.6574
v61	3052.63	31.3842	3052.56	32.3039
v62	3129.13	23.4474	3122.83	12.562
v63	3140.64	19.2915	3145.16	6.9561
v64	3142.6	17.2188	3154.23	7.3863
v65	3146.21	11.3026	3163.29	6.3356
v66	3191.18	2.7384	3179.42	13.7337
v67	3199.1	3.768	3191.42	6.5054
v68	3199.13	22.3112	3198.27	2.5384
v69	3210.27	11.9492	3210.13	7.2048
v70	3216.6	19.3863	3215.54	21.1767
v71	3222.83	10.9095	3223.04	16.8066
v72	3229.39	4.9053	3251.65	10.0707
	tsi17i19		**tsi17p9**	
v1	-677.02	21.4136	-865.98	5.6828

ν2	23.42	0.0789	9.28	0.0371
ν3	61.07	0.6705	40.61	0.2707
ν4	80.42	1.2542	68.88	1.8554
ν5	109.36	0.1579	124.17	0.1161
ν6	191.54	0.1903	129.06	0.5296
ν7	235.48	0.063	172.85	0.4272
ν8	249.5	0.2439	211.56	1.658
ν9	267.41	0.3846	215.93	1.1921
ν10	304.02	3.0628	232.2	1.4238
ν11	418.28	0.0829	308.17	1.4696
ν12	451.08	0.951	353.43	16.7595
ν13	466.32	4.0502	401.62	4.9303
ν14	482.22	2.0362	416.57	0.0027
ν15	510.55	26.298	425.13	1.5651
ν16	535.48	7.6866	450.72	18.0262
ν17	574.48	8.3766	481.58	16.502
ν18	636.19	4.5203	538.9	2.814
ν19	653.44	9.7045	546.66	4.5162
ν20	690.95	23.8595	597.05	8.2253
ν21	718.53	14.9201	632.12	2.0602
ν22	722.68	22.1593	649.26	1.1463
ν23	759.73	12.6181	686.23	4.1587
ν24	789.35	44.9445	701.7	1.5875
ν25	847.08	0.7181	718.78	34.6666
ν26	876.5	0.1177	791.82	39.1311
ν27	887.33	3.0537	874.07	0.0009
ν28	940.84	0.3971	891.97	0.0945
ν29	960.56	2.3718	900.56	2.5207
ν30	963.6	4.2546	955.79	47.6421
ν31	1010.08	4.44	958.99	4.8062
ν32	1014.32	0.0311	972.98	2.6045
ν33	1028.7	0.2474	1012.38	0.0198
ν34	1032.3	0.0381	1027.49	0.1468
ν35	1050.29	0.3917	1032.99	0.0104
ν36	1065.64	4.8057	1043.35	10.5266
ν37	1079.57	1.6985	1052.27	17.9739
ν38	1108.86	6.0978	1063.75	2.9556
ν39	1113.92	5.609	1068.54	6.9208
ν40	1133.99	6.8935	1114.71	5.8728

ν41	1189.86	0.0374	1143.05	4.5194
ν42	1212.37	0.2195	1190.95	0.0587
ν43	1244.94	0.9142	1212.32	0.2866
ν44	1272.39	1.8968	1235.95	1.8996
ν45	1317.88	0.297	1282.17	0.598
ν46	1319.3	0.699	1318.05	0.2554
ν47	1343.92	3.3488	1330.33	1.8424
ν48	1360.49	0.8405	1361.85	0.511
ν49	1400.7	2.6218	1390.02	19.5732
ν50	1417.16	5.4783	1421.68	6.5955
ν51	1491.78	4.722	1458.57	21.2824
ν52	1492.99	2.8246	1486.12	6.6004
ν53	1500.38	3.7913	1492.91	5.4715
ν54	1502.98	6.9312	1501.73	2.3026
ν55	1543.43	22.199	1546.48	29.8925
ν56	1647.78	3.7498	1588.35	6.7209
ν57	1649.14	4.3446	1646.85	1.7205
ν58	1677.53	9.1124	1676.6	4.3154
ν59	2087.24	0.1803	1679.07	11.6984
ν60	3052.94	35.9416	2344.82	5.7426
ν61	3055.43	15.0753	3052.96	21.1437
ν62	3132.87	19.5824	3125.24	10.0788
ν63	3136.97	26.6636	3152.79	11.3063
ν64	3140.47	9.5495	3155.74	6.8651
ν65	3149.25	11.1546	3171.72	6.5641
ν66	3189.61	20.1893	3182.22	5.8326
ν67	3191.29	0.909	3193.5	1.3867
ν68	3199.46	2.9238	3202.07	2.5118
ν69	3209.39	13.8846	3211.84	12.2013
ν70	3216.74	17.6022	3218.9	17.1398
ν71	3222.99	9.6119	3224.7	9.8996
ν72	3232.61	5.58	3250.46	8.4637
	tsi18i20		**tsi18p9**	
ν1	-373.06	2.6435	-748.95	10.819
ν2	36.97	0.0474	20.08	0.0338
ν3	63.69	0.3351	39.46	0.5724
ν4	73.21	0.4568	67.44	1.7661
ν5	142.82	1.0807	107.66	1.1008

ν6	175.61	0.0924	123.1	0.2214
ν7	201.52	0.2204	149.09	5.5982
ν8	229.15	0.1338	165.7	0.4088
ν9	259.46	0.1693	223.98	1.3771
ν10	331.9	2.8572	237.01	0.4605
ν11	363	1.1524	240.66	0.2835
ν12	416.23	0.081	307.55	1.5499
ν13	428.12	2.8683	379.71	2.2961
ν14	476.46	7.1816	415.78	0.0218
ν15	512.77	5.1101	434.42	0.5045
ν16	540.14	9.7663	463.07	10.3068
ν17	582.71	4.0612	486.77	28.3918
ν18	632.03	6.5568	535.68	1.2296
ν19	635.99	0.4498	550.12	1.2975
ν20	696.11	27.7005	605.39	3.6794
ν21	712.2	33.1793	627.42	3.4103
ν22	780.22	36.3221	646.84	1.1902
ν23	806.64	5.359	698.56	7.1918
ν24	841.34	15.9169	710.23	7.6273
ν25	863.4	0.0916	716.32	35.6977
ν26	884.13	1.0525	790	44.7962
ν27	911.4	9.2285	872.5	0.0072
ν28	936.73	0.7015	892.48	1.337
ν29	954.15	32.5059	916.74	0.5735
ν30	983.81	0.7166	957.03	2.2368
ν31	1003.75	3.166	963.83	48.9967
ν32	1006.61	0.0035	970.6	0.4932
ν33	1015.11	0.6289	1012.19	0.0052
ν34	1023.54	0.0511	1026.06	0.0831
ν35	1033.28	2.7333	1033	0.0064
ν36	1058.17	5.6451	1046.44	9.6965
ν37	1070.71	1.6577	1055.31	13.98
ν38	1113.23	5.8732	1062.92	2.5274
ν39	1128.13	1.4499	1077.02	5.147
ν40	1171.07	4.6842	1115.31	5.9134
ν41	1185.61	0.0882	1144.77	1.998
ν42	1193.72	4.5129	1190.77	0.0808
ν43	1217.88	0.8442	1211.24	0.3869
ν44	1298.76	0.4379	1234.44	1.0031

ν45	1308.67	0.5883	1289.6	1.1994
ν46	1338.06	2.7874	1318.31	0.3488
ν47	1357.87	0.2512	1334.02	2.2797
ν48	1394.47	4.703	1361.85	0.5975
ν49	1423.15	2.1119	1387.31	7.9919
ν50	1463.19	3.0301	1420.75	9.8549
ν51	1483.79	3.6317	1463.57	13.4843
ν52	1487.56	9.513	1480.55	9.8354
ν53	1500.89	11.5737	1492.09	5.562
ν54	1521.28	24.6253	1500.72	3.3116
ν55	1594.39	7.0442	1543.89	25.3678
ν56	1620.64	2.7305	1642.87	1.7852
ν57	1640.94	9.6158	1670.78	7.2678
ν58	1651.33	6.8328	1679.13	0.4033
ν59	1755.44	4.9884	1730.48	9.0965
ν60	3040.29	30.4238	2248.18	12.0334
ν61	3071.75	19.3621	3046.22	24.629
ν62	3097.35	17.3736	3108.85	10.6033
ν63	3137.48	16.8881	3143.02	16.7518
ν64	3150.92	10.7589	3154.16	6.8093
ν65	3160.53	30.385	3167	9.5844
ν66	3169.39	8.8651	3184.03	4.815
ν67	3188.96	3.7278	3194.2	1.4103
ν68	3195.36	2.2226	3202.87	2.6085
ν69	3206.97	7.2025	3212.45	11.1751
ν70	3212.18	22.0999	3219.63	15.5964
ν71	3220.66	15.3947	3225.24	10.1342
ν72	3251.4	6.5797	3247.62	9.605
	tsi19i20		**tsi20p3**	
ν1	-1542.6	16.9063	-812.64	5.9054
ν2	29.8	0.1065	50.45	0.2656
ν3	67.64	1.5591	60.81	0.0939
ν4	103.68	0.6866	93.09	0.8668
ν5	190.68	1.7991	122.06	0.5998
ν6	199.42	1.062	200.63	1.6831
ν7	222.25	2.129	254.04	0.042
ν8	291.18	1.455	296.93	0.2338
ν9	305.41	1.6852	330.67	1.7208

ν10	348.07	1.2428	348.87	2.038
ν11	418.04	0.0442	404.5	0.8003
ν12	435.46	6.4543	416.94	1.1797
ν13	455.28	1.0755	427.64	1.6657
ν14	505.54	22.6674	492.11	1.5184
ν15	556.15	7.6171	520.25	3.6736
ν16	598.84	6.4029	547.19	1.7928
ν17	617.5	3.9817	607.16	4.7438
ν18	638.62	0.4303	634.92	3.4712
ν19	687.49	4.3484	641.95	0.8076
ν20	714.78	35.9905	726.97	33.1856
ν21	742.75	72.0962	731.19	5.5193
ν22	789.58	27.4393	749.47	3.8337
ν23	819.64	13.6685	795.87	58.293
ν24	864.93	0.6667	826.38	14.7932
ν25	893.09	23.8939	877.62	0.6693
ν26	915.59	6.6691	882.98	1.595
ν27	942.77	5.6659	929.8	3.0422
ν28	955.43	17.9146	958.15	1.7117
ν29	988.62	8.6007	979.35	1.6556
ν30	993.59	36.8783	1013.21	0.2686
ν31	1007.96	0.9818	1014.63	2.2072
ν32	1015.68	2.6012	1017.82	0.2418
ν33	1022.58	1.2475	1028.14	0.3407
ν34	1028.24	0.3714	1031.44	0.0404
ν35	1051.83	9.7626	1037.3	1.9322
ν36	1071.05	9.3466	1061.99	4.2714
ν37	1121.72	5.5584	1070.18	7.0064
ν38	1144.21	7.7648	1083.85	2.2621
ν39	1187.75	0.2076	1120.4	5.1455
ν40	1191.71	0.4128	1128.49	3.3661
ν41	1197.55	0.081	1190.35	0.0145
ν42	1218.18	5.2474	1204.75	0.1485
ν43	1227.36	4.6591	1220.37	0.9047
ν44	1284.58	16.0196	1229.65	0.4213
ν45	1310.63	15.0801	1299.42	0.3342
ν46	1329.54	10.2921	1320.83	0.2215
ν47	1371.35	6.4458	1333.44	0.1327
ν48	1380.4	14.959	1356.76	0.124

ν49	1414.14	9.8262	1368.29	1.6352
ν50	1420.02	8.0673	1423.44	1.1678
ν51	1464.05	12.6387	1458.13	4.4507
ν52	1480.51	14.2923	1492.62	7.0332
ν53	1488.7	14.303	1495.84	7.6516
ν54	1498.01	7.2593	1509.92	6.0195
ν55	1507.66	35.3086	1528.34	38.5466
ν56	1541.75	17.647	1554.86	3.566
ν57	1641.12	4.5566	1626.21	9.5919
ν58	1665.86	6.2733	1653.69	7.0855
ν59	1692.89	15.5861	1668.78	30.5625
ν60	2124.56	35.9191	1680.89	4.5087
ν61	2998.96	21.2422	3048.28	27.5742
ν62	3045.88	40.0709	3112.08	14.3573
ν63	3111.33	17.0933	3136.26	13.5809
ν64	3113.17	8.7816	3186.16	11.8781
ν65	3141.76	10.2609	3186.69	2.5593
ν66	3175.44	6.7975	3188.25	4.6147
ν67	3187.38	3.3276	3192.77	0.5243
ν68	3195.42	8.7814	3200	11.7448
ν69	3198.86	26.7372	3201.99	1.395
ν70	3209.59	11.0453	3208.91	23.5772
ν71	3215.75	24.3776	3216.34	12.7259
ν72	3221.63	14.4011	3219.45	16.6583
	tsi26i27		**tsi27p12**	
ν1	-2330.1	53.5	-540.1	57.9715
ν2	27.98	0.0141	46.3	0.1893
ν3	62.44	0.6571	70.19	0.1892
ν4	75.76	0.5137	96.99	0.2601
ν5	157.91	0.2699	168.52	0.3175
ν6	186.75	1.1286	204.09	0.4331
ν7	243.85	0.2315	239.74	0.6608
ν8	257.09	0.9171	269	11.7792
ν9	304.3	0.3151	295.36	0.6794
ν10	356.5	1.317	312.66	1.5831
ν11	416.65	0.0185	360.76	3.078
ν12	464.17	1.8873	394.64	11.2502
ν13	492.11	6.2567	411.02	1.6076

ν14	525.37	2.3542	429.06	1.0606
ν15	552.13	2.8925	499.47	3.8244
ν16	637.08	1.921	578.05	1.1099
ν17	657.92	27.4756	603.05	9.2055
ν18	677.86	2.626	638.11	0.1696
ν19	715.97	33.4089	662.31	12.8831
ν20	719.8	35.5617	681.1	6.4413
ν21	770.17	15.7944	729.57	24.0504
ν22	776.39	5.1535	734.2	31.166
ν23	798.57	29.7323	771.07	27.3079
ν24	872.55	0.0939	797.41	20.1624
ν25	887.23	11.221	830.57	2.2481
ν26	900.62	38.2007	872.58	11.0438
ν27	919.06	0.6253	874.01	8.7776
ν28	952.82	3.9187	885.23	0.0961
ν29	973.46	3.5558	929.88	14.3444
ν30	1010.89	0.0658	963.34	0.4892
ν31	1023.29	0.3054	972.31	5.5301
ν32	1028.6	0.0337	997.32	2.1667
ν33	1039.56	8.6925	1020.4	0.5515
ν34	1046.7	6.9875	1028.88	1.2897
ν35	1062.69	2.3921	1037.2	0.799
ν36	1091.04	7.8534	1039.05	0.7337
ν37	1100.67	6.3314	1066.43	4.9729
ν38	1113.35	8.2755	1066.71	0.729
ν39	1127.04	4.0913	1112.22	2.0747
ν40	1147.64	10.3217	1118.35	6.3548
ν41	1173.99	1.8125	1142	30.4874
ν42	1187.9	0.036	1190.94	0.1878
ν43	1207.29	0.1239	1218.47	2.1437
ν44	1238.49	0.8983	1232.64	12.536
ν45	1275.49	0.9409	1255.94	1.2815
ν46	1297.69	2.1438	1301.25	1.7461
ν47	1312	0.6591	1332.6	0.0735
ν48	1346.03	1.4296	1368.15	0.9142
ν49	1359.05	0.2049	1384.29	11.2373
ν50	1379.01	4.9582	1413.6	2.3496
ν51	1420.24	3.0905	1429.62	2.3227
ν52	1487.69	3.8378	1490.06	14.2878

ν53	1501.7	7.8681	1495.25	7.1394
ν54	1503.16	9.451	1498.46	28.4363
ν55	1530.75	16.4326	1544.26	3.4311
ν56	1603.26	1.9443	1553.91	46.8037
ν57	1636.87	2.5553	1636.98	6.7438
ν58	1661.05	8.6905	1651.31	2.8843
ν59	1698.41	1.7175	1680.22	2.5485
ν60	1841.48	15.5476	1729.68	80.8805
ν61	3015.91	22.4539	3057.84	22.3212
ν62	3053.97	23.173	3125.13	15.2168
ν63	3124.66	11.801	3143.49	12.5627
ν64	3127.54	27.4413	3149.17	9.6461
ν65	3135.18	18.7279	3187.02	2.5249
ν66	3189.32	2.5368	3190.68	0.451
ν67	3196.46	1.3546	3200.15	3.2353
ν68	3197.31	4.6018	3209.69	19.6712
ν69	3206.94	9.4231	3220.44	18.2416
ν70	3213.07	24.8916	3221.14	7.7298
ν71	3220.9	15.1738	3232.15	7.5458
ν72	3226.76	23.3597	3252.38	13.268

	p3		**p7**	
ν1	37.39	0.2257	42.56	0.0407
ν2	60.21	0.0635	88.36	0.4085
ν3	91.58	0.7929	105.21	0.1428
ν4	114.13	0.2002	165.18	0.5607
ν5	217.7	1.5739	207.15	1.1619
ν6	257.7	0.0833	275.02	0.188
ν7	301.02	0.0513	299.84	0.3843
ν8	335.08	0.2044	335.27	0.7445
ν9	403.72	0.6782	416.58	0.6881
ν10	423.21	0.2265	423.31	0.4613
ν11	463.05	3.9653	473.17	4.9989
ν12	522.55	2.9298	532.78	4.1283
ν13	544.53	1.8968	566.93	1.4596
ν14	600.46	3.9823	583.2	3.3464
ν15	637	4.0267	637.54	2.5222
ν16	642.25	1.6055	641.91	2.4095
ν17	728.29	33.1406	730.62	42.4646

ν18	732.9	18.3819	739.94	0.9482
ν19	735.69	2.1235	759.61	14.6616
ν20	786.99	57.9548	779.73	52.7505
ν21	826.18	10.7878	808.85	12.9324
ν22	878.21	0.4769	829.26	0.5722
ν23	885.51	2.6736	880.37	0.081
ν24	924.92	2.9162	904	0.1563
ν25	942.49	2.2264	957.93	2.2766
ν26	964.8	1.381	986.45	0.6144
ν27	1012.97	0.3319	1013.68	0.4733
ν28	1016.18	1.3254	1019.34	1.6708
ν29	1018.38	0.2118	1022.91	0.0218
ν30	1026.38	0.2496	1030	0.3595
ν31	1030.63	0.0409	1031.7	0.1147
ν32	1030.87	0.1141	1039.53	8.8598
ν33	1062.94	3.9211	1070.67	3.0465
ν34	1073.43	6.8305	1072.8	0.5677
ν35	1092.01	1.8019	1089.63	3.8711
ν36	1119.29	4.9684	1114.8	5.1735
ν37	1136.65	4.7213	1156.25	3.1257
ν38	1190.06	0.02	1189.05	0.0035
ν39	1206.07	0.1052	1193.69	0.2555
ν40	1219.86	0.4402	1215.22	0.3079
ν41	1229.33	0.1779	1235.13	0.1284
ν42	1304.92	0.4804	1305.23	1.4307
ν43	1326.71	0.2137	1309.82	0.4517
ν44	1336.5	0.2921	1327.64	0.2882
ν45	1357.71	0.0621	1335.93	0.4087
ν46	1368.87	1.0205	1363.19	0.3607
ν47	1423.4	1.1577	1427.42	1.7661
ν48	1462.54	3.2539	1482.67	2.4987
ν49	1494	6.9916	1494.32	7.2758
ν50	1497.26	8.3726	1498.69	9.5417
ν51	1513.23	10.462	1511.22	14.3581
ν52	1536.51	33.3138	1535.82	33.1095
ν53	1558.82	0.9197	1559.31	1.5296
ν54	1649.95	8.1224	1645.72	1.1316
ν55	1664.91	3.6403	1657.24	1.3195
ν56	1681.75	22.2187	1679.33	5.1819

ν57	1685.81	9.4946	1684.82	2.3958
ν58	3049.6	29.0925	3054.81	20.9284
ν59	3113.82	14.9877	3117.9	14.4256
ν60	3136.13	13.9563	3140.28	16.4687
ν61	3182.95	4.9622	3181.68	8.8127
ν62	3183.89	9.2616	3187.12	3.2328
ν63	3187.22	4.0389	3190.07	1.9484
ν64	3192.19	1.2168	3192.36	0.0727
ν65	3196.47	16.2646	3201.54	15.303
ν66	3202.07	5.1605	3202.49	14.6104
ν67	3208.84	23.7736	3209.17	26.0682
ν68	3212.69	19.8704	3216.87	23.0861
ν69	3219.4	15.3808	3219.29	12.7652
	p12		**p8**	
ν1	38.55	0.1339	15.56	0.0567
ν2	59.27	0.0294	33.04	0.2071
ν3	92.39	0.1284	75.43	1.4639
ν4	174.4	0.2688	106.21	1.1695
ν5	204.45	0.2323	109.79	0.3073
ν6	237.14	1.2161	174.29	1.2856
ν7	277.02	7.5348	208.87	2.8835
ν8	291.6	0.2648	208.88	0.0104
ν9	362.29	2.0448	263.96	4.6786
ν10	408.46	1.2792	352	1.9642
ν11	427.7	0.8265	392.39	0.0669
ν12	495.36	5.0811	410.49	1.9308
ν13	580.79	0.789	417.03	0
ν14	600.19	8.9464	480.79	6.2114
ν15	638.61	0.1437	529.37	2.2215
ν16	668.31	5.769	547.89	0.4987
ν17	675.37	12.3937	576.48	7.3325
ν18	727.92	32.4358	641.92	0.1542
ν19	732.3	25.4254	681.61	8.5748
ν20	770.38	27.0995	719.09	33.9622
ν21	797.9	18.428	764.21	0.2162
ν22	830.48	1.1157	773	13.5003
ν23	871.99	1.1583	791.39	43.2331
ν24	880.28	14.2103	864.62	12.3256

ν25	881.24	0.1287	874.74	0.1801
ν26	925.79	13.5683	947.58	22.7064
ν27	960.78	0.2651	957.67	3.2096
ν28	966.39	5.5573	994.8	9.2714
ν29	991.39	1.82	996.07	13.7209
ν30	1015.83	0.2912	1012.34	0.0332
ν31	1028.88	1.6646	1027.52	0.0023
ν32	1033.95	0.1696	1031.79	0.2764
ν33	1039.27	0.4823	1033.82	22.5239
ν34	1066.04	4.2499	1064.85	5.0438
ν35	1071.21	1.9372	1076.38	0.5134
ν36	1109.77	3.3733	1105.04	0.4714
ν37	1116.44	5.2254	1114.47	5.4893
ν38	1140.63	25.7314	1165.7	0.2803
ν39	1190.8	0.1	1190.35	0.0472
ν40	1216.2	1.341	1212.71	0.0521
ν41	1235.67	13.0516	1252.86	3.5205
ν42	1255.21	0.308	1305.09	5.9079
ν43	1303.49	1.7586	1317.02	0.5022
ν44	1330.62	0.2657	1317.39	1.7638
ν45	1364.96	0.4787	1347.07	1.8253
ν46	1378.73	9.4131	1361.81	0.2977
ν47	1412.65	3.5091	1420.52	6.015
ν48	1430.94	1.8513	1449.56	5.9918
ν49	1485.77	14.1732	1484.13	7.1333
ν50	1494.96	2.1586	1492.67	5.4792
ν51	1501.04	24.6417	1496.77	20.7268
ν52	1546.23	7.5397	1546.63	34.0271
ν53	1600.32	65.829	1646.02	1.7884
ν54	1651.67	2.1449	1669.8	9.7166
ν55	1675.67	6.0827	1684.53	6.7382
ν56	1680.39	4.344	1747.56	36.8019
ν57	1733.12	54.1403	2344.01	2.0378
ν58	3053.32	25.5231	3039.41	33.0608
ν59	3115.6	13.2057	3095.63	15.4154
ν60	3130.23	24.4958	3128.01	4.2727
ν61	3146.64	9.8671	3150.45	27.5375
ν62	3188.44	2.6079	3165.61	2.9931
ν63	3194.78	0.2106	3173.43	6.3714

ν64	3204.29	9.3994	3192.14	1.9729
ν65	3212.43	21.3702	3193.87	21.0873
ν66	3216.41	10.1404	3200.6	2.698
ν67	3221.45	13.636	3210.8	12.7749
ν68	3229.42	8.6186	3217.69	18.3474
ν69	3251.11	13.8436	3223.63	10.7543
	p9		**vdW(i13)**	
ν1	14.36	0.0038	12.43	2.5856
ν2	40.79	0.277	26.19	3.5807
ν3	69.37	1.8469	40.7	0.3149
ν4	122.4	0.1139	62.21	1.011
ν5	126.98	0.5746	78.45	0.1486
ν6	162.4	0.3459	88.01	8.6967
ν7	211.9	1.954	130.77	13.0498
ν8	225.91	0.6236	147.67	4.0467
ν9	232.12	1.2998	148.23	4.357
ν10	310	1.2521	203.8	1.2985
ν11	385.41	0.0654	215.94	0.4929
ν12	416.98	0.0003	272.59	5.9016
ν13	428.69	0.939	277.06	52.275
ν14	479.77	10.3747	396.98	0.21
ν15	535.29	1.3907	461.73	0.3164
ν16	542.82	5.3808	480.57	4.4575
ν17	595.13	4.0908	490.01	1.507
ν18	628.45	3.8406	496.53	30.1731
ν19	648.23	1.4393	511.99	0.5452
ν20	700.99	4.4652	631.33	0.2222
ν21	703.94	5.8316	662.98	2.8933
ν22	719.21	35.4966	696.46	49.5314
ν23	792.02	40.8542	789.35	1.4868
ν24	874.65	0.0009	797.74	34.8678
ν25	894.73	0.2516	869.12	4.6072
ν26	916.17	0.1182	871.94	5.0328
ν27	958.87	1.9865	918.54	4.7731
ν28	963	51.2993	950.79	41.1027
ν29	971.35	0.9099	983.84	3.9618
ν30	1012.61	0.0063	999.53	6.5075
ν31	1027.53	0.0952	1004.84	20.3261

ν32	1032.95	0.0238	1019.82	6.4842
ν33	1048.39	10.3052	1025.89	0.5398
ν34	1055.32	14.2453	1042.16	0.1715
ν35	1063.86	2.8609	1053.74	0.5464
ν36	1076.4	6.2039	1062.29	47.6016
ν37	1114.68	5.8937	1079.95	5.8494
ν38	1144.81	2.6836	1110.07	0.403
ν39	1190.91	0.0514	1117.85	3.6968
ν40	1212.36	0.1983	1188.52	66.4898
ν41	1235.26	1.5414	1191.5	12.1024
ν42	1289.15	0.6116	1217.81	1.1816
ν43	1317.65	0.2392	1232.79	22.4083
ν44	1333.09	2.4366	1309.16	0.7961
ν45	1361.92	0.441	1326.99	5.0887
ν46	1393.67	13.1336	1335.85	0.9182
ν47	1421.93	6.3587	1356.66	2.6683
ν48	1464.55	15.7725	1359.98	6.4989
ν49	1482.74	7.7683	1420.04	4.4582
ν50	1492.94	5.2769	1460.8	6.7292
ν51	1501.27	3.4556	1482.94	8.5521
ν52	1547.29	31.1367	1483.93	8.6385
ν53	1646.35	1.7451	1497.21	9.2106
ν54	1672.66	5.6962	1515.3	2.8987
ν55	1682.36	4.9438	1614.82	0.7685
ν56	1730.44	14.1901	1640.27	117.811
ν57	2343.91	2.0015	1698.86	6.7557
ν58	3049.05	24.9238	1761.2	16.3953
ν59	3112.55	12.1574	1987.32	35.2654
ν60	3142.13	16.4386	3038.29	30.6488
ν61	3153.63	6.7275	3094.87	21.468
ν62	3167.05	9.1427	3123.67	9.4503
ν63	3180.6	5.3814	3142.73	3.0146
ν64	3192.98	1.8383	3149.58	2.1874
ν65	3201.09	2.4862	3151.82	21.4454
ν66	3211.4	11.325	3160.83	4.783
ν67	3217.93	17.7602	3199.46	0.4139
ν68	3224.14	10.9252	3211.89	3.2505
ν69	3247.1	9.8565	3219.81	5.9724
ν70			3228.69	5.5287

ν71			3238.11	2.3165
ν72			3243.91	8.1643
	vdW(i17)		**tsi13vdW**	
ν1	13.04	1.6084	-7.89	1.2284
ν2	23.82	1.456	33.16	1.7893
ν3	56.16	0.2178	43.62	0.0853
ν4	73.62	2.358	73.37	0.9349
ν5	84.85	1.4261	75.04	0.1546
ν6	109.41	7.5627	102.37	3.7
ν7	138.95	0.9043	130.56	10.0243
ν8	150.02	5.099	149.2	4.0901
ν9	172.21	4.9928	159.34	7.0183
ν10	204.22	2.0294	202.66	0.9904
ν11	212.59	0.6722	214.64	0.7149
ν12	278.01	17.2734	273.41	29.4103
ν13	321.4	23.8924	287.73	14.7296
ν14	399.96	0.0182	392.25	0.0446
ν15	462.71	0.2888	462.47	0.2174
ν16	476.76	2.4611	478.44	2.5265
ν17	489.58	0.3663	489.67	0.0256
ν18	508.16	27.6783	496.93	28.2342
ν19	514.03	5.5217	512.28	0.5676
ν20	633.55	0.1859	631.41	0.1742
ν21	654.95	1.9846	661.03	3.3236
ν22	697.78	43.2119	692.34	52.996
ν23	786.85	1.6757	788.64	0.7844
ν24	797.25	19.1738	797.57	26.7275
ν25	863.68	13.236	863.89	6.2021
ν26	869.95	1.0064	867.26	4.8003
ν27	919.65	3.3926	918.49	4.7523
ν28	947.05	32.3899	957.17	41.7161
ν29	976.2	0.2907	978.11	1.1852
ν30	994.33	57.2266	999.95	5.8062
ν31	999.54	7.6622	1002.48	27.6964
ν32	1021.14	3.5643	1019.9	4.6331
ν33	1021.47	0.5795	1021.48	0.6891
ν34	1041.38	0.0256	1041.12	0.1925

v35	1055.29	5.7962	1054.26	0.5603
v36	1056.72	44.6955	1068.8	44.6368
v37	1079.11	7.25	1074.95	4.3136
v38	1113.67	1.6333	1109.49	0.3171
v39	1115.43	4.8384	1116.47	4.1399
v40	1187.5	58.9813	1186.89	69.5648
v41	1191.22	2.2891	1191.1	3.9575
v42	1220.27	3.102	1216.88	0.4251
v43	1228.59	17.0657	1230.82	20.3458
v44	1308.23	0.7227	1307.66	0.9696
v45	1325.22	4.7193	1326.64	4.0967
v46	1330.9	9.7545	1334.61	0.9263
v47	1349.19	3.395	1351.57	2.175
v48	1358.17	5.9432	1359.22	6.4853
v49	1420.4	5.8229	1418.71	4.8727
v50	1459.85	9.7972	1460.57	8.8406
v51	1483.54	5.6888	1483.06	8.241
v52	1485.49	10.5011	1483.74	9.6447
v53	1500.23	16.4927	1497.15	11.027
v54	1517.49	0.8722	1515.28	2.2043
v55	1621.14	0.7656	1615.97	0.7606
v56	1643.92	82.3186	1640.67	89.721
v57	1687.54	16.6701	1699.17	5.3422
v58	1731.19	139.6986	1759.76	13.9651
v59	2009.89	100.6702	2010.18	17.1269
v60	3044.21	35.2781	3037.74	30.4605
v61	3109.87	6.9214	3094.19	22.1545
v62	3131.48	7.9154	3122.9	9.5411
v63	3145.52	5.0421	3141.64	3.3283
v64	3152.47	10.2299	3150.24	1.2456
v65	3160.89	1.3763	3151.72	27.6445
v66	3163.75	22.1218	3162.61	4.626
v67	3198.05	0.1894	3198.58	0.2177
v68	3209.73	3.7637	3210.8	3.5978
v69	3217.44	7.2317	3218.92	6.2085
v70	3227.52	5.3501	3228.59	3.8243
v71	3230.86	6.3962	3234.32	3.4981

ν72	3246.35	8.0472	3248.61	5.325
	tsi17vdW			
ν1	-5.74	2.2265		
ν2	22.21	1.0377		
ν3	43.91	0.1319		
ν4	62.49	0.118		
ν5	78.51	2.9491		
ν6	85.33	0.7038		
ν7	138.55	4.0525		
ν8	146.91	4.4542		
ν9	167.9	11.2328		
ν10	203.43	1.1321		
ν11	216.65	1.1777		
ν12	271.6	11.3076		
ν13	291.35	28.7278		
ν14	396.88	0.0466		
ν15	462.38	0.5469		
ν16	477.18	2.4011		
ν17	489.84	0.1158		
ν18	501.83	26.3163		
ν19	512.71	0.8436		
ν20	633.05	0.1913		
ν21	658.84	2.3393		
ν22	696.6	46.9324		
ν23	787.77	0.6532		
ν24	796.65	19.939		
ν25	861.38	4.4736		
ν26	868.99	0.7431		
ν27	918.19	5.0221		
ν28	947.88	41.8593		
ν29	976.92	0.4564		
ν30	993.63	35.7107		
ν31	998.08	8.4039		
ν32	1020.66	2.3561		
ν33	1021.24	1.9726		
ν34	1041.62	0.0892		
ν35	1054.76	36.7884		

v36	1055.49	11.6195
v37	1078.87	1.8637
v38	1113.65	0.4284
v39	1115.52	4.5584
v40	1186.84	62.9071
v41	1191.37	2.8215
v42	1217.92	1.9028
v43	1228.82	19.3042
v44	1307.31	1.0801
v45	1326.05	4.288
v46	1332.36	4.6678
v47	1350.37	3.3919
v48	1358.38	6.3165
v49	1423.38	5.2756
v50	1458.99	9.4721
v51	1481.6	9.0846
v52	1484.88	10.4509
v53	1495.53	21.3296
v54	1516.64	0.9125
v55	1619.82	0.9345
v56	1643.28	77.1544
v57	1693.17	3.3391
v58	1744.08	77.2733
v59	2019.81	52.1399
v60	3043.23	30.1195
v61	3107.52	7.4806
v62	3130.89	1.4312
v63	3146.82	19.1227
v64	3148.26	0.3092
v65	3155.01	19.0384
v66	3160.66	10.0132
v67	3198.01	0.2203
v68	3210.07	3.6397
v69	3217.45	6.5503
v70	3227.65	4.6802
v71	3231.02	5.7645
v72	3246.22	7.7347

	i34		i35	
ν1	11.61	0.0111	22.47	0.2808
ν2	34.39	0.354	50.51	0.2063
ν3	62.14	1.3595	71.16	0.6638
ν4	85.56	0.5563	83.54	0.4802
ν5	109.93	0.9323	125.77	0.5017
ν6	133.99	0.4997	190.47	0.6225
ν7	176.78	0.1696	196.04	0.9117
ν8	188.07	0.1314	208.43	0.6695
ν9	209.46	1.3906	250.85	3.0032
ν10	253.28	1.7733	329.18	2.2526
ν11	303.37	1.5346	377.89	4.7103
ν12	368.02	3.4403	412.08	1.2282
ν13	390.03	1.3304	418.38	1.1853
ν14	417.94	0.0028	465.15	2.1452
ν15	456.71	12.8775	482.87	5.3371
ν16	502.06	9.266	506.27	0.7558
ν17	532.09	24.8581	554.98	0.0781
ν18	547.39	7.0219	635.35	0.0056
ν19	585.53	13.611	673.82	0.5421
ν20	594.6	1.0221	696.7	32.852
ν21	644.91	0.0595	765.9	45.004
ν22	721.07	34.6715	807	14.5849
ν23	726.49	2.8813	829.67	8.787
ν24	792.61	39.534	844.84	0.3069
ν25	834.94	0.667	861.02	4.4401
ν26	877.31	0.0016	912.76	2.9643
ν27	901.27	0.5697	917.79	2.8937
ν28	941.92	11.6698	936.88	18.7328
ν29	960.34	3.6216	977.79	15.701
ν30	1008.37	43.1653	1000.31	0.0265
ν31	1014.15	0.0116	1001.64	9.2073
ν32	1027.99	0.1752	1004.22	46.749
ν33	1032.56	0.0741	1013.26	0.0035
ν34	1046.85	3.1874	1048.35	14.2981
ν35	1061.62	6.3613	1059.86	15.7146
ν36	1078.48	1.098	1067.7	0.997
ν37	1083.03	1.5068	1077.31	0.8926
ν38	1110.51	1.6562	1101.89	2.2746
ν39	1114.07	5.6505	1113.49	5.2768

ν40	1136.55	0.0958	1129.2	37.266
ν41	1190.34	0.0314	1180.77	0.3408
ν42	1212.8	0.2097	1198.36	17.6757
ν43	1239.23	2.4409	1202.26	4.5536
ν44	1279.79	1.1885	1277.11	0.3848
ν45	1317.07	0.2737	1305.3	0.7166
ν46	1326.03	12.7855	1320.47	11.635
ν47	1342.91	5.4791	1345.55	2.4304
ν48	1362.06	0.3184	1355.79	0.0627
ν49	1365.5	13.6671	1398.36	1.349
ν50	1422.92	3.7536	1424.81	3.2277
ν51	1454.42	1.1216	1468.79	3.171
ν52	1486.08	7.3627	1476.7	1.6603
ν53	1492.98	5.1459	1485.31	7.0096
ν54	1497.8	11.4399	1500.21	8.8919
ν55	1547.23	26.8853	1512.68	40.9295
ν56	1647.96	1.7059	1597.1	3.6612
ν57	1680.1	10.9103	1620.93	13.5463
ν58	1756.15	2.0632	1764.24	0.7362
ν59	2375.56	2.3003	1981.23	31.1685
ν60	3025.24	10.9778	3039.22	41.0943
ν61	3041.39	34.4347	3096.18	18.0189
ν62	3099.35	16.5489	3123.89	9.7208
ν63	3126.7	5.566	3129.93	16.9024
ν64	3146.94	27.0368	3142.14	5.5814
ν65	3163.49	13.7654	3150.26	25.9174
ν66	3165.24	14.0808	3160.55	15.8433
ν67	3191.65	0.9065	3190.51	4.8173
ν68	3200.49	3.3681	3196.63	4.4914
ν69	3210.72	14.1822	3211.13	7.6428
ν70	3217.84	18.3514	3215.78	22.0768
ν71	3223.41	8.5465	3220.34	5.1099
ν72	3282.65	7.1282	3222.99	12.9529
	i36		**i37**	
ν1	6.73	0.0034	26.57	0.3674
ν2	39.84	0.6298	55.35	0.1489
ν3	48.43	0.748	63.48	0.5011
ν4	62.25	0.4831	88.24	0.418
ν5	84.59	0.0541	149.54	0.3069
ν6	105.48	1.0465	177.57	0.1417

ν7	150.88	0.2838	197.6	0.4383
ν8	166.66	0.045	199.63	0.0874
ν9	250.22	2.4082	233.39	0.3153
ν10	283.12	1.0053	349.42	0.1961
ν11	322	0.6767	369.33	5.2907
ν12	401.2	2.5142	399.54	1.6842
ν13	417.66	0.0027	416.6	0.5482
ν14	418.76	11.9416	448.43	6.1986
ν15	426.59	1.8651	486.64	5.5898
ν16	469.17	17.3212	521.55	2.0369
ν17	549.38	3.1818	574.66	3.2816
ν18	575.7	2.9453	635.24	0.1174
ν19	583.94	4.6007	654.33	0.7632
ν20	644.27	0.1551	696.13	32.6818
ν21	690.49	25.9349	716.66	1.8689
ν22	720.79	34.7692	765.22	43.81
ν23	772.35	0.941	804.4	30.4514
ν24	792.39	39.3352	843.09	0.3397
ν25	876.48	0.0002	857.92	17.3927
ν26	881.67	1.4689	903.99	1.605
ν27	954.74	6.8368	912.02	3.1357
ν28	960.14	3.414	951.95	46.954
ν29	964.08	43.7151	997.45	0.6267
ν30	993.71	0.2585	999.18	0.1999
ν31	1013.44	0.0014	1005.92	13.5623
ν32	1027.48	0.074	1012.23	4.5217
ν33	1032.3	0.1078	1012.42	0.2781
ν34	1033.67	4.2827	1022.99	28.2595
ν35	1041.05	12.2462	1042.87	7.2446
ν36	1067.34	5.2662	1049.07	7.4519
ν37	1105.6	1.7229	1113.02	5.2872
ν38	1113.87	5.6025	1123.7	0.5721
ν39	1131.31	0.5216	1132.5	73.3407
ν40	1152.63	0.7155	1142.23	1.644
ν41	1190.03	0.0428	1179.94	0.3486
ν42	1212.75	0.2283	1199.83	4.301
ν43	1260.54	1.4035	1207.67	24.99
ν44	1277.45	6.3139	1289.83	1.2424
ν45	1313.96	23.123	1302.69	6.0173
ν46	1316.91	0.2467	1305.14	0.6968
ν47	1326.99	0.8208	1341.63	3.6281

ν48	1361.74	0.3095	1354.95	0.0373
ν49	1391.03	9.0117	1410.89	13.5151
ν50	1422.66	3.143	1423.88	3.1518
ν51	1455.94	6.0607	1473.18	0.5975
ν52	1476.32	8.8313	1476.34	1.6587
ν53	1489.2	3.0878	1495.08	2.4599
ν54	1492.86	5.0756	1504.36	12.2141
ν55	1547.02	26.6091	1513.26	36.7866
ν56	1647.94	1.69	1596.86	3.7547
ν57	1680	10.8808	1620.75	13.8059
ν58	1722.51	14.2449	1728.19	36.5097
ν59	2375.43	2.2544	1978.41	35.5565
ν60	2993.28	25.2022	3048.93	39.6726
ν61	3017.64	13.9628	3122.09	15.1272
ν62	3042.24	22.183	3125.58	12.6131
ν63	3132.6	18.4489	3142.59	18.5208
ν64	3149.49	8.6451	3148.76	0.5738
ν65	3175.62	3.4572	3154.38	20.2261
ν66	3192.13	0.8449	3162.85	7.1144
ν67	3201.02	3.3357	3190.02	4.8285
ν68	3208.38	8.5235	3196.1	4.3211
ν69	3211.12	14.2275	3210.5	7.3083
ν70	3218.34	18.0643	3215.07	21.795
ν71	3223.86	8.5861	3222.4	13.171
ν72	3240.74	11.5871	3245.68	11.3314
	tsi13i35		**tsi17i37**	
ν1	-675.9	3.4076	-659.07	11.6216
ν2	27.15	0.1457	34.62	0.3889
ν3	41.52	0.0249	43.27	0.0225
ν4	76.21	1.194	65.32	0.8523
ν5	94.29	1.3726	102.43	1.0016
ν6	127.65	0.4581	157.4	0.4235
ν7	183.25	2.1003	183.62	0.3089
ν8	198.44	1.1178	195.84	0.9295
ν9	213.85	0.1367	209.29	0.3188
ν10	266.8	2.2919	247.04	0.214
ν11	329.77	6.929	348.39	5.8947
ν12	396.68	5.7435	377.13	1.4377
ν13	416.13	0.0617	406.54	3.0667
ν14	428.27	2.2297	416.54	0.2623

ν15	441.65	3.6848	462.26	7.0458
ν16	469.44	3.2437	505.58	2.7717
ν17	512.91	2.6282	519.45	6.2238
ν18	552.81	0.0356	567.29	4.0982
ν19	640.98	0.0048	639.35	0.1733
ν20	708.03	10.1846	678.15	9.7558
ν21	709.35	24.143	704.12	2.608
ν22	774.74	47.2071	708.97	31.3693
ν23	796.53	0.4384	775.49	46.5514
ν24	837.16	2.6092	850.87	0.0772
ν25	858.14	0.0717	859.83	0.0356
ν26	910.46	5.1693	890.38	3.7958
ν27	929.4	3.8969	909.1	40.9007
ν28	957.99	3.2731	917.5	1.8655
ν29	978.29	10.8827	931.5	3.5426
ν30	998.01	29.3662	1004.26	0.3187
ν31	1002.92	0.0165	1004.47	0.1899
ν32	1015.5	8.4838	1014.92	5.027
ν33	1019.04	0.0428	1020.52	0.0447
ν34	1045.99	6.6726	1023.53	13.7528
ν35	1059.23	3.0728	1053.36	3.7991
ν36	1066	0.2382	1063.51	7.8915
ν37	1095.34	2.5231	1104.16	0.6144
ν38	1114.29	5.6579	1114.02	5.7347
ν39	1154.87	12.189	1166.15	19.1854
ν40	1180.71	6.7133	1178.71	3.6597
ν41	1185.39	0.2077	1184.99	0.1395
ν42	1204.92	12.5486	1206.78	3.5585
ν43	1213.82	12.4763	1230.81	26.017
ν44	1298.52	1.0036	1294.49	7.3788
ν45	1310.94	0.5833	1310.61	1.2674
ν46	1322.6	30.2718	1314.25	15.2122
ν47	1336.39	2.8282	1335	7.4983
ν48	1359.16	0.0123	1359.22	0.0036
ν49	1411.14	10.6941	1410.37	16.7411
ν50	1428	1.0284	1422.42	5.1459
ν51	1475.31	2.5171	1476.25	3.2015
ν52	1483.58	6.3911	1485.81	2.9299
ν53	1485.98	2.7263	1498.73	4.736
ν54	1499.51	11.3903	1504.29	6.9504
ν55	1529.9	54.6026	1530.41	51.6823

ν56	1620.05	3.2294	1620.43	3.1657
ν57	1644	44.3187	1637.08	60.8307
ν58	1679.45	1.5737	1653.77	14.3172
ν59	2066.2	0.3472	2058.4	0.7306
ν60	3033.61	50.4063	3055.13	34.1825
ν61	3087.2	18.1224	3107.4	4.6777
ν62	3103.21	26.6673	3134.85	22.4496
ν63	3121.47	12.0799	3138.92	21.2055
ν64	3138.76	11.9878	3149.89	13.217
ν65	3154.63	28.8371	3160.46	3.1191
ν66	3177.08	2.8742	3190.35	4.9984
ν67	3189.73	5.3175	3192.48	6.0635
ν68	3196.65	3.9341	3197.33	3.7175
ν69	3207.25	6.4016	3210.13	9.8041
ν70	3209.78	9.7501	3215.59	21.4169
ν71	3215.12	22.5953	3222.4	13.0801
ν72	3222.04	13.0778	3252.01	9.8202
	tsi34i35		**tsi36i37**	
ν1	-670.55	41.2168	-654.7	26.9018
ν2	34.11	0.4164	37.93	0.0601
ν3	37.51	0.05	40.37	0.3627
ν4	61.3	0.7834	59.2	0.8102
ν5	82.56	0.531	79.06	0.2003
ν6	129.45	0.4174	117.86	0.4181
ν7	185.49	0.4482	138.28	0.582
ν8	203.88	0.7181	165.28	0.257
ν9	213.45	0.1332	215.46	0.5881
ν10	250.53	1.0864	236.27	0.364
ν11	324.88	2.6937	344.33	3.5381
ν12	353.48	2.0361	354.78	0.1957
ν13	411.37	0.6469	399.31	1.3019
ν14	416.94	0.0744	416.53	0.0163
ν15	462.62	0.7022	426.85	4.1393
ν16	495.28	4.8405	503.36	3.7173
ν17	519.84	5.9039	520.58	4.9736
ν18	538.68	0.9677	563.13	0.4874
ν19	628.93	1.6668	640.66	0.0783
ν20	643.86	0.6984	661.51	3.6121
ν21	659.89	16.7659	694.12	9.763
ν22	712.65	31.7081	712.67	31.4301

ν23	729.02	2.8932	767.58	3.9237
ν24	778.6	45.3372	777.45	45.0915
ν25	836.44	0.425	862.26	0.0147
ν26	863.12	0.0029	893	12.6734
ν27	892.08	1.2136	934.6	2.7568
ν28	937.26	3.2257	944.83	10.7962
ν29	962.09	15.9266	971.51	39.1686
ν30	987.64	2.6399	1004.43	0.0212
ν31	1005.19	0.0278	1006.4	13.4116
ν32	1009.71	35.9939	1017.73	1.5879
ν33	1019.52	4.9235	1021.27	0.0425
ν34	1022.49	0.0915	1038.51	5.1245
ν35	1060.46	6.7059	1042.29	10.9887
ν36	1077.03	3.0984	1061.68	7.0761
ν37	1080.17	0.3713	1080.45	6.9184
ν38	1114.02	5.6871	1114.14	5.8285
ν39	1142.22	17.9187	1166.78	26.5193
ν40	1172.91	8.3079	1177.36	0.341
ν41	1186.23	0.0906	1186.41	0.1643
ν42	1207.55	0.9892	1204.59	0.9941
ν43	1216.38	8.2242	1209.76	3.3522
ν44	1273.22	0.5381	1282.12	2.945
ν45	1310.13	23.3451	1311.73	0.3321
ν46	1312.22	0.3528	1314.66	32.8903
ν47	1344.79	1.8458	1340.64	4.6246
ν48	1360.1	0.0075	1360.44	0.0025
ν49	1393.46	7.5008	1400.51	15.4941
ν50	1424.15	4.9827	1424.86	5.3696
ν51	1450.15	2.5557	1470.71	3.9075
ν52	1485.72	6.7275	1483.66	6.6478
ν53	1488.13	3.3404	1488.06	3.2195
ν54	1499.12	11.6413	1496.96	10.6779
ν55	1534.91	52.9546	1534.83	60.1756
ν56	1628.53	2.8508	1627.24	3.1556
ν57	1654.93	42.6337	1654.59	57.0162
ν58	1773.68	2.214	1739.1	15.1188
ν59	2109.11	9.1017	2115.39	21.4677
ν60	3042.48	35.0794	3010.78	57.7638
ν61	3101.05	16.0005	3084.28	10.9294
ν62	3109.72	9.4922	3098.24	9.5605
ν63	3127.56	6.8954	3122.77	15.8007

ν64	3150.31	15.4092	3153.28	9.5325
ν65	3155.88	24.1749	3170.51	3.8886
ν66	3182.31	6.3883	3189.9	5.1755
ν67	3190.51	4.0864	3196.81	3.4881
ν68	3197.86	3.5888	3208.99	9.4417
ν69	3210.08	11.1183	3209.58	9.7308
ν70	3215.85	21.8884	3214.82	22.8389
ν71	3222.44	12.2829	3222.03	13.0734
ν72	3305.24	1.8111	3244.5	11.0003

Table S8. **(a)** k_3 (**i1→p2)** analysis at zero collision energy.

	k_7 (**c6 → p1**) 2.62 × 10^8 s^{-1}	k_3 (**i1 → p2**) 2.78 s^{-1}
number of states (**ts**)	8.63 × 10^6 (**tsc6p1**)	5.95 × 10^{14} (**tsi1p2**)
density of states (**intermediate**)	1.98 × 10^9 (**c6**)	1.28 × 10^{25} (**i1**)

$$\frac{k_7}{k_3} \propto \frac{\frac{number\ of\ states\ (\boldsymbol{tsc6p1})}{density\ of\ states\ (\boldsymbol{c6})}}{\frac{number\ of\ states\ (\boldsymbol{tsi1p2})}{density\ of\ states\ (\boldsymbol{i1})}} \approx 10^8$$

(b) Number of states (zero collision energy) and **frequencies** (cm^{-1})

$C_2H + C_2H_4$ CCSD(T)/cc-pVQZ// B3LYP/6-311G(d,p)	$C_6H_5CC+C_4D_6$ CCSD(T)/cc-pVTZ// *w*B97XD/cc-pVTZ
8.63×10^6 (**tsc6p1**) (k_7, **c6** → **p1**, 2.62×10^8 s^{-1})	5.95×10^{14} (**tsi1p2**) (k_3, **i1** → **p2**, 2.78 s^{-1})
-741.1331	-571.5631
220.8862	11.5708
281.2715	41.0526
389.9083	72.3213
418.1062	113.6533
554.4333	121.8362
649.4072	180.1196
677.4378	196.0092
686.2903	257.2621
885.3291	260.9275
914.5351	349.2534
1012.5147	359.7981
1106.1016	416.3073
1296.6117	423.7918
1433.0593	440.0346
1591.4473	536.2308
2210.7440	547.4793
3144.0101	582.3694
3150.2065	641.2384
3245.0019	658.5665
3477.1532	665.7317
	718.4427

	738.2888
	742.6543
	758.6011
	784.7155
	791.4305
	833.8025
	874.1867
	874.2977
	937.5360
	958.8121
	969.7932
	1012.4920
	1027.5828
	1032.7249
	1058.5078
	1064.1167
	1096.9426
	1114.7606
	1190.8066
	1212.1635
	1237.6048
	1317.7443
	1331.6066
	1361.8166
	1492.7611
	1531.6860
	1558.4405
	1602.3986
	1646.4528

	1678.9918
	2300.1954
	2336.6834
	2344.9651
	2358.8661
	2367.7870
	2421.9790
	3193.4906
	3202.1283
	3211.7279
	3218.9901
	3224.7351

(c) Density of states (zero collision energy) and **frequencies** (cm^{-1})

$C_2H + C_2H_4$ CCSD(T)/cc-pVQZ// B3LYP/6-311G(d,p)	$C_6H_5CC+C_4D_6$ CCSD(T)/cc-pVTZ// *w*B97XD/cc-pVTZ
1.98×10^9 (**c6**) (k_7, **c6** → **p1**, 2.62×10^8 s^{-1})	1.28×10^{25} (**i1**) (k_3, **i1** → **p2**, 2.78 s^{-1})
46.5231	6.3803
207.3390	40.4576
318.1048	64.0240
435.7973	98.3267
526.0302	123.9341
661.3982	175.6246
680.3857	240.1005
833.7489	273.9109
878.9712	319.2211
1045.8597	394.9053
1083.3448	405.6534
1197.4887	417.6833
1344.7288	428.1657
1446.8915	540.8525
1454.1079	556.5464
2227.1626	571.7122
2942.6291	631.5157
2974.1212	642.5586
3149.2941	651.5161
3264.7874	715.3767
3478.5307	720.8787
	741.1525

	767.6370
	792.6104
	820.0357
	820.6838
	876.9872
	902.4658
	919.9334
	944.0992
	960.4850
	1014.0652
	1028.2489
	1033.1884
	1053.2266
	1055.9708
	1064.3948
	1096.7098
	1113.9785
	1189.5745
	1189.6936
	1213.3177
	1316.9073
	1317.4419
	1330.3433
	1361.7930
	1427.5877
	1493.0670
	1547.2282
	1648.1094
	1680.2507

	2196.0135
	2248.9203
	2291.8300
	2333.5270
	2345.0158
	2379.8825
	2428.6948
	3192.3052
	3200.9303
	3210.9662
	3217.9940
	3223.7378

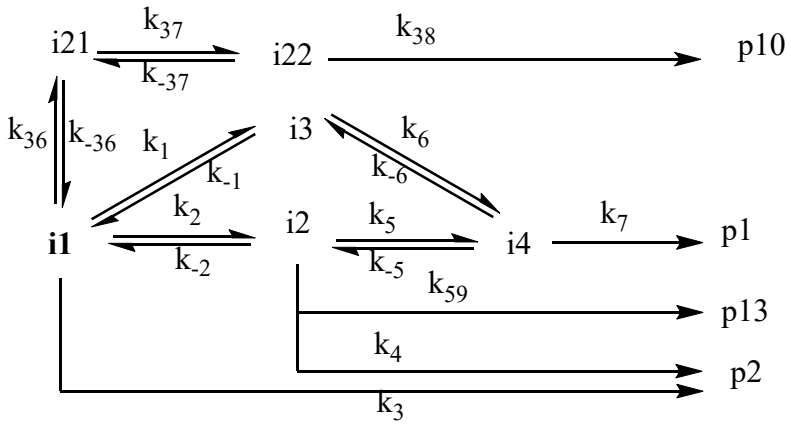
Table S9. **(a)** Branching ratios at zero collision energy according to reaction paths in Figures S4, S5a, S5b, S6a, and S6b based on rate constants from Tables S2, S3, and S4, respectively.

$C_6H_5CC + C_4D_6$		**p1**	**p2**	**p10**	**phenylacetylene**
(Fig S4.)	**i1**	9.951×10^{-1}	4.776×10^{-3}	1.603×10^{-4}	-

C_6H_5CC + isoprene		**p3**	**p4**	**p11**
(Fig S5a.)	**i5**	9.991×10^{-1}	2.994×10^{-4}	3.209×10^{-4}
		p5	**p6**	**p11'**
(Fig S5b.)	**i9**	9.838×10^{-1}	1.467×10^{-2}	1.511×10^{-3}

C_6H_5CC + 1,3-pentadiene		**p7**	**p8**	**p12**
(Fig S6a.)	**i13**	9.701×10^{-1}	2.958×10^{-2}	3.296×10^{-4}
		p3	**p9**	**p12**
(Fig S6b.)	**i17**	9.953×10^{-1}	4.659×10^{-3}	1.411×10^{-6}

(b) The $C_6H_5CC + C_4D_6$ reaction mechanism and rate equations according to reaction paths in Figure S4 based on rate constants from Table S2.



$$\frac{d[i1]}{dt} = k_{-2}[i2] + k_{-1}[i3] + k_{-36}[i21] - (k_1+k_2+k_3+k_{36})[i1]$$

$$\frac{d[i2]}{dt} = k_2[i1] + k_{-5}[i4] - (k_{-2}+k_5+k_4+k_{59})[i2]$$

$$\frac{d[i3]}{dt} = k_1[i1] + k_{-6}[i4] - (k_{-1}+k_6)[i3]$$

$$\frac{d[i4]}{dt} = k_5[i2] + k_6[i3] - (k_{-5}+k_{-6}+k_7)[i4]$$

$$\frac{d[i21]}{dt} = k_{36}[i1] + k_{-37}[i22] - (k_{-36}+k_{37})[i21]$$

$$\frac{d[i22]}{dt} = k_{37}[i21] - (k_{-37}+k_{38})[i22]$$

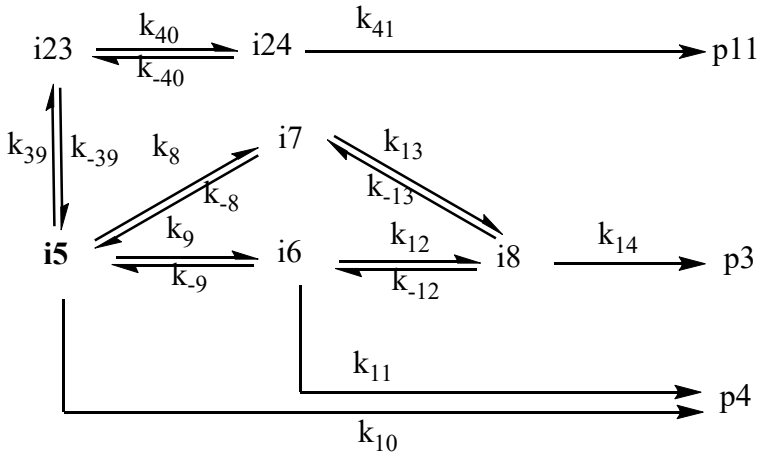
$$\frac{d[p1]}{dt} = k_7[i4]$$

$$\frac{d[p2]}{dt} = k_3[i1] + k_4[i2]$$

$$\frac{d[p10]}{dt} = k_{38}[i22]$$

$$\frac{d[p13]}{dt} = k_{59}[i2]$$

(c). The C_6H_5CC + isoprene reaction mechanism and rate equations according to reaction paths in Figure S5 based on rate constants from Table S3.



$$\frac{d[i5]}{dt} = k_{-8}[i7] + k_{-9}[i6] + k_{-39}[i23] - (k_8+k_9+k_{10} + k_{39})[i5]$$

$$\frac{d[i6]}{dt} = k_9[i5] + k_{-12}[i8] - (k_{-9}+k_{12}+k_{11})[i6]$$

$$\frac{d[i7]}{dt} = k_8[i5] + k_{-13}[i8] - (k_{-8}+k_{13})[i7]$$

$$\frac{d[i8]}{dt} = k_{12}[i6] + k_{13}[i7] - (k_{-12}+k_{-13}+k_{14})[i8]$$

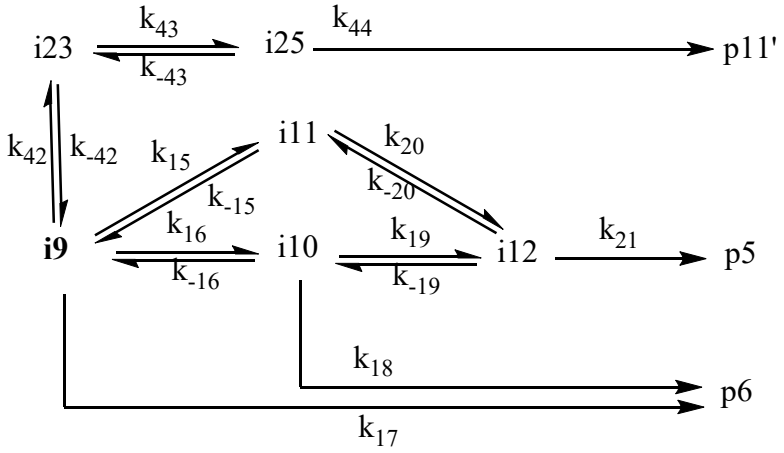
$$\frac{d[i23]}{dt} = k_{39}[i5] + k_{-40}[i24] - (k_{-39}+k_{40})[i23]$$

$$\frac{d[i24]}{dt} = k_{40}[i23] - (k_{-40}+k_{41})[i24]$$

$$\frac{d[p3]}{dt} = k_{14}[i8]$$

$$\frac{d[p4]}{dt} = k_{10}[i5] + k_{11}[i6]$$

$$\frac{d[p11]}{dt} = k_{41}[i24]$$



$$\frac{d[i9]}{dt} = k_{-15}[i11] + k_{-16}[i10] + k_{-42}[i23] - (k_{15}+k_{16}+k_{17}+k_{42})[i9]$$

$$\frac{d[i10]}{dt} = k_{16}[i9] + k_{-19}[i12] - (k_{-16}+k_{18}+k_{19})[i10]$$

$$\frac{d[i11]}{dt} = k_{15}[i9] + k_{-20}[i12] - (k_{-15}+k_{20})[i11]$$

$$\frac{d[i12]}{dt} = k_{19}[i10] + k_{20}[i11] - (k_{-19}+k_{-20}+k_{21})[i12]$$

$$\frac{d[i23]}{dt} = k_{42}[i9] + k_{-43}[i25] - (k_{-42}+k_{43})[i23]$$

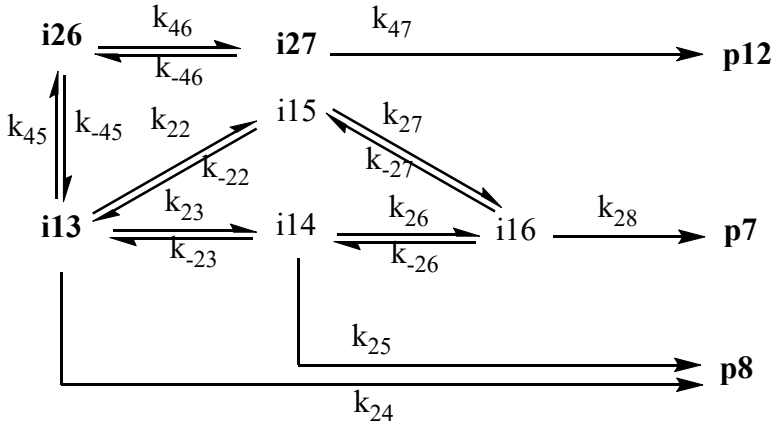
$$\frac{d[i25]}{dt} = k_{43}[i23] - (k_{-43}+k_{44})[i25]$$

$$\frac{d[p5]}{dt} = k_{21}[i12]$$

$$\frac{d[p6]}{dt} = k_{17}[i9] + k_{18}[i10]$$

$$\frac{d[p11']}{dt} = k_{44}[i25]$$

(d). The C_6H_5CC + 1,3-pentadiene reaction mechanism and rate equations according to reaction paths in Figure S6 based on rate constants from Table S4.



$$\frac{d[i13]}{dt} = k_{-22}[i15] + k_{-23}[i14] + k_{-45}[i26] - (k_{22}+k_{23}+k_{24}+k_{45})[i13]$$

$$\frac{d[i14]}{dt} = k_{23}[i13] + k_{-26}[i16] - (k_{-23}+k_{26}+k_{25})[i14]$$

$$\frac{d[i15]}{dt} = k_{22}[i13] + k_{-27}[i16] - (k_{-22}+k_{27})[i14]$$

$$\frac{d[i16]}{dt} = k_{26}[i14] + k_{27}[i15] - (k_{-26}+k_{-27}+k_{28})[i14]$$

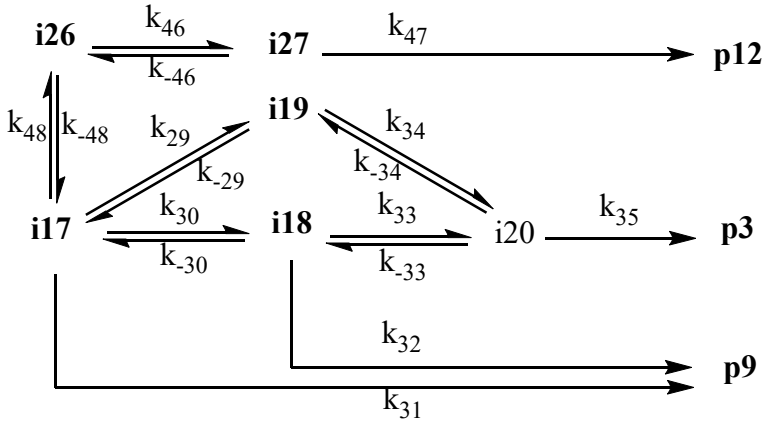
$$\frac{d[i26]}{dt} = k_{45}[i13] + k_{-46}[i27] - (k_{-45}+k_{46})[i26]$$

$$\frac{d[i27]}{dt} = k_{46}[i26] - (k_{-46}+k_{47})[i27]$$

$$\frac{d[p7]}{dt} = k_{28}[i16]$$

$$\frac{d[p8]}{dt} = k_{24}[i13] + k_{25}[i14]$$

$$\frac{d[p12]}{dt} = k_{47}[i27]$$



$$\frac{d[i17]}{dt} = k_{-29}[i19] + k_{-30}[i18] + k_{-48}[i26] - (k_{29}+k_{30}+k_{31}+k_{48})[i17]$$

$$\frac{d[i18]}{dt} = k_{30}[i17] + k_{-33}[i20] - (k_{-30}+k_{33}+k_{32})[i18]$$

$$\frac{d[i19]}{dt} = k_{29}[i17] + k_{-34}[i20] - (k_{-29}+k_{34})[i19]$$

$$\frac{d[i20]}{dt} = k_{33}[i18] + k_{34}[i19] - (k_{-33}+k_{-34}+k_{35})[i20]$$

$$\frac{d[i26]}{dt} = k_{48}[i17] + k_{-46}[i27] - (k_{-48}+k_{46})[i26]$$

$$\frac{d[i27]}{dt} = k_{46}[i26] - (k_{-46}+k_{47})[i27]$$

$$\frac{d[p3]}{dt} = k_{35}[i20]$$

$$\frac{d[p9]}{dt} = k_{31}[i17] + k_{32}[i18]$$

$$\frac{d[p12]}{dt} = k_{47}[i27]$$

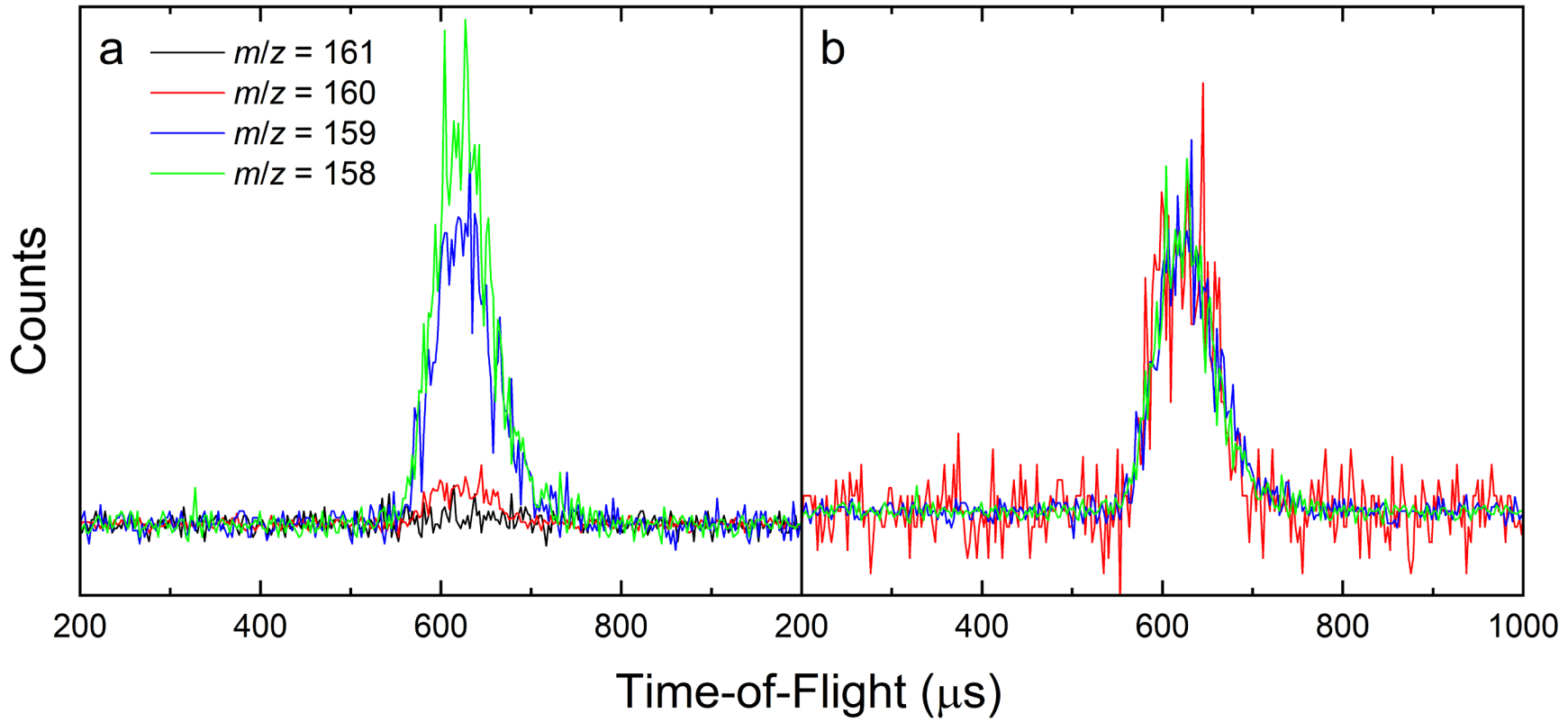


Fig. S1 Absolute (**a**) and normalized (**b**) time-of-flight (TOF) mass spectra for the reaction of phenylethynyl radicals (C_6H_5CC) with 1,3-butadiene-d_6 (C_4D_6) at m/z = 158–161.

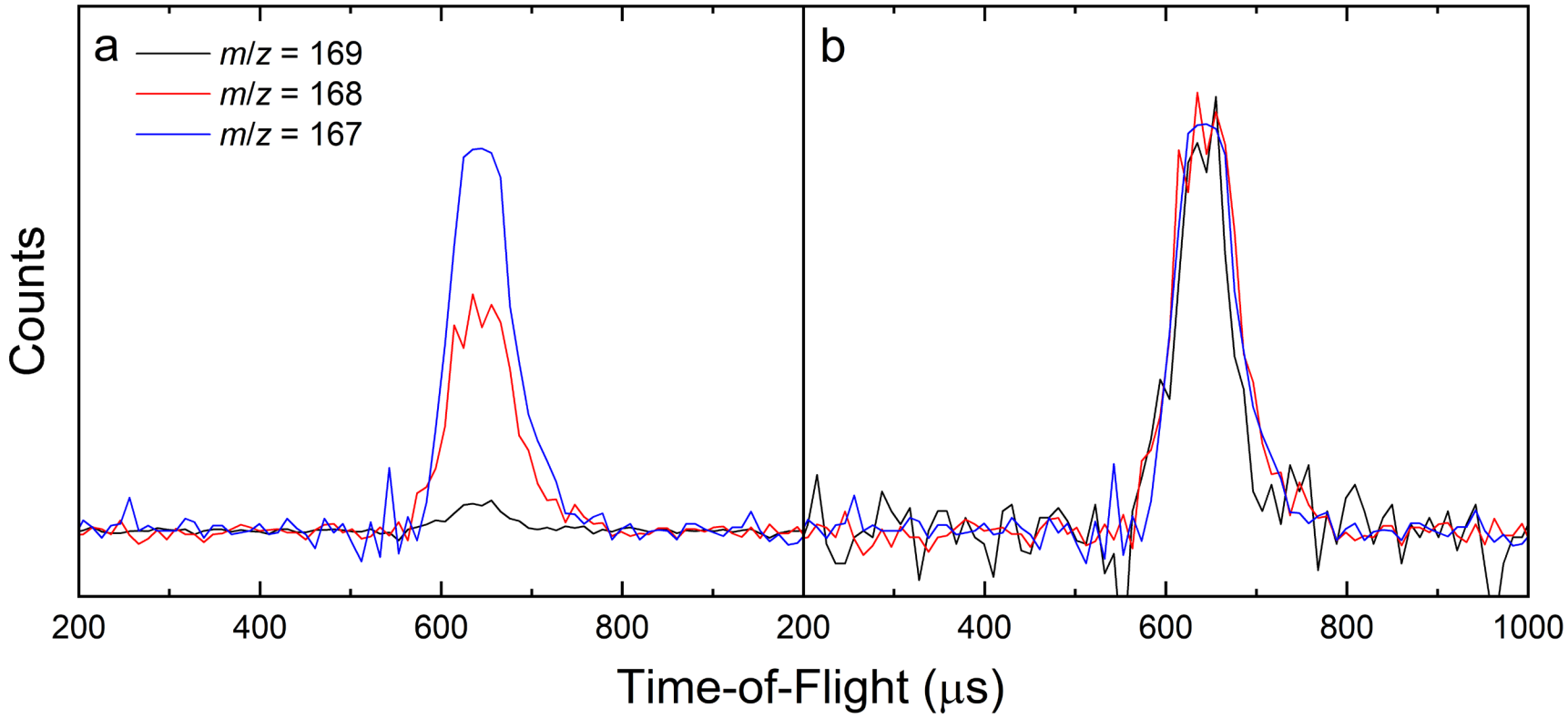


Fig. S2 Absolute (**a**) and normalized (**b**) time-of-flight (TOF) mass spectra for the reaction of phenylethynyl radicals (C_6H_5CC) with isoprene ($CH_2C(CH_3)CHCH_2$) at m/z = 167–169.

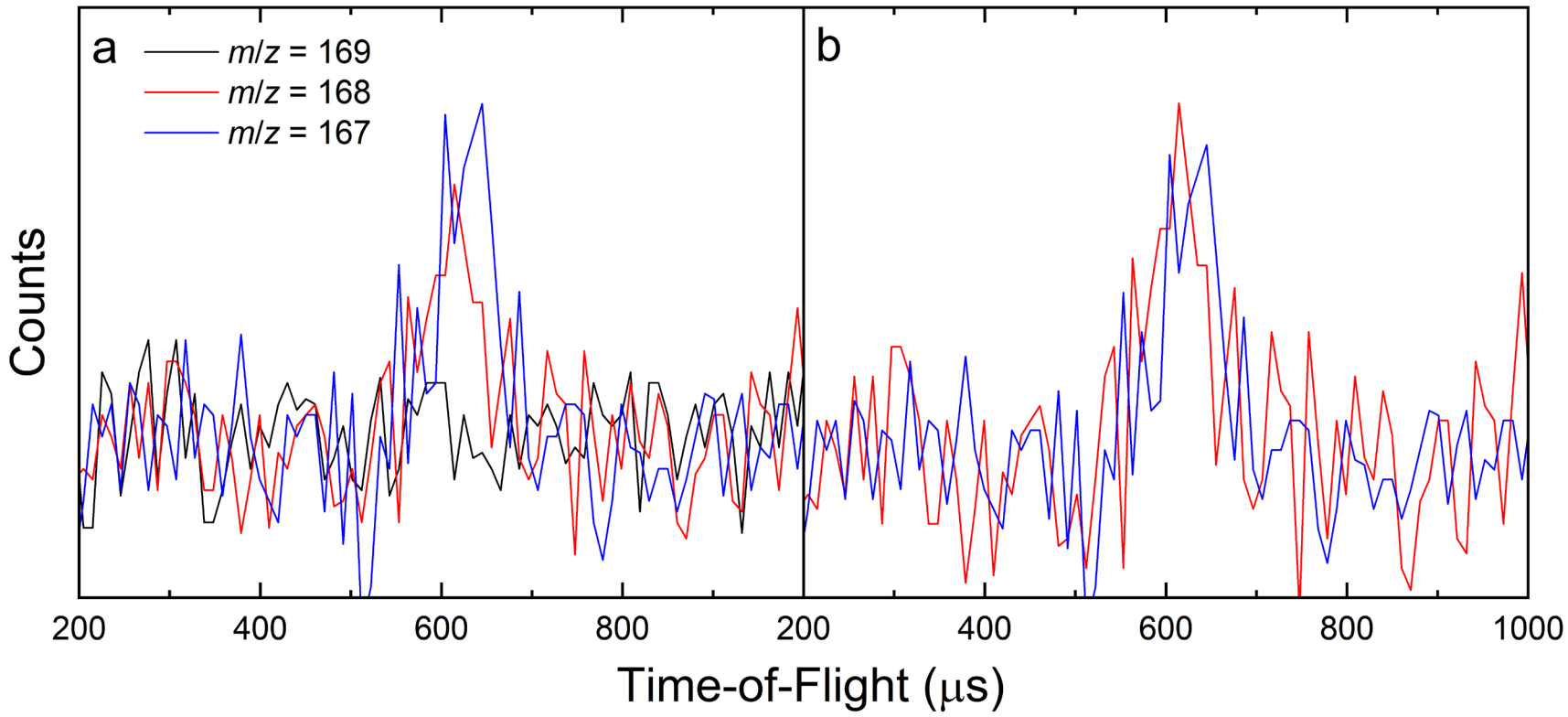


Fig. S3 Absolute (**a**) and normalized (**b**) time-of-flight (TOF) mass spectra for the reaction of phenylethynyl radicals (C_6H_5CC) with 1,3-pentadiene ($CH_2CHCHCHCH_3$) at m/z = 167–169.

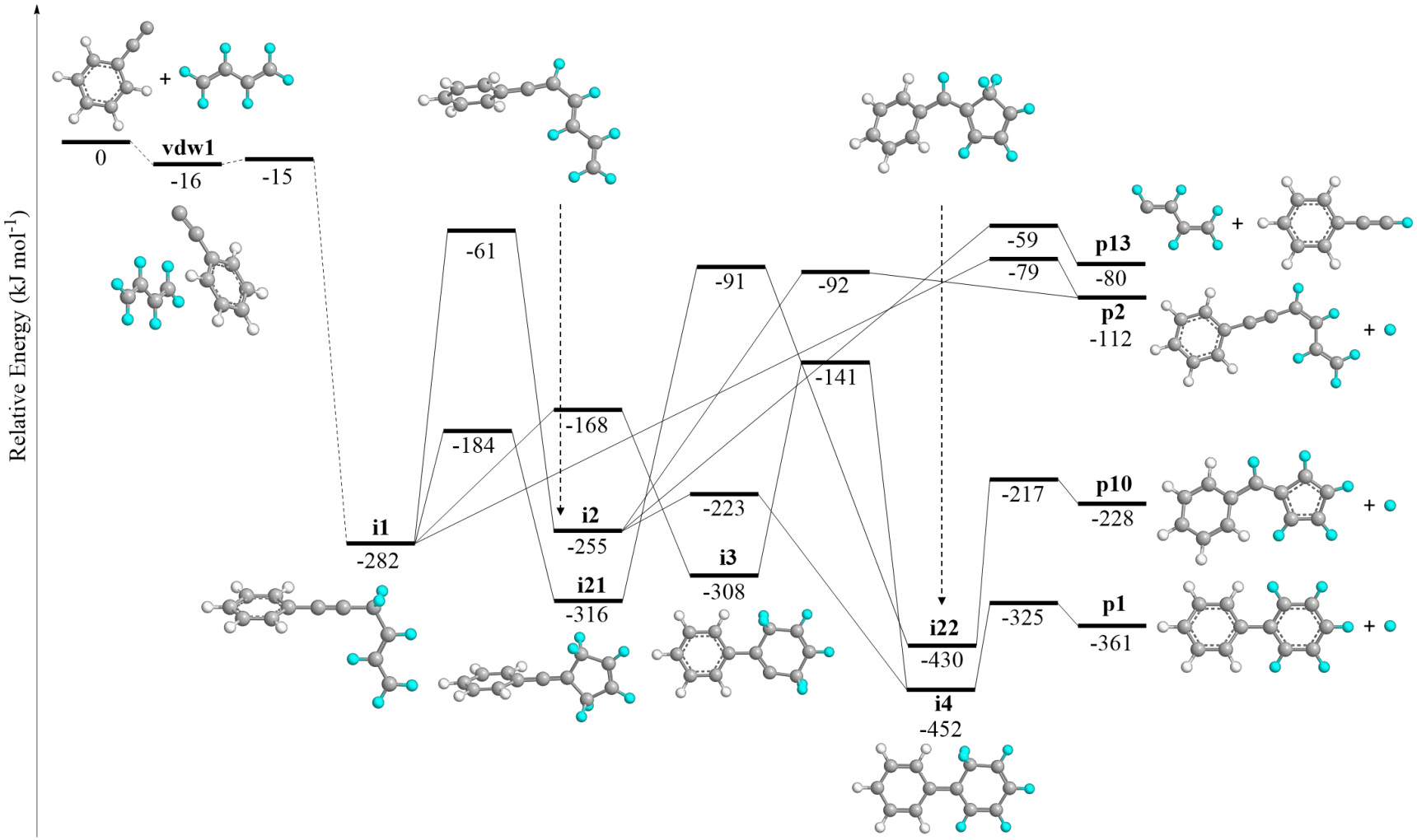


Fig. S4 Schematic potential energy surface for the reaction of phenylethynyl (C_6H_5CC) with 1,3-butadiene-d_6 (C_4D_6) calculated at the CCSD(T)/cc-pVTZ//*w*B97X-D/cc-pVTZ level. Carbon atoms are colored gray, hydrogens are white, and deuteriums are light blue.

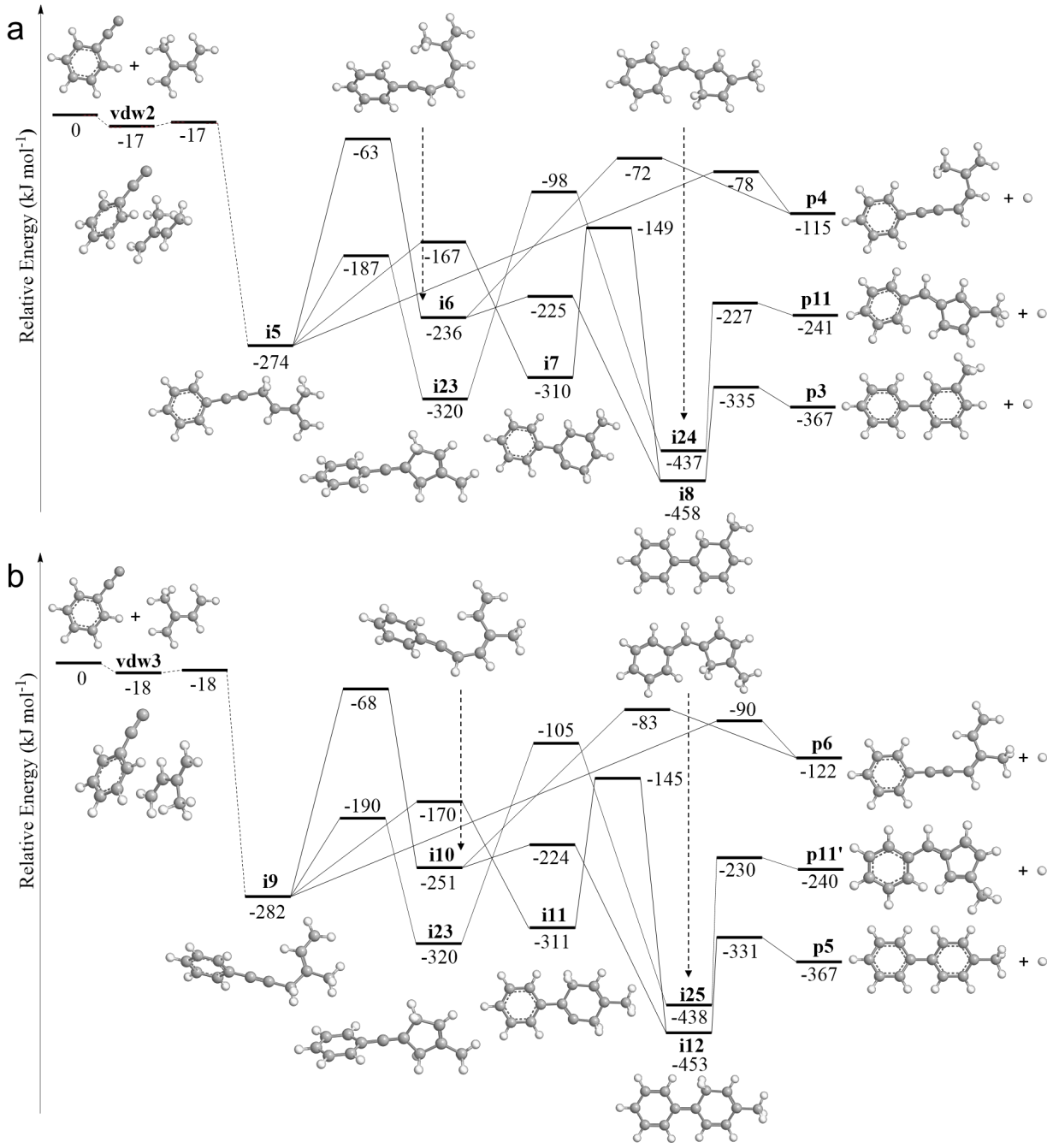


Fig. S5 Schematic potential energy surface for the reaction of phenylethynyl (C_6H_5CC) with isoprene ($CH_2C(CH_3)CHCH_2$) calculated at the CCSD(T)/cc-pVTZ//*w*B97X-D/cc-pVTZ level for phenylethynyl addition to the C4 (**a**) and C1 (**b**) carbons of isoprene. Carbons are colored as gray and hydrogens are white.

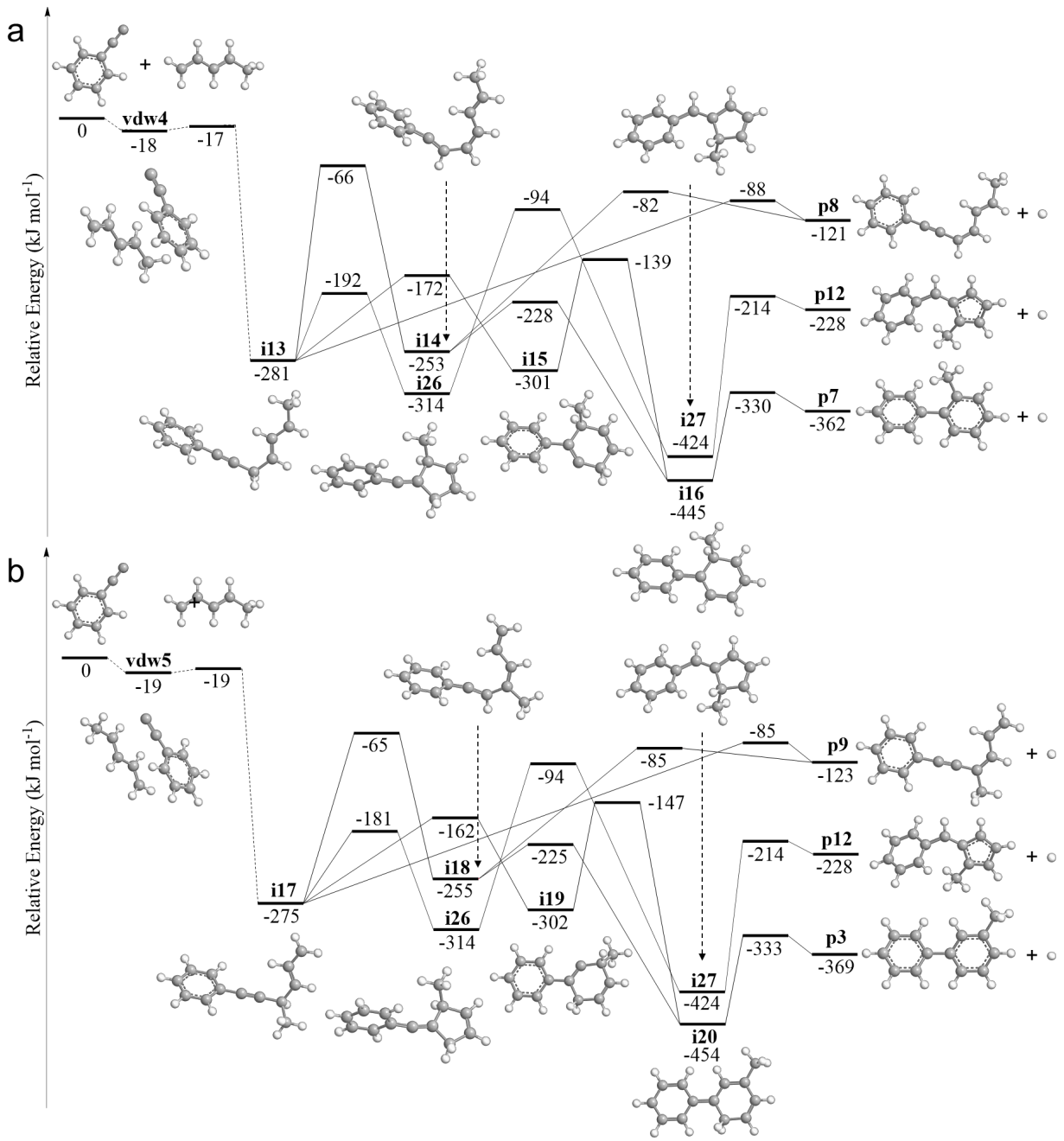


Fig. S6 Schematic potential energy surface for the reaction of phenylethynyl (C_6H_5CC) with 1,3-pentadiene ($CH_2CHCHCHCH_3$) calculated at the CCSD(T)/cc-pVTZ//*w*B97X-D/cc-pVTZ level for phenylethynyl addition to the C1 (**a**) and C4 (**b**) carbons of 1,3-pentadiene. Carbons are colored as gray and hydrogens are white.

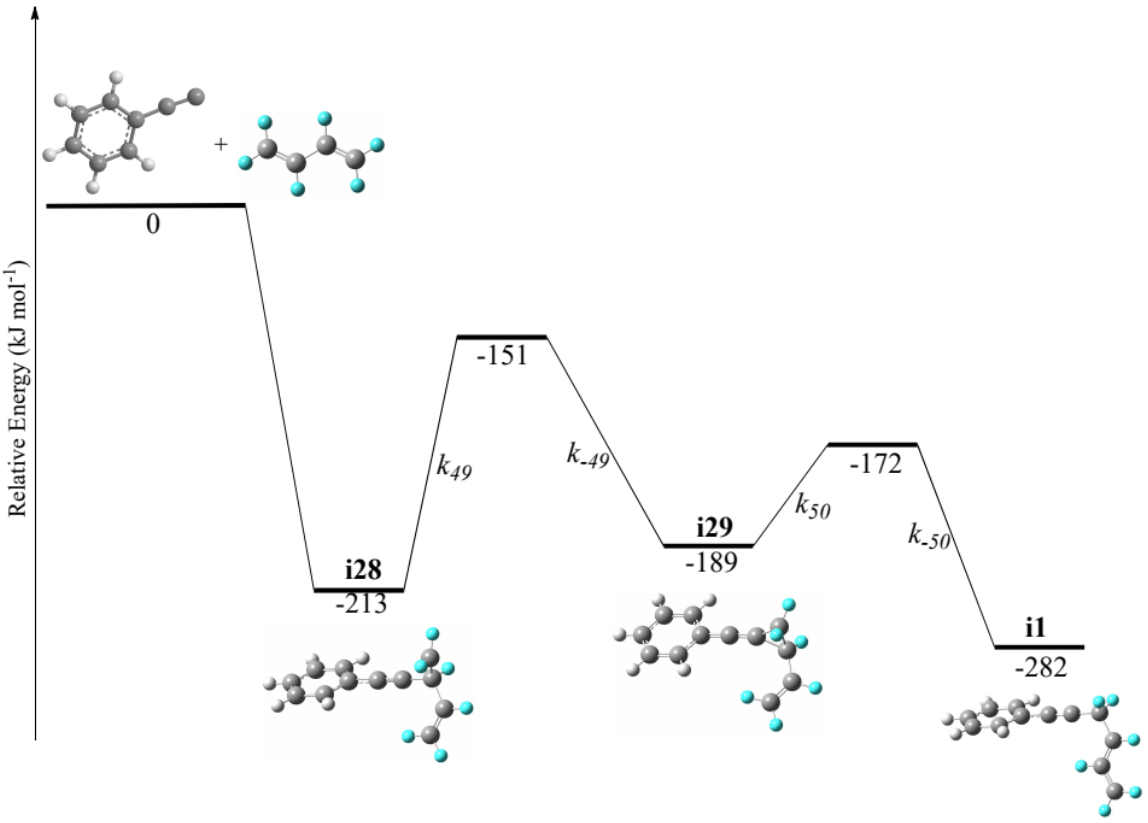


Fig S7 Schematic potential energy surface for the reaction of phenylethynyl (C_6H_5CC) with 1,3-butadiene-d_6 (C_4D_6) calculated at the CCSD(T)/cc-pVTZ//*w*B97X-D/cc-pVTZ level for phenylethynyl addition to the C2 carbons of 1,3-butadiene-d_6. Carbon atoms are colored gray, hydrogens are white, and deuteriums are light blue.

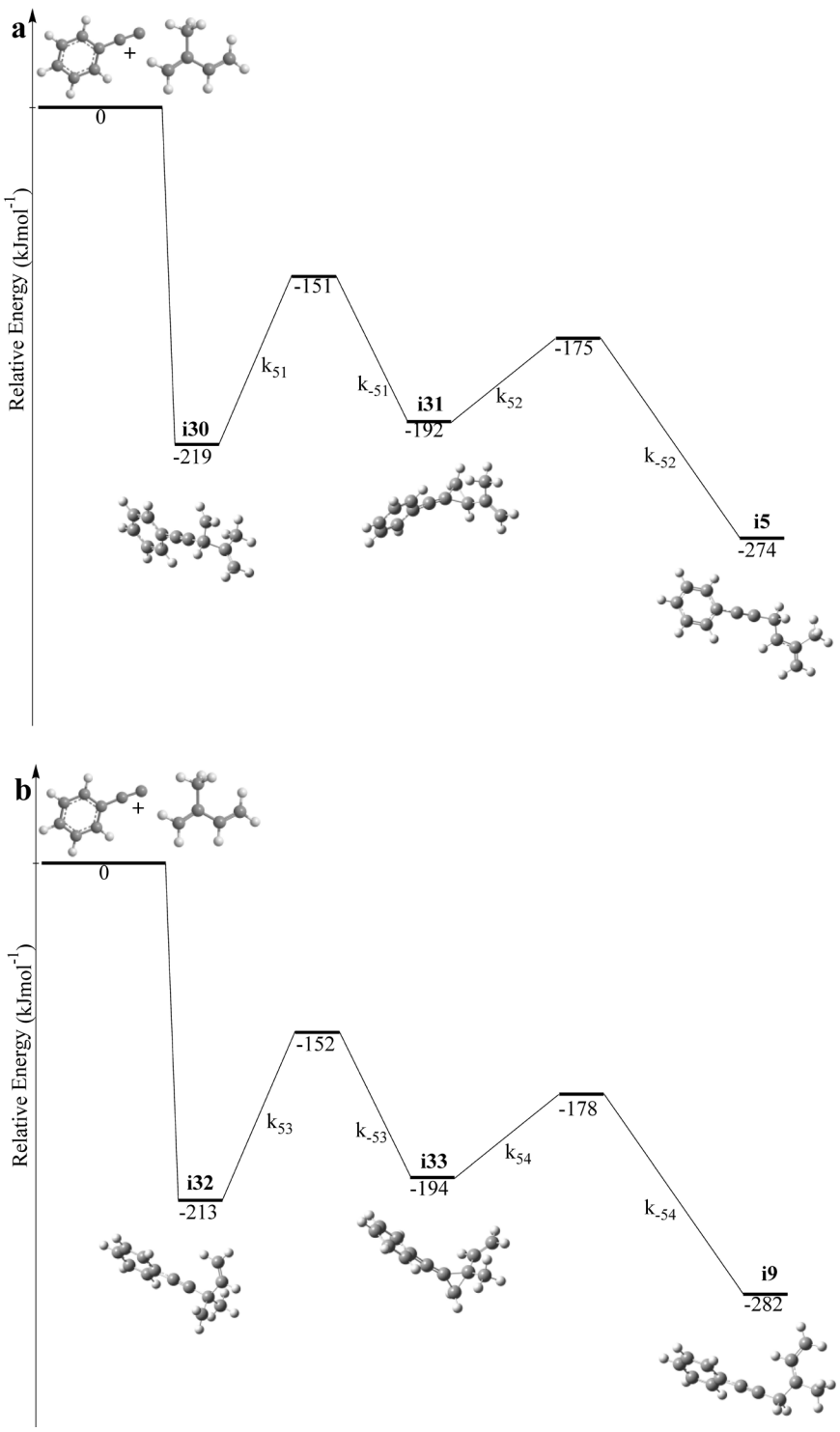


Fig. S8 Schematic potential energy surface for the reaction of phenylethynyl (C_6H_5CC) with isoprene ($CH_2C(CH_3)CHCH_2$) calculated at the CCSD(T)/cc-pVTZ//*w*B97X-D/cc-pVTZ level for phenylethynyl addition to the C2 (**a**) and C3 (**b**) carbons of isoprene. Carbons are colored as gray and hydrogens are white.

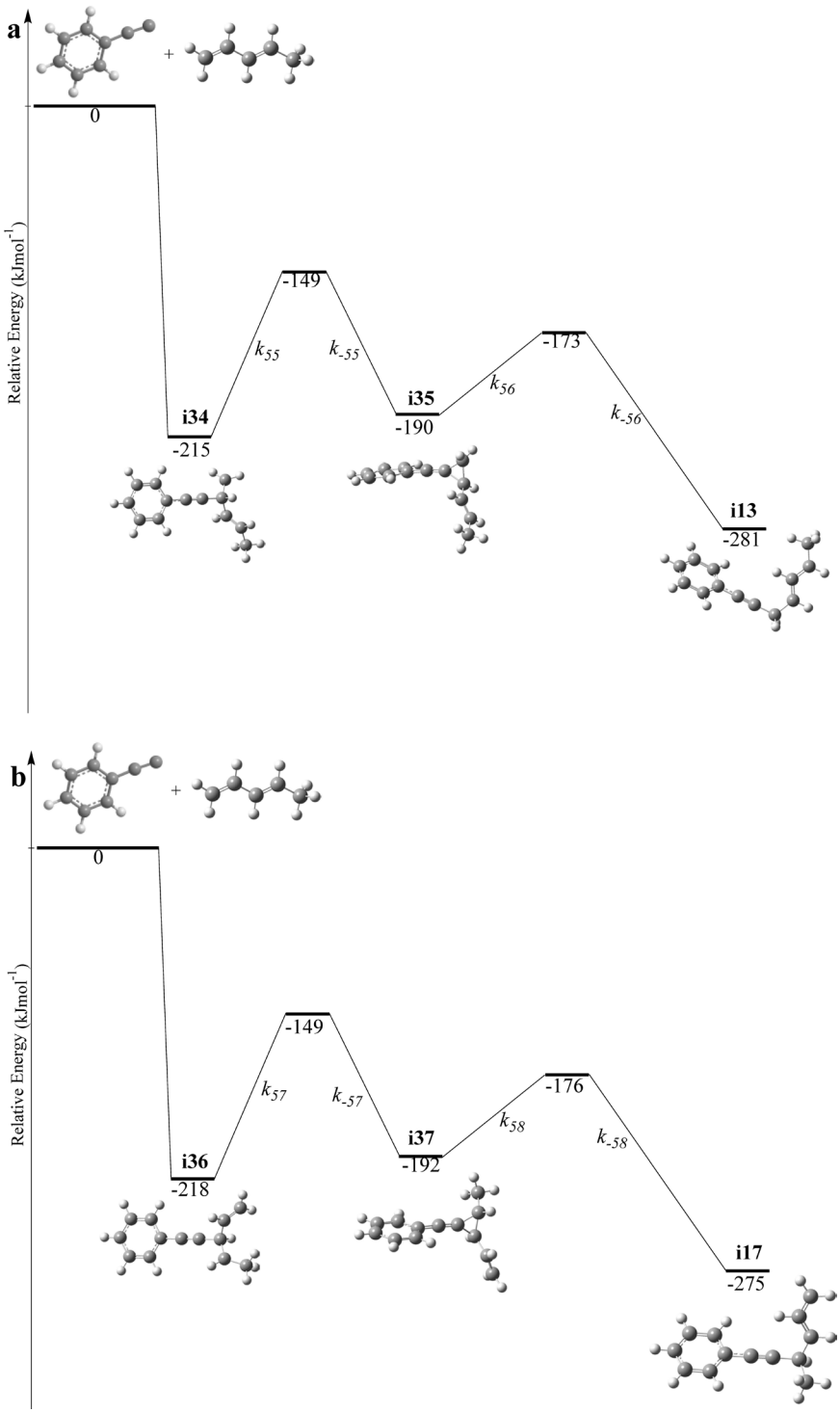


Fig. S9 Schematic potential energy surface for the reaction of phenylethynyl (C_6H_5CC) with 1,3-pentadiene ($CH_2CHCHCHCH_3$) calculated at the CCSD(T)/cc-pVTZ//*w*B97X-D/cc-pVTZ level for phenylethynyl addition to the C2 (**a**) and C3 (**b**) carbons of 1,3-pentadiene. Carbons are colored as gray and hydrogens are white.

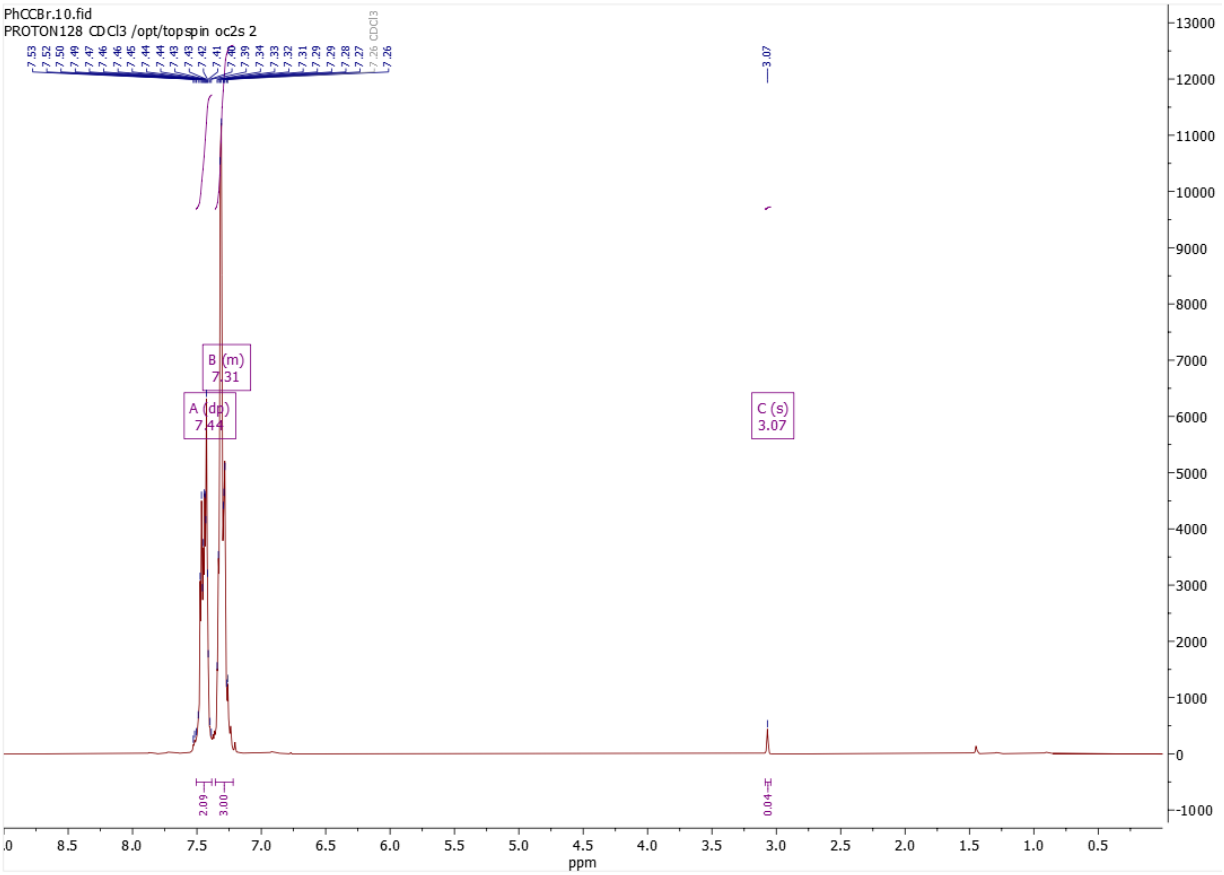


Fig. S10 ^{1}H NMR spectrum of (2-bromoethynyl)benzene. A small impurity of phenylacetylene is still observed at 3.07 ppm and was later removed by distillation.

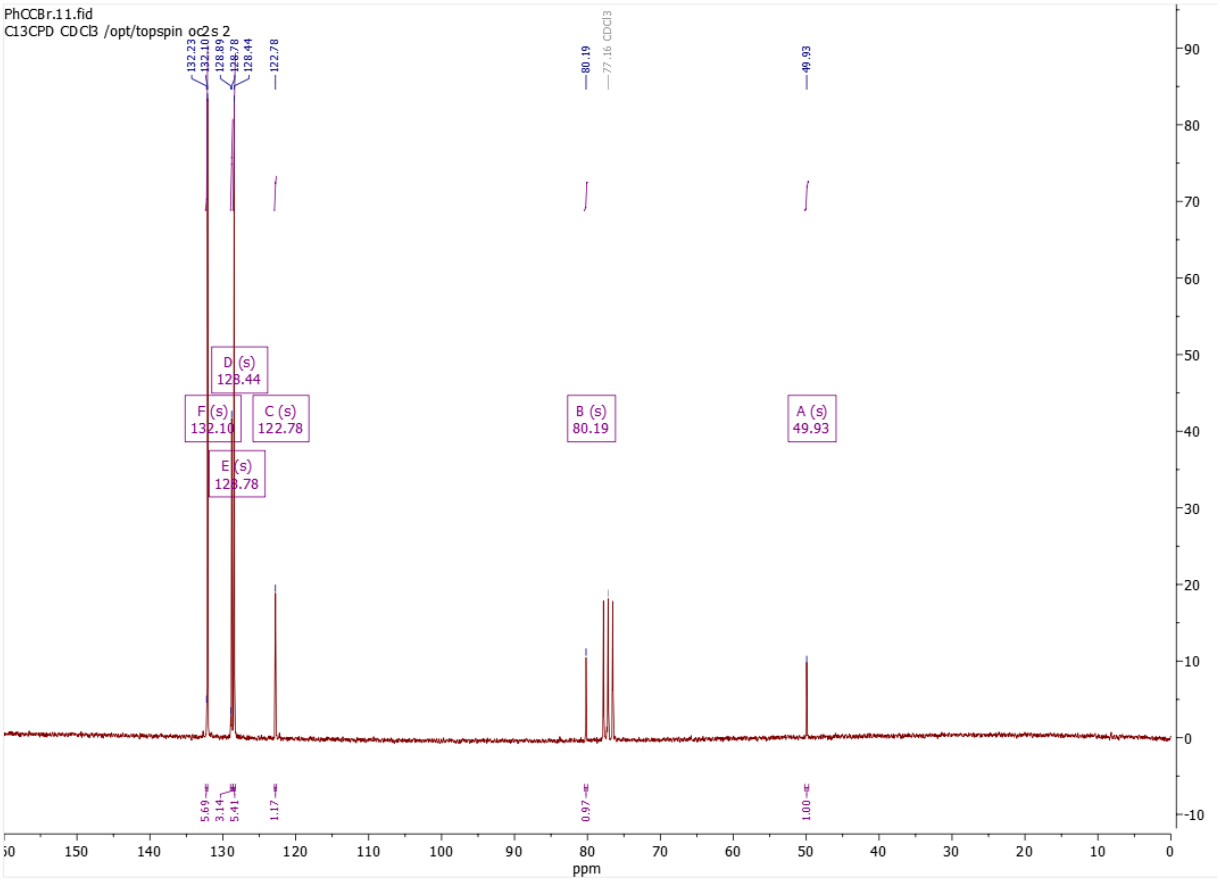


Fig. S11 ^{13}C NMR spectrum of (2-bromoethynyl)benzene.

Supplementary References

1 M. V. Russo, C. Lo Sterzo, P. Franceschini, G. Biagini and A. Furlani, Synthesis of highly ethynylated mono and dinuclear Pt(II) tethers bearing the 4,4′-bis(ethynyl)biphenyl (debp) unit as central core, *J. Organomet. Chem.*, 2001, **619**, 49-61.

2 M. X.-W. Jiang, M. Rawat and W. D. Wulff, Contingency and serendipity in the reactions of Fischer carbene complexes with conjugated triynes, *J. Am. Chem. Soc.*, 2004, **126**, 5970-5971.