Supplementary Material

Initiation Reactions in the High Temperature Decomposition of Styrene

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Travis Sikes [1], Colin Banyon [1], Rachel A. Schwind [2], Patrick T. Lynch [3], Andrea Comandini [4], Raghu Sivaramakrishnan [1], and Robert S. Tranter [1]

[1] *Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700 South Cass Ave., Lemont, IL 60439, USA*

[2] *Chemical and Environmental Engineering, School of Engineering, Brown University, 184 Hope St., Providence, RI, 02912, USA*

[3] *Department of Mechanical and Industrial Engineering, University of Illinois at Chicago, 842 W. Taylor St., Chicago IL 60607, USA*

[4] *INSIS, CNRS, 1C Avenue de la Recherche Scientifique, 45071 Orléans Cedex 2, France*

Corresponding author:

Robert S. Tranter (tranter@anl.gov)
Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL 60439
Tel: +1-630-252-6505

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1. Species Information

Table S1. Species name translations for mechanism names, chemical names, and InChI. InChiKey is suitable for internet and PubChem database searching.

Mechanism Name	Chemical Name	InChIKey	InChI
C16H10	pyrene	BBEAQIROQSPTKN-UHFFFAOYSA-N	InChI=1S/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H
C2HC6H4C6H4C2H	diethynyl-biphenyl	QBZOHZXEKPNLSP-UHFFFAOYSA-N	InChI=1S/C16H10/c1-3-13-7-5-9-15(11-13)16-10-6-8-14(4-2)12-16/h1-2,5-12H
C6H5CCHC6H5		NIXPGVLLMKFPPA-UHFFFAOYSA-N	InChI=1S/C14H11/c1-12(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h1-11H
C14H10	phenanthrene	YNPNZTXNASCQKK-UHFFFAOYSA-N	InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)13/h1-10H
C6H5CCC6H5	diphenylacetylene	JRXXLCKWQFKACW-UHFFFAOYSA-N	InChI=1S/C14H10/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-10H
C13H8CH2	9-methylene-fluorene	ZYASLTYCYTYKFC-UHFFFAOYSA-N	InChI=1S/C14H10/c1-10-11-6-2-4-8-13(11)14-9-5-3-7-12(10)14/h2-9H,1H2
C6H4(C2H)C6H5	ethyl-biphenyl	PIARMLHJPVJQKG-UHFFFAOYSA-N	InChI=1S/C14H10/c1-2-12-7-6-10-14(11-12)13-8-4-3-5-9-13/h1,3-11H
C12H10	biphenyl	ZUOUZKKEUPVFJK-UHFFFAOYSA-N	InChI=1S/C12H10/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-10H
C10H7	1-naphthyl	ZHZZWIQPCAMTIM-UHFFFAOYSA-N	InChI=1S/C10H7/c1-2-6-10-8-4-3-7-9(10)5-1/h1-7H
C9H6CH	benzofulvenyl	NGKKPHSSSRLRTM-UHFFFAOYSA-N	InChI=1S/C10H7/c1-8-6-7-9-4-2-3-5-10(8)9/h1-7H
C10H6_12	3,4-didehydronaphthalene	GWNSUXNLALZEML-UHFFFAOYSA-N	InChI=1S/C10H6/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-7H
C6H4(C2H)2	1,2-diethynylbenzene	CBYDUPRWILCUIC-UHFFFAOYSA-N	InChI=1S/C10H6/c1-3-9-7-5-6-8-10(9)4-2/h1-2,5-8H
C8H8	styrene	PPBRXRYQALVLMV-UHFFFAOYSA-N	InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H/1H2
oiC8H8	ortho-iso-styrene	JZMQWMRCIBSWQI-UHFFFAOYSA-N	InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h3-6H,1,7H2
aC8H7	alpha-styryl	HVOAOEQOQJYIGP-UHFFFAOYSA-N	InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h3-7H/1H2
bC8H7	beta-styryl	XXZXPSKZWQWGKG-UHFFFAOYSA-N	InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h1-7H
oC8H7	ortho-styryl	YQFQMJCKLXLQOX-UHFFFAOYSA-N	InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h2-6H/1H2
mC8H7	meta-styryl	PCPQORSTCJDFDI-UHFFFAOYSA-N	InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h2-4,6-7H,1H2
pC8H7	para-styryl	PWLRAMSGTKOJDW-UHFFFAOYSA-N	InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h2,4-7H,1H2
C8H6	phenylacetylene	UEXCJVNBTNXOEH-UHFFFAOYSA-N	InChI=1S/C8H6/c1-2-8-6-4-3-5-7-8/h1,3-7H
C6H4C2H	2-	RNNZJEBQMQRHQJ-	InChI=1S/C8H5/c1-2-8-6-4-3-5-7-8/h1,3-6H

	ethynylphenyl	UHFFFAOYSA-N	
C8H2	tetracetylene	CDGAYCHXIBGGNI-UHFFFAOYSA-N	InChI=1S/C8H2/c1-3-5-7-8-6-4-2/h1-2H
C8H	1,3,5,7-octatetrynyl	GTEOCQSGHJLKQX-UHFFFAOYSA-N	InChI=1S/C8H/c1-3-5-7-8-6-4-2/h1H
Benzene	benzene	UHOVQNZJYSORNB-UHFFFAOYSA-N	InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H
Fulvene	fulvene	UHOVQNZJYSORNB-UHFFFAOYSA-N	InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H
HD5Y13	1,3-hexadiene-5-yne	OGWJYLKDZYZYBA-UHFFFAOYSA-N	InChI=1S/C6H6/c1-3-5-6-4-2/h1,4-6H,2H2
HD15	1,5-hexadiyne	YFIBSNDOVCWPBL-UHFFFAOYSA-N	InChI=1S/C6H6/c1-3-5-6-4-2/h1-2H,5-6H2
DMCB34	3,4-dimethylenecyclobutene	WHCRVRGGFVUMOK-UHFFFAOYSA-N	InChI=1S/C6H6/c1-5-3-4-6(5)2/h3-4H,1-2H2
C6H5	phenyl	CIUQDSCDWFSTQR-UHFFFAOYSA-N	InChI=1S/C6H5/c1-2-4-6-5-3-1/h1-5H
l-C6H5	CHCCHCHCHCH	QKDIQSQLXPANKK-UHFFFAOYSA-N	InChI=1S/C6H5/c1-3-5-6-4-2/h1-3,5-6H
o-C6H4	o-benzyne	KLYCPFXDDDMZNQ-UHFFFAOYSA-N	InChI=1S/C6H4/c1-2-4-6-5-3-1/h1-4H
C6H4	(Z)-hex-3-en-1/5-diyne	KIWAUQFHKHLABA-WAYWQWQTSA-N	InChI=1S/C6H4/c1-3-5-6-4-2/h1-2,5-6H/b6-5-
C6H3	HCCCHCCCH (linear)	RYHFXBYSIUWIFK-UHFFFAOYSA-N	InChI=1S/C6H3/c1-3-5-6-4-2/h1H,2H2
C6H2	triacetylene	MZHROOGPARRVHS-UHFFFAOYSA-N	InChI=1S/C6H2/c1-3-5-6-4-2/h1-2H
l-C5H5	1-vinylpropargyl	MOHCYMPYDWGDHY-UHFFFAOYSA-N	InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2
C5H5	cyclopentadienyl	HPYIUKIBUJFXII-UHFFFAOYSA-N	InChI=1S/C5H5/c1-2-4-5-3-1/h1-5H
n-C5H3	HCCCHCCH	FEOOCZDIRHAFDB-UHFFFAOYSA-N	InChI=1S/C5H3/c1-3-5-4-2/h1-2,5H
H2CCCCCH	2,4-pentadiynyl-1	FLUJJNYXRYEAOV-UHFFFAOYSA-N	InChI=1S/C5H3/c1-3-5-4-2/h1H,2H2
i-C4H5	CH2CHCCH2	ZQHGTWBTOVSLEJ-UHFFFAOYSA-N	InChI=1S/C4H5/c1-3-4-2/h3H,1-2H2
C4H4	vinylacetylene	WFYPICNXBKQZGB-UHFFFAOYSA-N	InChI=1S/C4H4/c1-3-4-2/h1/4H/2H2
i-C4H3	CH2CCCH	QJBRNNNJBVJKPK-UHFFFAOYSA-N	InChI=1S/C4H3/c1-3-4-2/h1H,2H2
n-C4H3	CHCHCCH	GQMYNBIOBOYFNG-UHFFFAOYSA-N	InChI=1S/C4H3/c1-3-4-2/h1-3H
C4H2	diacetylene	LLCSWKVOHICRDD-UHFFFAOYSA-N	InChI=1S/C4H2/c1-3-4-2/h1-2H
C4H	1,3-butadiynyl	GRADOOOISCPIDG-UHFFFAOYSA-N	InChI=1S/C4H/c1-3-4-2/h1H
C4	buta-1,3-diyn-	FMIYQRFAIMZVNM-	InChI=1S/C4/c1-3-4-2

	1,4-diyl	UHFFFAOYSA-N	
p-C3H4	propyne	MWWATHDPGQKSAR-UHFFFAOYSA-N	InChI=1S/C3H4/c1-3-2/h1H,2H3
a-C3H4	allene	IYABWNGZIDDRAK-UHFFFAOYSA-N	InChI=1S/C3H4/c1-3-2/h1-2H2
c-C3H4	cyclopropene	OOXWYYGXTJLWHA-UHFFFAOYSA-N	InChI=1S/C3H4/c1-2-3-1/h1-2H,3H2
C3H3	propargyl	DITHIFQMPPCBCU-UHFFFAOYSA-N	InChI=1S/C3H3/c1-3-2/h1H,2H2
c-C3H2	1,2-cyclopropadiene	VVLPCWSYZYKZKR-UHFFFAOYSA-N	InChI=1S/C3H2/c1-2-3-1/h1-2H
CHCCH	propynylidene triplet	OUSWHEMIRJJMAW-UHFFFAOYSA-N	InChI=1S/C3H2/c1-3-2/h1-2H
CHCCH(s)	propynylidene singlet	OUSWHEMIRJJMAW-UHFFFAOYSA-N	InChI=1S/C3H2/c1-3-2/h1-2H
C3H	C3H radical	WWDRUPNDOSDMRD-UHFFFAOYSA-N	InChI=1S/C3H/c1-3-2/h1H
C2H5	ethyl	QUPDWYMUPZLYJZ-UHFFFAOYSA-N	InChI=1S/C2H5/c1-2/h1H2,2H3
C2H4	ethylene	VGGSQFUCUMXWEO-UHFFFAOYSA-N	InChI=1S/C2H4/c1-2/h1-2H2
C2H3	vinyl	ORGHESHFQPYLAO-UHFFFAOYSA-N	InChI=1S/C2H3/c1-2/h1H/2H2
CH2C	vinylidene	SNVLJLYUUXKWOJ-UHFFFAOYSA-N	InChI=1S/C2H2/c1-2/h1H2
C2H2	acetylene	HSFWRNGVRCDJHI-UHFFFAOYSA-N	InChI=1S/C2H2/c1-2/h1-2H
C2H	ethynyl	XEHVFKKSDRMODV-UHFFFAOYSA-N	InChI=1S/C2H/c1-2/h1H
C2	ethyne	LBVWYGNGGJURHQ-UHFFFAOYSA-N	InChI=1S/C2/c1-2
H2	hydrogen	UFHFLCQGNIYNRP-UHFFFAOYSA-N	InChI=1S/H2/h1H
H	hydrogen-atom	YZCKVEUIGOORGS-UHFFFAOYSA-N	InChI=1S/H
He	helium	SWQJXJOGLNCZEY-UHFFFAOYSA-N	InChI=1S/He
Ar	argon	XKRFYHLGVUSROY-UHFFFAOYSA-N	InChI=1S/Ar
Kr	krypton	DNNSSWSSYDEUBZ-UHFFFAOYSA-N	InChI=1S/Kr
Ne	neon	GKAOGPIIYCISHV-UHFFFAOYSA-N	InChI=1S/Ne

Table S2. List of density, refractive index, and molar refractivity for mixture species.

Mechanism Name	ρ / g^{-1} cm^3	n	K_L / m^3 mol^{-1}	Reference
C8H8	0.9016	1.5440	36.47	ρ, n: PubChem
Kr	3.698×10^{-3}	1.0004	6.37	ρ, n: PubChem K_L: Gardiner 1981[a]

[a] DOI: 10.1016/0010-2180(81)90124-3

2. TOF-MS Figures

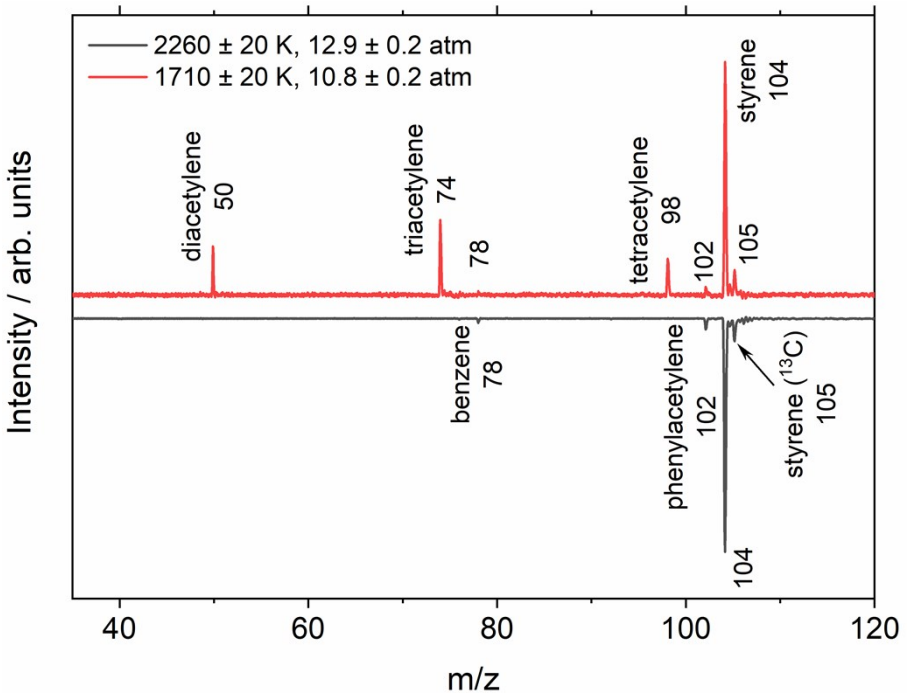

Figure S1. Mass spectra on a linear scale taken with MgF_2 window ~150 μs after the shock front arrival in a 0.06% C_8H_8/99.94% Ar mixture. Mass spectra are integrated from 8 – 10.5 eV.

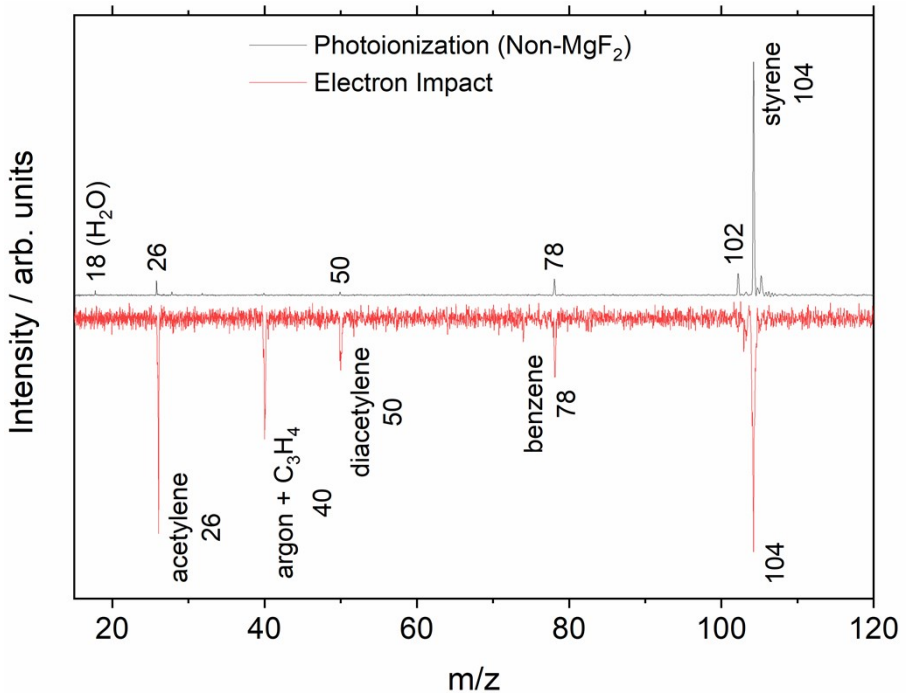

Figure S2. Mass spectra on a linear scale from photoionization (top) and electron impact (bottom) TOF-MS experiments ~150 μs post-shock. PI spectra were taken at 1875 ± 25 K, 11.3 ± 0.2 atm, 0.25% C_8H_8/99.75% Ar, and integrated from 8 – 10.5 eV. EI spectra were taken at 1830 ± 25 K, 368 ± 7 Torr, 0.5% C_8H_8/1.0% Ar/98.5% Ne and 21 eV.

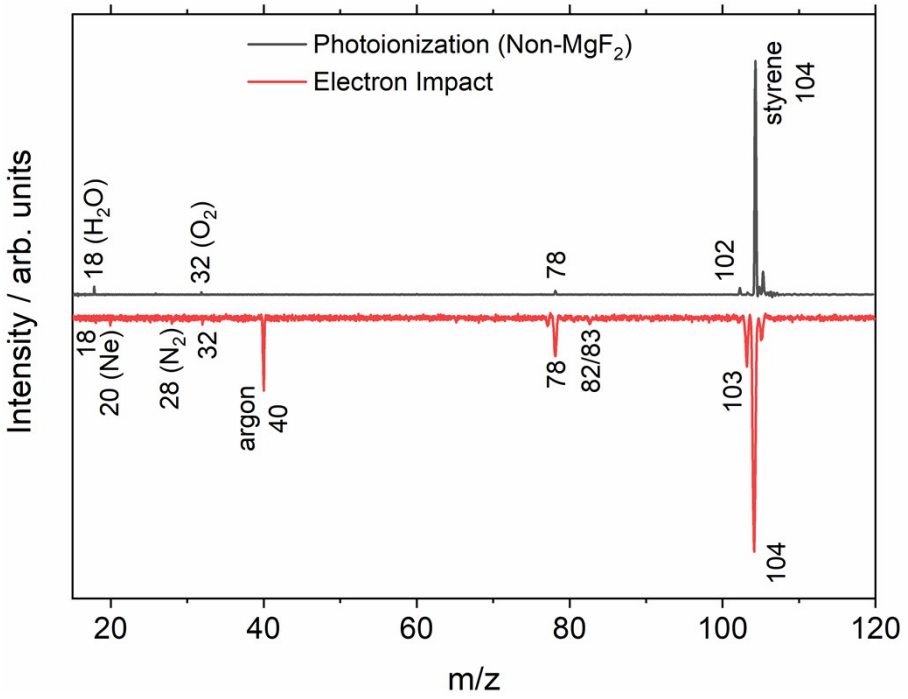

Figure S3. Mass spectra on a linear scale from photoionization (top) and electron impact (bottom) TOF-MS experiments pre-shock/non-reactive. PI spectra were taken at 1875 ± 25 K, 11.3 ± 0.2 atm, 0.25% C_8H_8/99.75% Ar, and integrated from 8 – 10.5 eV. EI spectra were taken at 1830 ± 25 K, 368 ± 7 Torr, 0.5% C_8H_8/1.0% Ar/98.5% Ne and 21 eV.

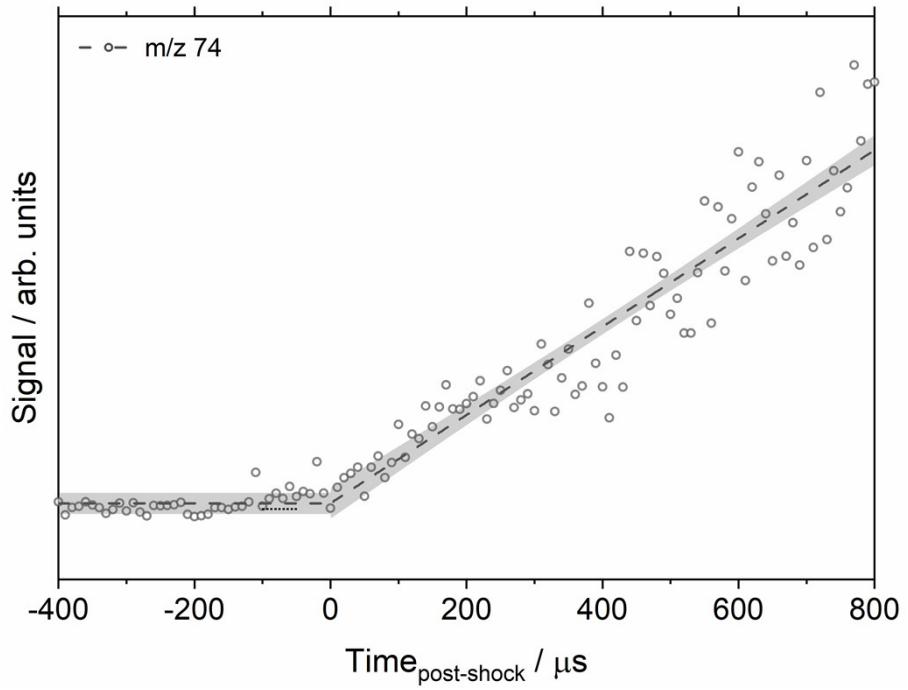

Figure S4. EI time history of m/z 74 at 1830 ± 25 K, 368 ± 7 Torr, 0.5% C_8H_8/1.0% Ar/98.5% Ne and 21 eV. Symbols represent the data, lines are experimental fits for clarity only, and shading is the 95% confidence interval of the experimental fit.

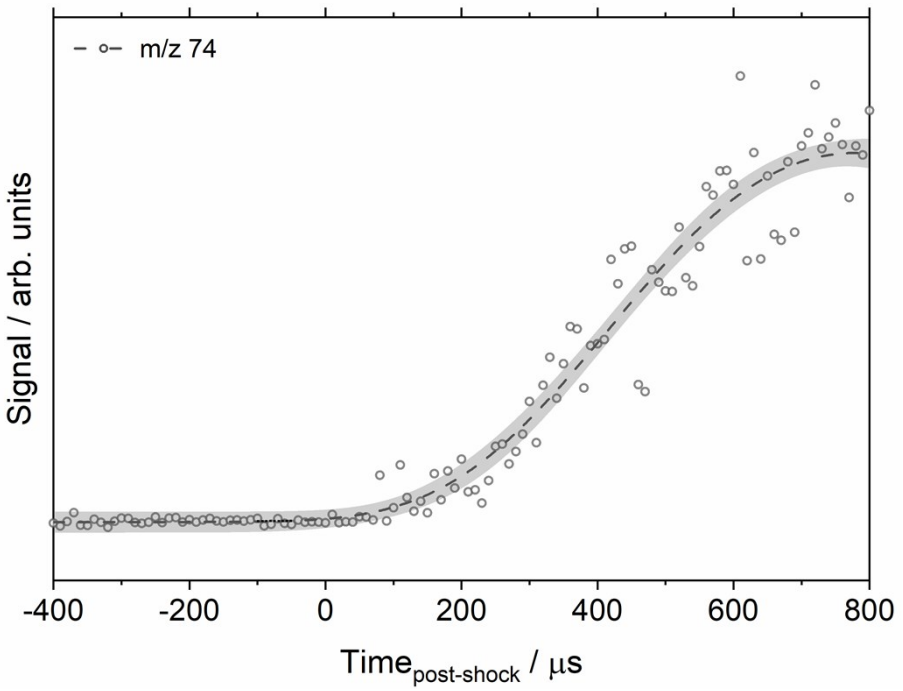

Figure S5. PI time history of m/z 74 with the MgF_2 filter at 1875 ± 25 K, 11.3 ± 0.2 atm, 0.25% C_8H_8/99.75% Ar, and integrated from 8 – 10.5 eV. Symbols represent the data, lines are experimental fits for clarity only, and shading is the 95% confidence interval of the experimental fit.

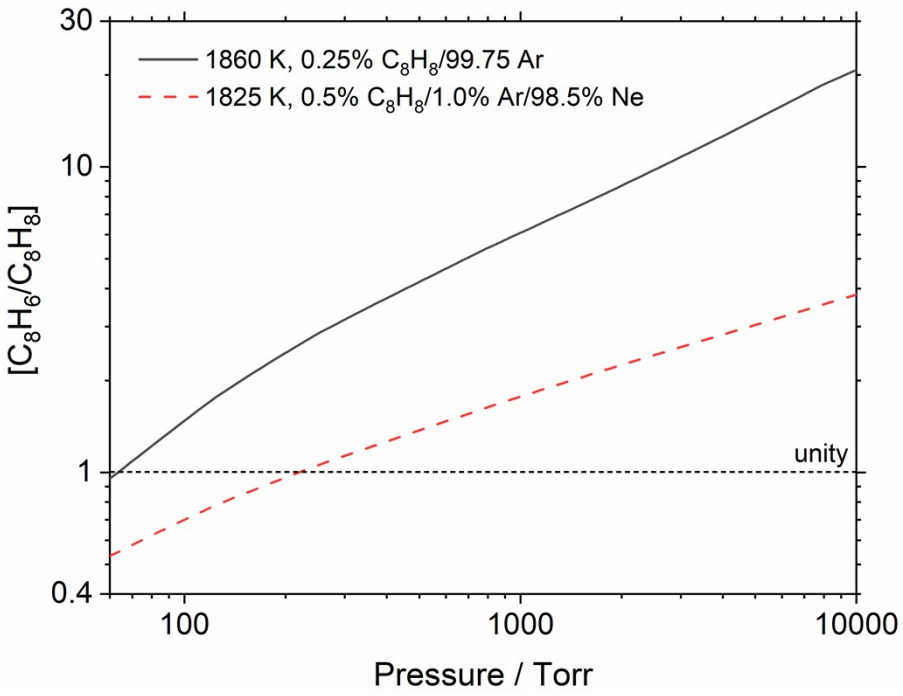

Figure S6. Simulation of $[C_8H_6]/[C_8H_8]$ at 150 μs in a constant volume reactor showing the effect of pressure.

3. Mechanism Analysis Figures

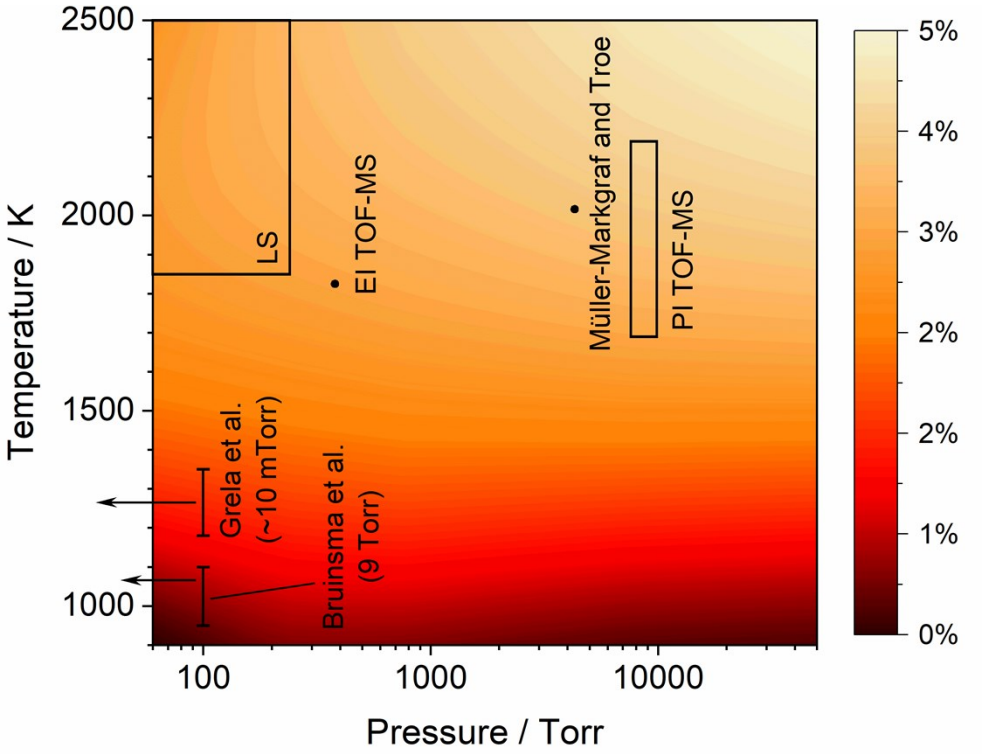

Figure S7. Percentage that R2: $C_8H_8 \rightarrow \beta\text{-}C_8H_7 + H$ comprises of the total styrene decomposition rate based upon the current mechanism. The conditions of the current study and literature studies are emphasized.

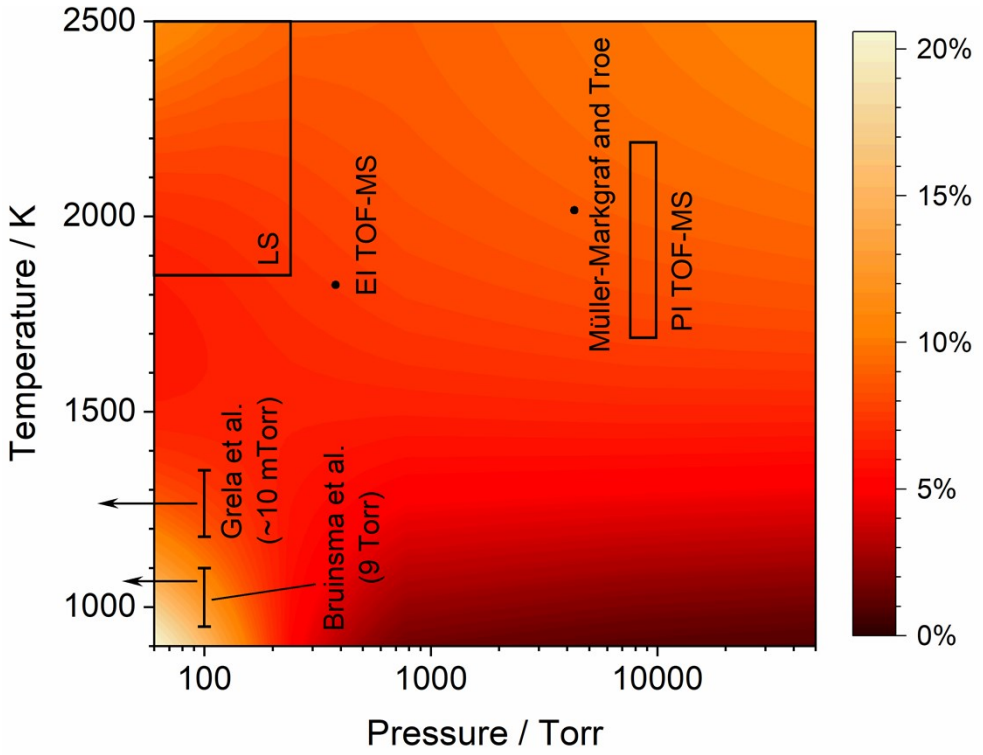

Figure S8. Percentage that R3: $C_8H_8 \rightarrow o\text{-}C_8H_7 + H$ comprises of the total styrene decomposition rate based upon the current mechanism. The conditions of the current study and literature studies are emphasized.

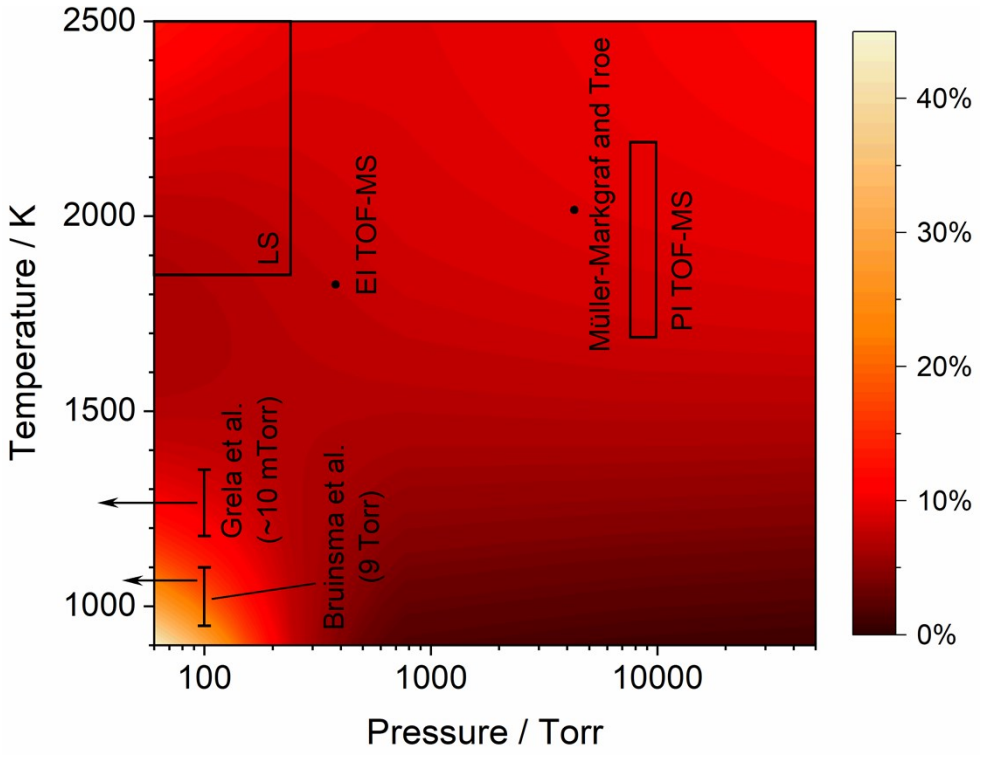

Figure S9. Percentage that R4: $C_8H_8 \rightarrow m\text{-}C_8H_7 + H$ comprises of the total styrene decomposition rate based upon the current mechanism. The conditions of the current study and literature studies are emphasized.

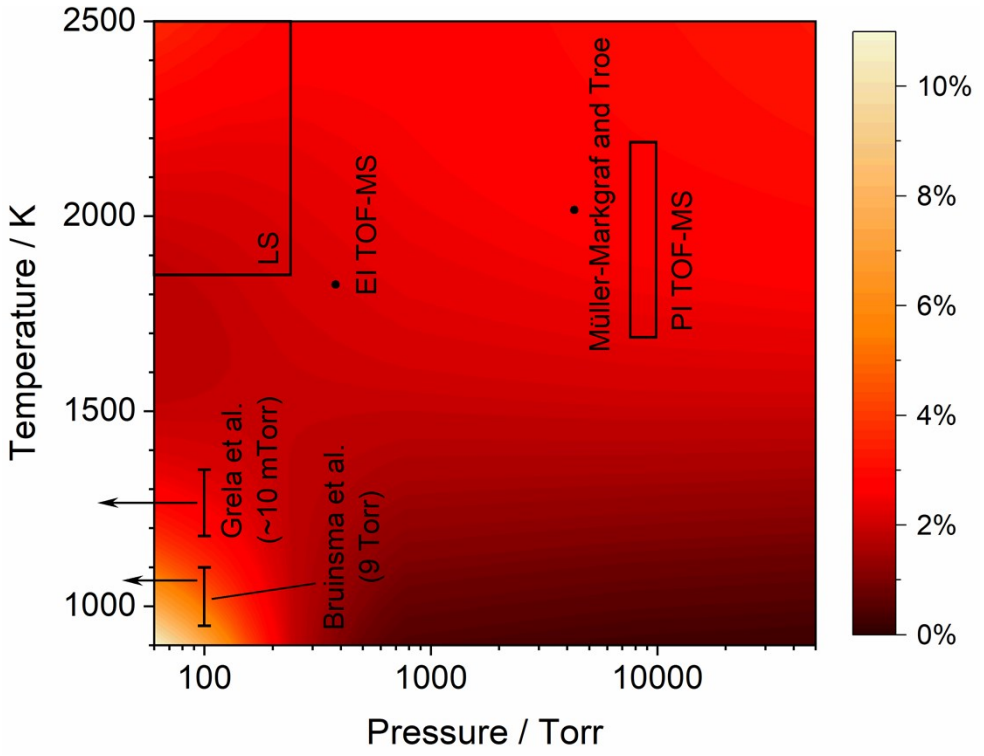

Figure S10. Percentage that R5: $C_8H_8 \rightarrow p\text{-}C_8H_7 + H$ comprises of the total styrene decomposition rate based upon the current mechanism. The conditions of the current study and literature studies are emphasized.

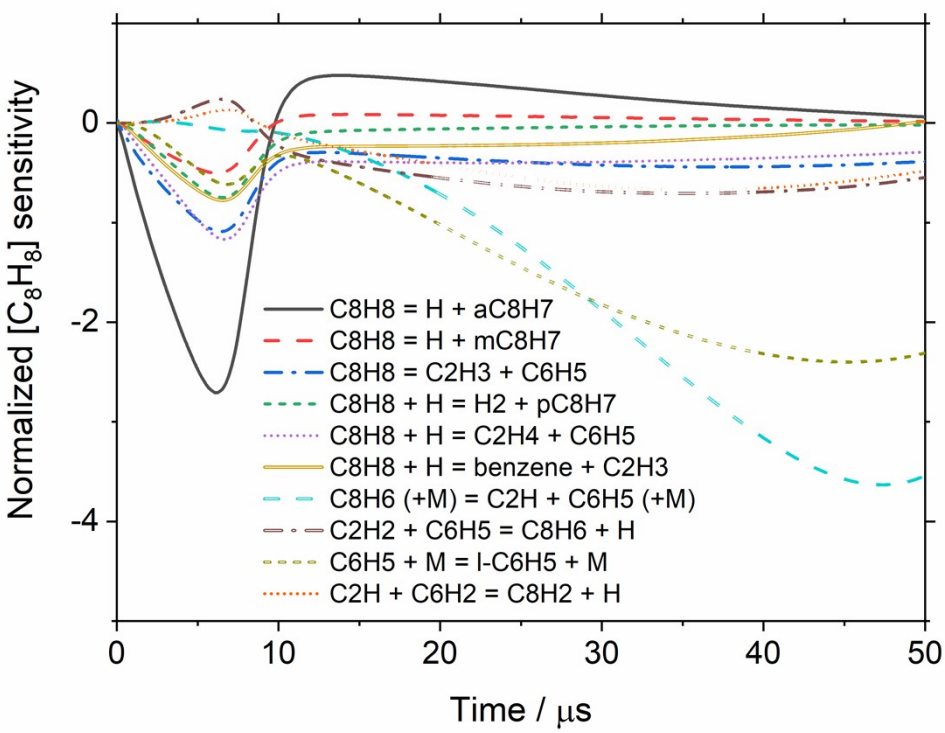

Figure S11. CHEMKIN-based normalized [C_8H_8] sensitivity of the current mechanism while simulating the Müller-Markgraf and Troe study.

4. Styrene Data Tables

Table S3. List of LS experimental conditions and rate coefficients for k_{decomp} (the total rate of styrene decomposition) at 60 Torr.

C_8H_8	T_1 / K	P_1 / Torr	T_2 / K	P_2 / Torr	k_{decomp} / s^{-1}
2%	298.0	1.90	1838	52	6.26×10^{3}
2%	298.0	2.00	1858	55	6.83×10^{3}
2%	293.0	2.10	1915	61	1.42×10^{4}
2%	298.0	2.10	1944	61	1.25×10^{4}
2%	297.8	1.95	1947	57	1.61×10^{4}
2%	296.5	1.85	1974	55	1.56×10^{4}
2%	296.6	1.88	1985	56	1.95×10^{4}
2%	298.0	1.90	1985	57	1.78×10^{4}
2%	296.6	1.85	1990	56	2.01×10^{4}
2%	296.7	1.95	1992	59	1.77×10^{4}
2%	293.1	1.90	2016	59	2.50×10^{4}
2%	296.7	1.90	2017	58	2.52×10^{4}
2%	296.8	1.85	2023	57	2.32×10^{4}
2%	297.9	1.95	2024	60	2.08×10^{4}
2%	298.0	2.05	2027	63	2.22×10^{4}
2%	293.1	1.85	2041	58	3.02×10^{4}
2%	297.9	2.00	2045	62	2.74×10^{4}
2%	298.0	2.30	2049	71	2.80×10^{4}
2%	296.5	1.90	2053	59	2.61×10^{4}
2%	293.1	1.80	2096	59	4.17×10^{4}
2%	292.3	1.75	2111	58	3.63×10^{4}
2%	292.3	1.70	2196	59	5.54×10^{4}
2%	292.3	1.65	2225	58	5.61×10^{4}
2%	297.0	1.65	2231	57	5.73×10^{4}
2%	297.0	1.62	2240	56	5.64×10^{4}
2%	297.8	1.60	2261	56	6.48×10^{4}
2%	296.9	1.80	2279	64	6.84×10^{4}
2%	297.7	1.50	2294	54	7.17×10^{4}
2%	292.3	1.60	2303	59	7.89×10^{4}
2%	297.8	1.50	2315	54	6.94×10^{4}
2%	297.7	1.50	2366	56	9.97×10^{4}
2%	292.4	1.55	2372	59	9.22×10^{4}
2%	292.4	1.50	2423	58	1.08×10^{5}
2%	292.4	1.45	2478	58	1.19×10^{5}
2%	292.4	1.40	2513	57	1.20×10^{5}
2%	297.7	1.65	2553	67	1.49×10^{5}
4%	296.7	1.60	1944	58	1.28×10^{4}
4%	296.2	1.44	1998	54	1.84×10^{4}
4%	296.4	1.44	2064	56	2.83×10^{4}
4%	296.2	1.55	2111	62	3.47×10^{4}

Table S4. List of LS experimental conditions and rate coefficients for k_{decomp} (the total rate of styrene decomposition) at 120 Torr.

C_8H_8	T_1 / K	P_1 / Torr	T_2 / K	P_2 / Torr	k_{decomp} / s^{-1}
1%	296.85	4.7	1873	116	9.62×10^{3}
1%	296.95	4.7	1889	117	7.97×10^{3}
1%	291.85	4.7	1897	120	1.08×10^{4}
1%	296.85	4.65	1944	120	1.52×10^{4}
1%	296.95	4.6	1965	120	1.56×10^{4}
1%	296.95	4.5	1991	120	2.04×10^{4}
1%	291.85	4.6	1992	125	2.19×10^{4}
1%	291.85	4.5	2016	124	2.99×10^{4}
1%	291.95	4.4	2045	123	3.39×10^{4}
1%	291.95	4.3	2085	123	4.94×10^{4}
1%	291.95	4.2	2131	124	6.22×10^{4}
1%	297.15	4.15	2177	123	6.68×10^{4}
1%	291.95	4.1	2179	124	9.08×10^{4}
1%	297.45	3.85	2210	116	8.89×10^{4}
1%	291.95	4	2214	123	8.06×10^{4}
1%	291.95	3.9	2264	123	1.18×10^{5}
1%	291.95	3.8	2271	120	1.16×10^{5}
1%	291.95	3.8	2284	121	1.32×10^{5}
1%	297.55	3.8	2306	120	1.32×10^{5}
1%	297.85	3.9	2310	123	1.51×10^{5}
1%	292.15	3.7	2346	122	1.59×10^{5}
1%	297.45	3.75	2347	121	1.53×10^{5}
1%	297.65	3.85	2349	124	1.73×10^{5}
1%	297.85	3.45	2355	112	1.81×10^{5}
1%	297.85	3.45	2359	112	1.64×10^{5}
1%	292.15	3.6	2389	121	1.84×10^{5}
1%	292.15	3.6	2400	122	2.09×10^{5}
1%	297.85	3.45	2422	115	2.65×10^{5}
1%	297.75	3.66	2426	123	2.04×10^{5}
1%	292.15	3.6	2427	123	2.10×10^{5}
1%	292.15	3.5	2448	121	2.20×10^{5}
1%	297.75	3.55	2464	121	2.53×10^{5}
2%	292.95	4.7	1812	128	6.06×10^{3}
2%	293.05	5	1900	127	1.19×10^{4}
2%	292.95	4.2	1923	123	1.66×10^{4}
2%	292.95	4.1	1961	123	2.13×10^{3}
2%	292.95	2.1	1974	129	1.96×10^{4}
2%	293.05	4	2002	123	2.38×10^{3}
2%	293.05	1.9	2037	126	2.44×10^{4}
2%	293.05	3.9	2039	123	2.36×10^{4}

2%	293.15	3.8	2078	122	3.05×10^{4}
2%	292.95	3.75	2101	122	3.94×10^{4}
2%	292.95	5	2145	128	4.87×10^{4}
2%	293.15	3.65	2174	124	5.98×10^{4}
2%	292.25	1.75	2302	128	1.36×10^{5}
4%	296.65	3.7	1829	123	5.30×10^{3}
4%	296.75	3.4	1898	119	7.74×10^{3}
4%	296.65	3.15	1919	111	1.97×10^{3}
4%	296.65	3.1	1977	114	1.45×10^{4}

Table S5. List of LS experimental conditions and rate coefficients for k_{decomp} (the total rate of styrene decomposition) at 240 Torr.

C_8H_8	T_1 / K	P_1 / Torr	T_2 / K	P_2 / Torr	k_{decomp} / s^{-1}
1%	297.95	10.45	1790	243	5.33×10^{3}
1%	297.95	10.05	1818	238	5.00×10^{3}
1%	297.65	8.3	1924	211	1.17×10^{4}
1%	297.95	8.55	1973	224	1.93×10^{4}
1%	297.65	6.21	2052	171	3.17×10^{4}
1%	296.85	8.4	2057	232	3.20×10^{4}
1%	297.15	7.6	2249	234	1.06×10^{5}
1%	297.95	7.45	2267	230	1.39×10^{5}
1%	298.05	7.3	2268	226	1.36×10^{5}
1%	297.45	6.6	2305	208	1.66×10^{5}
1%	298.05	7	2313	221	1.85×10^{5}
1%	297.15	6.7	2377	220	2.33×10^{5}
2%	292.35	8	1845	223	8.16×10^{3}
2%	292.35	8	1904	232	1.29×10^{4}

5. Electronic Structure Theory Results

Table S6. Stationary point energies for the thermal decomposition reactions of Styrene.

Saddle Point	CC/M06	G4
H + $C_6H_5CCH_2$	102.02	101.35
H + C_6H_5CHCH	109.91	101.82
H + o-$C_6H_4CHCH_2$ (IP)	111.25	109.28
H + o-$C_6H_4CHCH_2$ (OP)	111.85	109.86
H + m-$C_6H_4CHCH_2$ (IP)	111.50	109.37
H + m-$C_6H_4CHCH_2$ (OP)	111.69	109.58
H + p-$C_6H_4CHCH_2$	112.00	110.11
C_6H_5 + C_2H_3	114.96	114.43
C_8H_8 → H_2CC: + C_6H_6 (TS)	94.66	94.59
C_8H_8 → C_2H_2 + C_6H_6 (TS)	110.50	
C_8H_8 → C_2H_4 + o-C_6H_4 (TS)	120.35	
C_8H_8 → H_2 + C_6H_5CCH (TS)	110.15	
C_8H_8 → o-iso-C_8H_8 (TS)	95.16	94.67
o-iso-C_8H_8 → H_2 + C_6H_5CCH (TS)	94.24	93.64
o-iso-C_8H_8 → m-iso-C_8H_8 (TS)	98.39	97.96
m-iso-C_8H_8 → p-iso-C_8H_8 (TS)	100.00	99.48
o-iso-C_8H_8	42.88	42.85
m-iso-C_8H_8	73.40	72.96
p-iso-C_8H_8	39.66	39.59
C_2H_2 + C_6H_6	38.20	
H_2CC: + C_6H_6	81.09	81.59
C_2H_4 + o-C_6H_4	86.09	
H_5 + C_6H_5CCH	39.20	38.35

Table S7. Structures and frequencies for relevant molecules and reactions on the C_8H_8 PES at the M06-2X/cc-pvtz level of theory.

Species:	**Styrene (C_8H_8)**		
Frequencies (cm^{-1}):	23.5, 205.5, 244.4, 414, 442.3, 458.6, 559.1, 633.5, 666.9, 722.1, 795, 814.5, 873.7, 955, 963.5, 1010.2, 1022.3, 1029.2, 1045.1, 1045.6, 1069.2 1120.7 1177.8, 1208.3, 1239.8, 1317.5, 1342, 1364.7, 1458.7, 1495.1, 1544.7 1652.6, 1678.3, 1728.5, 3167.9, 3179.1, 3193.1, 3201.7, 3210.7, 3219, 3227.5, 3261.7		
Cartesian Coordinates:	6	2.946817000	0.336682000	0.069037000
	6	1.947981000	-0.529505000	-0.051347000
	6	0.509211000	-0.223112000	-0.031035000
	6	-0.404516000	-1.275652000	0.001162000
	6	0.013763000	1.082670000	-0.043915000
	6	-1.770752000	-1.038240000	0.031818000

6	-2.247751000	0.263131000	0.025709000
6	-1.348398000	1.322613000	-0.014191000
1	-0.034025000	-2.293324000	0.005698000
1	0.699334000	1.918014000	-0.087064000
1	-2.461413000	-1.870088000	0.058953000
1	-3.311884000	0.454007000	0.047322000
1	-1.713848000	2.340584000	-0.026766000
1	2.186988000	-1.581704000	-0.167884000
1	3.974430000	0.003584000	0.041622000
1	2.782287000	1.397409000	0.204693000

Species: **$C_6H_5CCH_2$ (α-C_8H_7)**

Frequencies (cm^{-1}): 77.8, 149.5, 213.6, 389.5, 447.2, 459.1, 477.7, 554.8, 629, 691.7, 764, 771.9, 843.2, 913.2, 915.5, 964.5, 988.1, 1000.3, 1013.6, 1047, 1111.2, 1143.6, 1168.8, 1215.9, 1297, 1345.9, 1435.9, 1471.8, 1496.4, 1591.5, 1614.1, 1907.6, 3088.3, 3150, 3201.9, 3207.2, 3221.8, 3225.1, 3232.1

Cartesian Coordinates:

6	3.206147000	0.000022000	0.000110000
6	1.912660000	-0.000054000	-0.000166000
6	0.543363000	-0.000043000	-0.000059000
6	-0.190219000	-1.219766000	-0.000031000
6	-0.190141000	1.219728000	-0.000031000
6	-1.565835000	-1.205235000	0.000022000
6	-2.268069000	0.000046000	0.000044000
6	-1.565758000	1.205283000	0.000022000
1	3.780358000	0.000021000	-0.924052000
1	3.779952000	0.000013000	0.924527000
1	0.353942000	-2.153649000	-0.000053000
1	0.354083000	2.153575000	-0.000051000
1	-2.106359000	-2.142236000	0.000045000
1	-3.348642000	0.000080000	0.000080000
1	-2.106223000	2.142318000	0.000044000

Species: **C_6H_5CHCH (β-C_8H_7)**

Frequencies (cm^{-1}): 81.4, 222.5, 224.9, 416.1, 451.9, 467.4, 552.8, 633.6, 667.5, 720.9, 766.7, 796.8, 874, 888, 901.7, 961.5, 1013.7, 1022.8, 1032.8, 1063.9, 1113.6, 1177.9, 1204.3, 1227.1, 1277.2, 1329.7, 1357.8, 1493.6, 1541.6, 1649.9, 1677.4, 1688.7, 3085.4, 3192.6, 3196.5, 3206.5, 3215.2, 3226.1, 3278

Cartesian Coordinates:

6	-2.957049000	0.429732000	0.000000000
6	-2.008262000	-0.472583000	0.000000000
6	-0.559957000	-0.206596000	0.000000000
6	0.336321000	-1.272197000	0.000000000
6	-0.056083000	1.095726000	0.000000000

6	1.705621000	-1.047485000	0.000000000
6	2.195447000	0.249096000	0.000000000
6	1.308162000	1.320479000	0.000000000
1	-4.033517000	0.431318000	0.000000000
1	-2.293199000	-1.526409000	0.000000000
1	-0.045771000	-2.285528000	0.000000000
1	-0.748959000	1.927900000	0.000000000
1	2.388605000	-1.886050000	0.000000000
1	3.261952000	0.427645000	0.000000000
1	1.685693000	2.334092000	0.000000000

Species: **C_6H_5CHCH (*β*-C_8H_7)**

Frequencies (cm^{-1}): 81.4, 222.5, 224.9, 416.1, 451.9, 467.4, 552.8, 633.6, 667.5, 720.9, 766.7, 796.8, 874, 888, 901.7, 961.5, 1013.7, 1022.8, 1032.8, 1063.9, 1113.6, 1177.9, 1204.3, 1227.1, 1277.2, 1329.7, 1357.8, 1493.6, 1541.6, 1649.9, 1677.4, 1688.7, 3085.4, 3192.6, 3196.5, 3206.5, 3215.2, 3226.1, 3278

Cartesian Coordinates:

6	-2.957049000	0.429732000	0.000000000
6	-2.008262000	-0.472583000	0.000000000
6	-0.559957000	-0.206596000	0.000000000
6	0.336321000	-1.272197000	0.000000000
6	-0.056083000	1.095726000	0.000000000
6	1.705621000	-1.047485000	0.000000000
6	2.195447000	0.249096000	0.000000000
6	1.308162000	1.320479000	0.000000000
1	-4.033517000	0.431318000	0.000000000
1	-2.293199000	-1.526409000	0.000000000
1	-0.045771000	-2.285528000	0.000000000
1	-0.748959000	1.927900000	0.000000000
1	2.388605000	-1.886050000	0.000000000
1	3.261952000	0.427645000	0.000000000
1	1.685693000	2.334092000	0.000000000

Species: **o-$C_6H_4CHCH_2$ (*o*-C_8H_7) In-plane (IP)**

Frequencies (cm^{-1}): 82.2, 204.3, 210.5, 418.8, 443.3, 466.2, 556.7, 629.3, 657.7, 741.7, 788, 795.6, 885.7, 970.3, 975, 995.6, 1017.3, 1039.8, 1045.1, 1056.6, 1136.8, 1172.9, 1242.1, 1262.2, 1319.8, 1339.9, 1447.2, 1471, 1495.4, 1606.4, 1668.4, 1723.6, 3167.4, 3180.4, 3188.7, 3200.1, 3212.2, 3224.5, 3261.1

Cartesian Coordinates:

6	-2.929724000	-0.439936000	0.000002000
6	-1.983953000	0.491279000	-0.000001000
6	-0.541688000	0.219863000	-0.000001000
6	0.392035000	1.261559000	0.000000000
6	-0.003001000	-1.050905000	-0.000001000

6	1.756744000	1.003184000	0.000001000
6	2.229283000	-0.300883000	0.000001000
6	1.324434000	-1.366482000	-0.000001000
1	-3.977344000	-0.175518000	0.000001000
1	-2.678470000	-1.493700000	0.000005000
1	-2.261648000	1.539712000	-0.000004000
1	0.033741000	2.284246000	0.000000000
1	2.455926000	1.827893000	0.000002000
1	3.293125000	-0.497018000	0.000001000
1	1.669884000	-2.391688000	-0.000001000

Species:	**o-$C_6H_4CHCH_2$ (*o*-C_8H_7) Out-of-plane (OP)**
Frequencies (cm^{-1}):	17.4, 200.5, 232.5, 411.7, 438.6, 463.1, 549.9, 628.5, 651.4, 742.8, 789.5, 790.8, 881.8, 964.1, 975, 994.7, 1018.3, 1037.4, 1047.8, 1068.5, 1139.1, 1171.1, 1222.4, 1290.9, 1318.5, 1338.8, 1447.7, 1470.5, 1498.2, 1609.9, 1666.4, 1726, 3176.5, 3184.6, 3197, 3203.7, 3213, 3225.1, 3263.8

Cartesian Coordinates:

6	2.961368000	0.286842000	0.022140000
6	1.959406000	-0.582860000	-0.016529000
6	0.524936000	-0.259489000	-0.009772000
6	-0.422253000	-1.259310000	0.000420000
6	0.010665000	1.045329000	-0.014025000
6	-1.781489000	-1.097484000	0.010423000
6	-2.256390000	0.211951000	0.008151000
6	-1.355394000	1.272134000	-0.004591000
1	3.987313000	-0.051944000	0.013083000
1	2.801654000	1.356014000	0.066071000
1	2.182320000	-1.643154000	-0.053933000
1	0.690298000	1.887445000	-0.028039000
1	-2.459407000	-1.940295000	0.019238000
1	-3.321487000	0.401257000	0.015016000
1	-1.725780000	2.288006000	-0.008734000

Species:	**m-$C_6H_4CHCH_2$ (*m*-C_8H_7) In-plane (IP)**
Frequencies (cm^{-1}):	21.5, 204.2, 246, 411.2, 443.9, 466.3, 554.2, 625.2, 654.3, 718.5, 788.2, 805.9, 889.1, 930.8, 966.6, 1000.3, 1009.6, 1041.8, 1045.7, 1081.3, 1105.7, 1180, 1222.2, 1284.8, 1312.6, 1346.4, 1453.5, 1463.9, 1505.9, 1594.2, 1668.5, 1725.8, 3169.4, 3179.2, 3196.2, 3207.9, 3208.8, 3220.4, 3261.9

Cartesian Coordinates:

6	-2.927749000	-0.277176000	0.074393000
6	-1.900318000	0.553342000	-0.054028000
6	-0.474395000	0.192828000	-0.033543000
6	0.483187000	1.207236000	0.002176000
6	-0.033508000	-1.139773000	-0.050314000

6	1.842405000	0.926585000	0.033744000
6	2.285938000	-0.393360000	0.026137000
6	1.312934000	-1.360276000	-0.016801000
1	-3.943533000	0.090256000	0.046670000
1	-2.798772000	-1.341842000	0.217936000
1	-2.100146000	1.612745000	-0.177381000
1	0.151120000	2.237562000	0.008907000
1	-0.739627000	-1.957914000	-0.099269000
1	2.559973000	1.735965000	0.063438000
1	3.340016000	-0.633208000	0.049119000

Species: **m-$C_6H_4CHCH_2$ (*m*-C_8H_7) Out-of-plane (OP)**

Frequencies (cm^{-1}): 37.6, 202.8, 245.4, 421, 442.6, 465.2, 554.9, 626.2, 654.4, 719.3, 787.6, 804.7, 898.4, 928, 968.2, 1003.3, 1011.4, 1042.7, 1044.4, 1075.7, 1113.5, 1186.8, 1214.3, 1305.8, 1310.5, 1345.4, 1442.2, 1465.9, 1510.6, 1592.9, 1671.7, 1727.1, 3170.2, 3179.8, 3191.7, 3198.1, 3215.3, 3224.1, 3262.2

Cartesian Coordinates:

6	2.880515000	-0.431189000	0.092277000
6	1.928889000	0.479850000	-0.070344000
6	0.477030000	0.243358000	-0.041217000
6	-0.384871000	1.346902000	0.008564000
6	-0.083702000	-1.036849000	-0.062143000
6	-1.731705000	1.107659000	0.049665000
6	-2.319755000	-0.127858000	0.039505000
6	-1.455002000	-1.223359000	-0.020557000
1	3.924310000	-0.153966000	0.055041000
1	2.658963000	-1.474167000	0.275901000
1	2.219939000	1.513141000	-0.228279000
1	0.019787000	2.351545000	0.019082000
1	0.563162000	-1.900866000	-0.125097000
1	-3.392411000	-0.260938000	0.069797000
1	-1.862138000	-2.225828000	-0.040948000

Species: **p-$C_6H_4CHCH_2$ (*p*-C_8H_7)**

Frequencies (cm^{-1}): 39.9, 215.9, 245.1, 404.7, 439.6, 460.8, 559.3, 616.5, 646.9, 743, 778.6, 836.6, 841, 963.8, 979, 993.3, 1002.7, 1043.2, 1049.3, 1066.1, 1117.9, 1188.5, 1231.5, 1302.5, 1320.4, 1345.5, 1412.3, 1463.1, 1504.9, 1628.5, 1648.8, 1727.9, 3168.7, 3179, 3191.1, 3202.5, 3212.9, 3217.9, 3261.7

Cartesian Coordinates:

6	2.881616000	0.296983000	0.099707000
6	1.872004000	-0.546373000	-0.078081000
6	0.437241000	-0.220140000	-0.045139000
6	-0.487662000	-1.263958000	0.002732000
6	-0.031379000	1.096564000	-0.062131000

6	-1.857649000	-1.014735000	0.050536000
6	-2.246147000	0.297388000	0.041433000
6	-1.392975000	1.370710000	-0.016344000
1	3.904764000	-0.047721000	0.055994000
1	2.730044000	1.348949000	0.302698000
1	2.097267000	-1.593259000	-0.253830000
1	-0.129459000	-2.286439000	0.007661000
1	-2.569823000	-1.827706000	0.090867000
1	0.670743000	1.917319000	-0.125924000
1	-1.753827000	2.390224000	-0.033734000

Species: **ortho-iso-C_8H_8 (oiC_8H_8)**

Frequencies (cm^{-1}): 62.9, 149.7, 206.8, 322.3, 415.5, 468.4, 536, 582, 593.7, 619.3, 724.3, 740, 813.4, 909.1, 935.3, 949.9, 981.1, 1001.7, 1009.5, 1017.2, 1020.8, 1164.9, 1201.6, 1212.6, 1262, 1269.9, 1358.4, 1403.9, 1448.7, 1461.8, 1488.3, 1667.7, 1736.5, 2065.1, 3012.9, 3107.8, 3139, 3192.9, 3203, 3213.9, 3215, 3225.1

Cartesian Coordinates:

6	3.177985000	0.006735000	-0.191288000
6	1.887402000	0.009944000	-0.042091000
6	0.586884000	0.012365000	0.111989000
6	-0.163627000	1.269937000	0.166203000
6	-0.198408000	-1.279288000	0.268625000
6	-1.493133000	1.279226000	0.023837000
6	-2.236410000	0.043003000	-0.215425000
6	-1.639798000	-1.143852000	-0.133123000
1	3.843726000	-0.005834000	0.664136000
1	3.630467000	0.018014000	-1.176138000
1	0.397391000	2.187739000	0.277585000
1	0.287161000	-2.082532000	-0.284338000
1	-0.168234000	-1.579070000	1.323633000
1	-2.032780000	2.216342000	0.040561000
1	-3.285759000	0.111825000	-0.468926000
1	-2.197339000	-2.054898000	-0.308872000

Species: **m-iso-C_8H_8**

Frequencies (cm^{-1}): 128.7, 184.5, 270.7, 348.6, 404.1, 493.5, 523.9, 569.9, 693.1, 710.6, 812.7, 822.3, 824.4, 873.4, 926.5, 933.5, 961.6, 976.4, 1009.5, 1029.5, 1041.2, 1082.1, 1149.8, 1187.8, 1200.1, 1272.6, 1332.1, 1338.8, 1385.4, 1450.6, 1475.6, 1692.4, 1724, 1903.1, 3039.7, 3115.6, 3120.5, 3169.5, 3182.3, 3198.7, 3205.1, 3258.1

Cartesian Coordinates:

6	2.860540000	-0.072980000	-0.351607000
6	1.603069000	-0.084259000	0.039360000
6	0.389161000	-0.747396000	0.326777000
6	0.452357000	0.705453000	0.606378000

6	-0.677688000	-1.421981000	-0.066406000
6	-0.629775000	1.431610000	-0.124270000
6	-1.770833000	0.786498000	-0.348019000
6	-1.985808000	-0.671079000	0.046384000
1	3.407335000	0.855969000	-0.434078000
1	3.374818000	-0.992179000	-0.597076000
1	0.622659000	1.026498000	1.631518000
1	-0.628715000	-2.367164000	-0.591611000
1	-2.382116000	-0.714137000	1.066254000
1	-0.502836000	2.466556000	-0.416121000
1	-2.595341000	1.292038000	-0.836361000
1	-2.741951000	-1.122776000	-0.594101000

Species: **p-iso-C_8H_8**

Frequencies (cm^{-1}): 90.3, 150.3, 220.6, 373.4, 384.6, 443.8, 560.4, 567.2, 607.7, 617.6, 725.1, 772.6, 798.7, 892.4, 905.3, 968.1, 970.8, 1001.7, 1011, 1019.8, 1031, 1154.7, 1205.3, 1224.4, 1271.7, 1292.3, 1379.7, 1421.5, 1432.9, 1465.7, 1489, 1707, 1759.4, 2061.5, 3024.2, 3036.8, 3138, 3188.7, 3189.3, 3212.3, 3214.6, 3216.1

Cartesian Coordinates:

6	-3.237056000	0.000000000	0.000001000
6	-1.939016000	0.000001000	-0.000001000
6	-0.625215000	0.000001000	-0.000001000
6	0.146179000	1.249284000	0.000000000
6	0.146178000	-1.249283000	0.000000000
6	1.475799000	1.249813000	0.000000000
6	2.300843000	-0.000001000	0.000001000
6	1.475798000	-1.249813000	0.000000000
1	-3.800248000	0.000000000	-0.926434000
1	-3.800246000	-0.000001000	0.926437000
1	-0.409638000	2.177315000	-0.000001000
1	-0.409640000	-2.177314000	-0.000001000
1	2.007742000	2.193298000	0.000000000
1	2.971618000	-0.000001000	0.867031000
1	2.971619000	-0.000001000	-0.867029000
1	2.007740000	-2.193299000	0.000000000

Species: **phenylacetylene (C_6H_5CCH)**

Frequencies (cm^{-1}): 141.4, 158.6, 370.9, 412.7, 472.4, 543.6, 558.6, 636.3, 692.9, 717.3, 725.6, 780.2, 791.8, 875.5, 961.8, 1012.4, 1022.5, 1033.3, 1062.4, 1111.2, 1180.2, 1202.2, 1234.3, 1308.1, 1351.9, 1489.7, 1538, 1647, 1676.9, 2254.1, 3203.8, 3212.4, 3220.9, 3227.6, 3232.5, 3487.7

Cartesian Coordinates:

6	-3.215472000	0.000000000	0.000001000
6	-2.016667000	-0.000001000	0.000000000

6	-0.584863000	-0.000001000	-0.000001000
6	0.119229000	-1.205447000	-0.000001000
6	0.119227000	1.205447000	-0.000001000
6	1.504031000	-1.201719000	0.000000000
6	2.199249000	0.000001000	0.000000000
6	1.504029000	1.201721000	0.000000000
1	-4.277865000	0.000001000	0.000001000
1	-0.429970000	-2.136489000	-0.000001000
1	-0.429973000	2.136488000	-0.000001000
1	2.042321000	-2.139517000	0.000001000
1	3.280586000	0.000002000	0.000000000
1	2.042318000	2.139518000	0.000000000

Species: **benzene (C_6H_6)**

Frequencies (cm^{-1}): 413.3, 413.7, 619.9, 620.1, 695.8, 733.7, 880.8, 883.6, 1010.3, 1012.6, 1021.3, 1033.4, 1042.7, 1073.2, 1074.1, 1167.1, 1200.8, 1202.6, 1326.8, 1381.9, 1525.5, 1526.7, 1669.7, 1669.9, 3195, 3204.9, 3204.9, 3219.8, 3219.9, 3229.4

Cartesian Coordinates:

6	0.000004000	1.388115000	0.000000000
6	-1.202143000	0.694063000	0.000000000
6	1.202143000	0.694061000	0.000000000
6	-1.202143000	-0.694061000	0.000000000
6	-0.000004000	-1.388115000	0.000000000
6	1.202143000	-0.694063000	0.000000000
1	-2.138868000	1.234873000	0.000000000
1	2.138879000	1.234865000	0.000000000
1	-2.138879000	-1.234865000	0.000000000
1	0.000004000	-2.469758000	0.000000000
1	2.138868000	-1.234873000	0.000000000
1	-0.000004000	2.469758000	0.000000000

Species: **phenyl (C_6H_5)**

Frequencies (cm^{-1}): 403.3, 430.2, 600.9, 617.2, 691.5, 734.4, 842.3, 916.1, 989.6, 994.1, 1024.6, 1037.1, 1062.3, 1084.8, 1174.3, 1179.6, 1306.1, 1319.6, 1475.7, 1490.3, 1611.6, 1664.7, 3195.6, 3200.9, 3211.8, 3214.8, 3226

Cartesian Coordinates:

6	0.000000000	1.393487000	0.000000000
6	0.000000000	0.766066000	1.218006000
6	0.000000000	0.766066000	-1.218006000
6	0.000000000	-0.628572000	1.206573000
6	0.000000000	-1.316735000	0.000000000
6	0.000000000	-0.628572000	-1.206573000
1	0.000000000	1.316628000	2.149055000
1	0.000000000	1.316628000	-2.149055000

	1	0.000000000	-1.172850000	2.141851000
	1	0.000000000	-2.398001000	0.000000000
	1	0.000000000	-1.172850000	-2.141851000

Species:	**ortho-benzyne (o-C_6H_4)**			
Frequencies (cm^{-1}):	395.5, 423.7, 471.9, 624.5, 627.7, 763.8, 846.9, 892.7, 953.9, 1004.8, 1013.1, 1083.4, 1120.2, 1163.2, 1276.6, 1311.7, 1442.2, 1497.7, 1499.4, 2065.1, 3197.4, 3212.5, 3236.3, 3239.6			
Cartesian Coordinates:	6	0.000000000	-1.227062000	0.617953000
	6	0.000000000	-1.227062000	-0.617953000
	6	0.000000000	-0.132413000	1.456123000
	6	0.000000000	-0.132413000	-1.456123000
	6	0.000000000	1.048787000	-0.700360000
	6	0.000000000	1.048787000	0.700360000
	1	0.000000000	-0.133515000	2.535509000
	1	0.000000000	-0.133515000	-2.535509000
	1	0.000000000	1.997641000	-1.221565000
	1	0.000000000	1.997641000	1.221565000

Species:	**ethylene (C_2H_4)**			
Frequencies (cm^{-1}):	829.1, 990.4, 1002.9, 1071, 1243.1, 1388.1, 1473.8, 1718.6, 3159.7, 3175.8, 3235.5, 3261.9			
Cartesian Coordinates:	6	0.000000000	0.000000000	0.660746000
	6	0.000000000	0.000000000	-0.660746000
	1	0.000000000	0.921739000	1.227744000
	1	0.000000000	-0.921739000	1.227744000
	1	0.000000000	-0.921739000	-1.227744000
	1	0.000000000	0.921739000	-1.227744000

Species:	**vinyl (C_2H_3)**			
Frequencies (cm^{-1}):	730.8, 867.8, 946.4, 1067, 1399.1, 1680.1, 3098, 3184.8, 3261			
Cartesian Coordinates:	6	-0.599833000	0.087227000	-0.767266000
	6	0.466963000	0.082375000	-0.021446000
	1	-1.550661000	-0.420606000	-0.776663000
	1	0.549954000	-0.557843000	0.855290000
	1	1.320055000	0.715876000	-0.240216000

Species:	**acetylene (C_2H_2)**			
Frequencies (cm^{-1}):	705.2, 705.2, 789.7, 789.7, 2105.2, 3428.9, 3541.1			
Cartesian Coordinates:	6	0.000000000	0.000000000	0.596958000

	6	0.000000000	0.000000000	-0.596958000
	1	0.000000000	0.000000000	1.659774000
	1	0.000000000	0.000000000	-1.659774000

Species:	**vinylidene (CH_2C)**			
Frequencies (cm^{-1}):	309.6, 764.3, 1213.1, 1738.8, 3147.9, 3232.8			
Cartesian Coordinates:	6	0.475253000	0.000000000	-0.000001000
	6	-0.814427000	-0.000001000	0.000000000
	1	1.017518000	0.940645000	0.000002000
	1	1.017528000	-0.940640000	0.000002000

Species:	**hydrogen (H_2)**			
Frequencies (cm^{-1}):	4468.3			
Cartesian Coordinates:	1	0.000000000	0.000000000	0.369500000
	1	0.000000000	0.000000000	-0.369500000

Transition State:	**C_8H_8 → CH_2C: + C_6H_6**			
Frequencies (cm^{-1}):	i835.1, 53.5, 119.5, 166.8, 317.3, 404.8, 498.2, 549.8, 615.5, 697.1, 714.2, 752.5, 791, 874, 910.5, 952.9, 961.5, 996.4, 1010.8, 1030.6, 1035.6, 1057.4, 1100.3, 1179.6, 1183.1, 1195.7, 1324, 1337.1, 1392.5, 1491.6, 1512.1, 1624.3, 1646.3, 1667.2, 2238.6, 3133.7, 3199.3, 3204.8, 3211.2, 3218.7, 3219, 3227.3			
Cartesian Coordinates:	6	0.285806000	0.209700000	-0.723747000
	6	1.119963000	1.221438000	-0.292000000
	6	0.484655000	-1.115407000	-0.391447000
	6	2.192658000	0.889925000	0.525924000
	6	2.407081000	-0.435358000	0.884374000
	6	1.559951000	-1.437381000	0.426850000
	1	0.927227000	2.246607000	-0.580188000
	1	-0.193439000	-1.876201000	-0.755501000
	1	2.859049000	1.662907000	0.883915000
	1	3.241669000	-0.689291000	1.523491000
	1	1.736570000	-2.466664000	0.708126000
	6	-1.553299000	0.738072000	-1.374849000
	6	-2.136276000	0.839822000	-0.196885000
	1	-1.714704000	0.678607000	0.786205000
	1	-3.183641000	1.125918000	-0.240742000
	1	-0.439274000	0.452320000	-1.760306000

Transition State:	**$C_8H_8 \rightarrow C_2H_2 + C_6H_6$**
Frequencies (cm^{-1}):	i743.9, 126, 200.3, 219.4, 406.4, 414.6, 485.1, 569, 616.5, 641.5, 705.6, 742.8, 848.5, 877.9, 895.2, 935.7, 983.2, 1013.3, 1023, 1045.6, 1053.2, 1071.3, 1089.1, 1112.1, 1181.4, 1194.7, 1293.7, 1336.7, 1341.6, 1498.4, 1503.1, 1599.5, 1659.8, 1682.7, 2146.7, 3104.7, 3166.4, 3199.7, 3206.6, 3212.9, 3222.2, 3230
Cartesian Coordinates:	6 -0.004649000 0.717626000 0.192572000 6 1.195000000 1.417479000 0.193471000 6 -0.047424000 -0.663363000 0.056354000 6 2.378560000 0.717785000 0.023661000 6 2.352180000 -0.663995000 -0.119111000 6 1.142890000 -1.351965000 -0.095734000 1 1.197128000 2.493489000 0.313250000 1 -1.016926000 -1.144737000 0.044782000 1 3.320596000 1.247852000 0.006678000 1 3.277321000 -1.206947000 -0.255484000 1 1.130485000 -2.426734000 -0.213184000 6 -2.616722000 0.930594000 -0.155815000 6 -1.509802000 1.635983000 -0.090611000 1 -3.452439000 1.510019000 -0.556060000 1 -1.143206000 2.647579000 -0.220711000 1 -0.871556000 1.163246000 0.933546000

Transition State:	**$C_8H_8 \rightarrow C_2H_4 + o\text{-}C_6H_4$**
Frequencies (cm^{-1}):	i651, 97.2, 168.5, 232.5, 366.7, 406.1, 453, 501.3, 559.5, 637, 688.2, 754.3, 825.2, 886, 898.7, 940.9, 963.4, 977.2, 1026.4, 1030.7, 1039.9, 1070.6, 1128.7, 1153.9, 1176.1, 1259.4, 1313.7, 1361.8, 1403, 1451.8, 1471.2, 1604.2, 1613.3, 1664.7, 2274.9, 3156.7, 3184, 3186.5, 3195.9, 3224.3, 3241.6, 3276
Cartesian Coordinates:	6 0.203126000 0.910915000 -0.216628000 6 1.333135000 1.629187000 -0.023238000 6 -0.008182000 -0.472560000 -0.289737000 6 2.427715000 0.780623000 0.276821000 6 2.329648000 -0.598086000 0.231483000 6 1.108930000 -1.236660000 -0.053879000 1 -0.973610000 -0.922576000 -0.483129000 1 3.394465000 1.215378000 0.508588000 1 3.206739000 -1.209728000 0.409142000 1 1.045893000 -2.315616000 -0.073354000 1 -0.657412000 1.483263000 -1.079526000 6 -2.407947000 1.467730000 0.210463000 6 -1.197922000 1.925437000 -0.109199000 1 -3.141340000 2.136480000 0.638304000 1 -2.685105000 0.429956000 0.093243000

	1	-0.856321000	2.941738000	0.018234000

Transition State:	**C_8H_8 → H_2 + C_6H_5CCH**
Frequencies (cm^{-1}):	i1369.4, 68.4, 134, 223.3, 317.5, 412.5, 473.9, 504.7, 534.4, 631.4, 688.2, 722.2, 765.9, 784.6, 870, 911.5, 920.3, 937.1, 1004, 1015.8, 1022.1, 1062.9, 1108.7, 1175.4, 1194.8, 1212.5, 1297.3, 1350.2, 1396.5, 1473, 1505, 1527.4, 1635.5, 1666.6, 1777.1, 3184.1, 3194.6, 3201.1, 3211.4, 3218.4, 3227.6, 3233.4

Cartesian Coordinates:

6	-0.986611000	1.508570000	0.402347000
6	0.170430000	0.660611000	0.228580000
6	1.426907000	1.226156000	-0.017931000
6	0.079244000	-0.733431000	0.343918000
6	2.540455000	0.421284000	-0.191916000
6	2.441504000	-0.958003000	-0.067322000
6	1.206775000	-1.526931000	0.215305000
1	1.514842000	2.302428000	-0.074089000
1	-0.882636000	-1.184024000	0.550500000
1	3.498492000	0.877536000	-0.403194000
1	3.317526000	-1.581348000	-0.179720000
1	1.117043000	-2.600018000	0.321607000
6	-2.079318000	1.469956000	-0.274383000
1	-2.622455000	1.031827000	-1.096732000
1	-2.819664000	2.635125000	-0.102190000
1	-3.118424000	2.053412000	0.427634000

Transition State:	**C_8H_8 → oiC_8H_8**
Frequencies (cm^{-1}):	i1793.9, 129.8, 166.9, 339.1, 392.2, 447, 506.3, 539.7, 608.1, 644.7, 738.5, 766.5, 784.3, 838.7, 896.7, 901.1, 970.3, 996.4, 1006.8, 1021.5, 1040.5, 1076.6, 1170.3, 1185.9, 1230.2, 1285.8, 1332.9, 1408.2, 1434.6, 1461.5, 1495, 1561.7, 1653.1, 1683.6, 1838, 3126.9, 3132.4, 3197, 3209.2, 3219.1, 3221.7, 3228.1

Cartesian Coordinates:

6	-0.205872000	0.521731000	-0.494228000
6	0.948240000	1.393977000	-0.342355000
6	-0.058830000	-0.884821000	-0.576729000
6	2.102249000	0.805388000	0.287970000
6	2.153410000	-0.549160000	0.401624000
6	1.114534000	-1.394760000	-0.104491000
1	1.150660000	2.074897000	-1.164918000
1	-0.885405000	-1.521800000	-0.859001000
1	2.943635000	1.416687000	0.585418000
1	3.028124000	-1.016772000	0.833704000
1	1.245883000	-2.466620000	-0.041810000
6	-1.255642000	1.373093000	-0.278477000
1	-0.053792000	2.313312000	-0.036566000

	6	-2.394921000	1.577488000	0.355194000
	1	-2.795739000	0.835691000	1.040081000
	1	-2.949513000	2.499606000	0.246375000

Transition State:	**oiC_8H_8 → H_2 + C_6H_5CCH**

Frequencies (cm^{-1}): i1763.6, 168, 252, 350, 420.4, 501.9, 558.6, 564.7, 619.2, 661.8, 706.7, 770.9, 809.8, 839.4, 891.7, 920.4, 971.6, 1003.6, 1020.6, 1027.9, 1037.2, 1092, 1140.6, 1186.4, 1196.5, 1270.2, 1288.2, 1314.6, 1336.4, 1380.3, 1471.4, 1515.7, 1560.7, 1604.5, 1684.7, 1938.7, 3194.5, 3202.6, 3211, 3221.8, 3229.8, 3335.9

Cartesian Coordinates:

6	-2.043266000	1.081839000	-1.020001000
1	-2.949774000	1.640259000	-1.152556000
6	-1.544320000	-0.063519000	-0.859345000
1	-0.972875000	1.893365000	-0.695832000
6	-0.282693000	-0.403380000	-0.409538000
6	0.658996000	-1.164442000	-1.141188000
6	0.179079000	0.436801000	0.664273000
6	1.977830000	-1.150560000	-0.788632000
6	2.424139000	-0.402228000	0.329245000
6	1.547956000	0.340475000	1.059954000
1	0.313702000	-1.741842000	-1.987177000
1	-0.536303000	0.751347000	1.412637000
1	2.692907000	-1.726442000	-1.360058000
1	3.464906000	-0.453934000	0.618741000
1	1.875892000	0.853859000	1.953766000
1	-0.164180000	1.708957000	-0.093773000

Transition State:	**oiC_8H_8 → m-iso-C_8H_8**

Frequencies (cm^{-1}): i407.8, 76.5, 141.4, 169.1, 368.3, 387.9, 451.8, 511.1, 555.6, 565.7, 617.4, 625.3, 745.6, 756.1, 795.1, 868.7, 932.5, 969.7, 991.3, 996.3, 1031.9, 1065, 1140.9, 1184.5, 1218.9, 1274.9, 1285.3, 1365.5, 1425.4, 1443.6, 1487.4, 1507.4, 1592.6, 2012.4, 2753.1, 3084.9, 3144.6, 3145.9, 3190.9, 3209, 3216.6, 3261.3

Cartesian Coordinates:

6	-2.785364000	-0.114205000	-1.150669000
6	-1.543022000	0.031071000	-0.794349000
6	-0.249379000	0.065386000	-0.497764000
6	0.803691000	0.723704000	-1.288116000
6	0.322975000	-0.678644000	0.587215000
6	2.029209000	1.056189000	-0.762647000
6	2.453046000	0.626995000	0.489220000
6	1.584584000	-0.290645000	1.181232000
1	-3.109711000	-0.921892000	-1.804856000
1	-3.565191000	0.566183000	-0.816359000
1	0.573767000	0.976000000	-2.314152000

	1	-0.251632000	-1.462370000	1.064102000
	1	2.708504000	1.633106000	-1.378140000
	1	3.403726000	0.902642000	0.914657000
	1	2.051181000	-1.027557000	1.830419000
	1	0.975793000	0.358298000	1.890323000

Transition State:	**m-iso-C_8H_8 → p-iso-C_8H_8**			
Frequencies (cm^{-1}):	i637.5, 56.7, 143.8, 165.7, 362, 382.4, 459.7, 534.6, 558, 578.5, 616.2, 629.8, 681.3, 750, 808.6, 869.7, 933.8, 967.4, 987.7, 994.5, 1036.4, 1068, 1145.7, 1185.3, 1229.5, 1258.1, 1274.3, 1359.8, 1430.2, 1466.1, 1480.6, 1504.9, 1603.6, 2033.8, 2664.7, 3089.2, 3149, 3171.6, 3195.4, 3214.4, 3226, 3259.7			
Cartesian Coordinates:	6	-1.984018000	1.095962000	-2.058346000
	6	-1.129230000	0.745722000	-1.141532000
	6	-0.270520000	0.294131000	-0.242446000
	6	1.170764000	0.126627000	-0.487256000
	6	-0.639928000	-0.224046000	1.056933000
	6	2.095373000	0.036125000	0.517394000
	6	1.726447000	-0.122450000	1.852790000
	6	0.299120000	-0.264506000	2.122658000
	1	-2.439795000	0.372192000	-2.731269000
	1	-2.286768000	2.130766000	-2.199300000
	1	1.503106000	0.124808000	-1.517091000
	1	-1.663626000	-0.516500000	1.242374000
	1	3.147285000	0.039938000	0.261487000
	1	2.426267000	-0.112756000	2.672335000
	1	0.010243000	-0.790498000	3.026262000
	1	0.378296000	0.844423000	2.406957000