Supplementary Material

Literature data

V. P. Zhukov, V. A. Sechenov, A. Yu. Starikovskii, Self-ignition of a lean mixture of *n*-pentane and air over a wide range of pressures, Combust. Flame 140 (2005) 196–203.

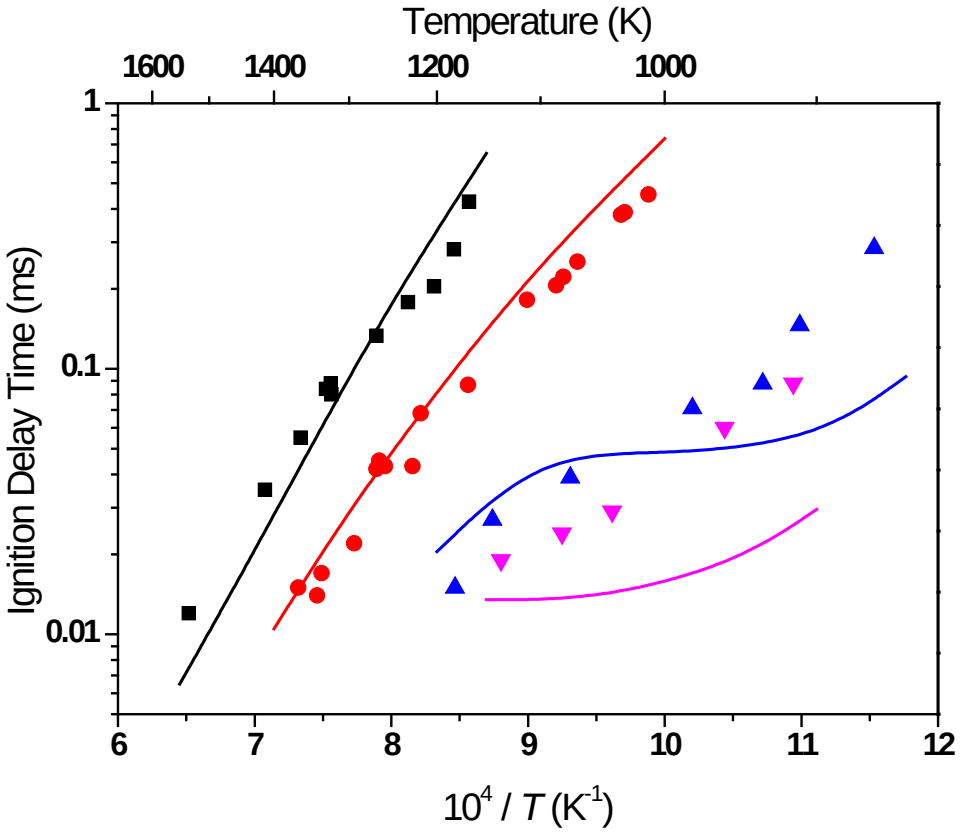

Figure S1. Comparison of experimental and model simulated ignition delay times for *n*-pentane in 'air' mixtures, φ = 0.5, at pressures near ■ – 12 atm, ● – 60 atm, ▲ – 250 atm, and ▼ – 530 atm. Symbols represent experimental data and lines refer to model simulations.

M. A. Oehlschlaeger, D. F. Davidson, J. T. Herbon, R. K. Hanson, Shock Tube Measurements of Branched Alkane Ignition Times and OH Concentration Time Histories, Int. J. Chem. Kin. 36 (2004) 67–78.

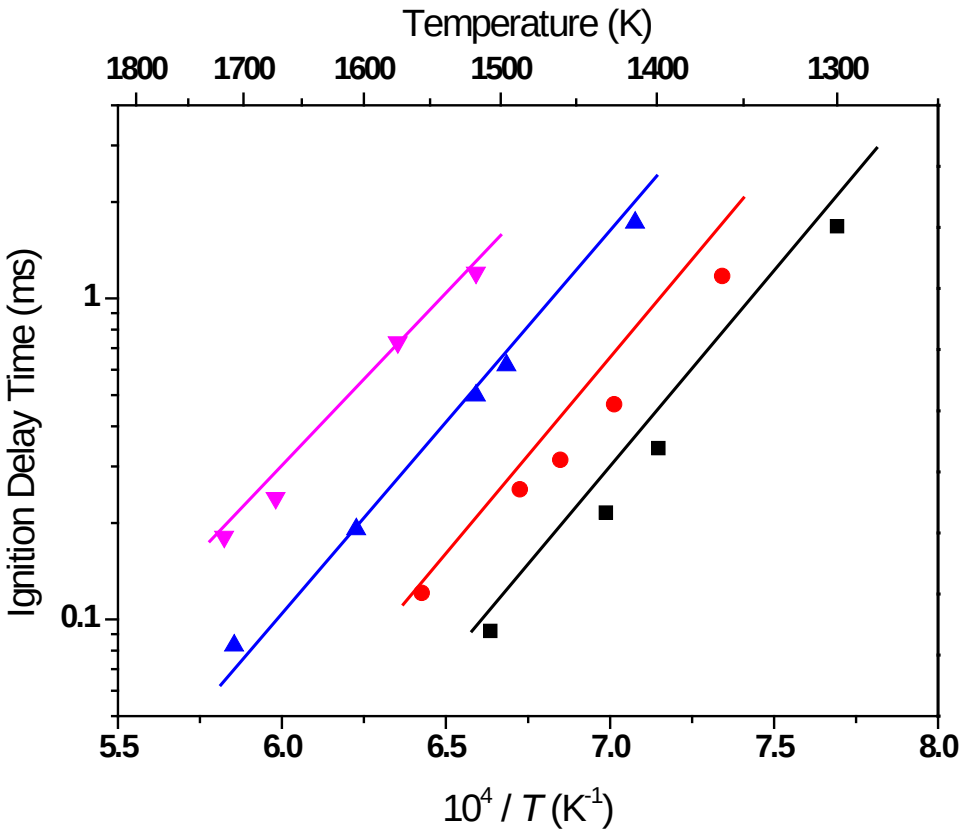

Figure S2. Comparison of experimental and model simulated ignition delay times for *iso*-pentane/argon mixtures with 0.8% O_2, at pressures near 2 atm, and at fuel concentrations near ■ – 0.025%, ● – 0.05%, ▲ – 0.1%, and ▼ – 0.2%. Symbols represent experimental data and lines refer to model simulations.

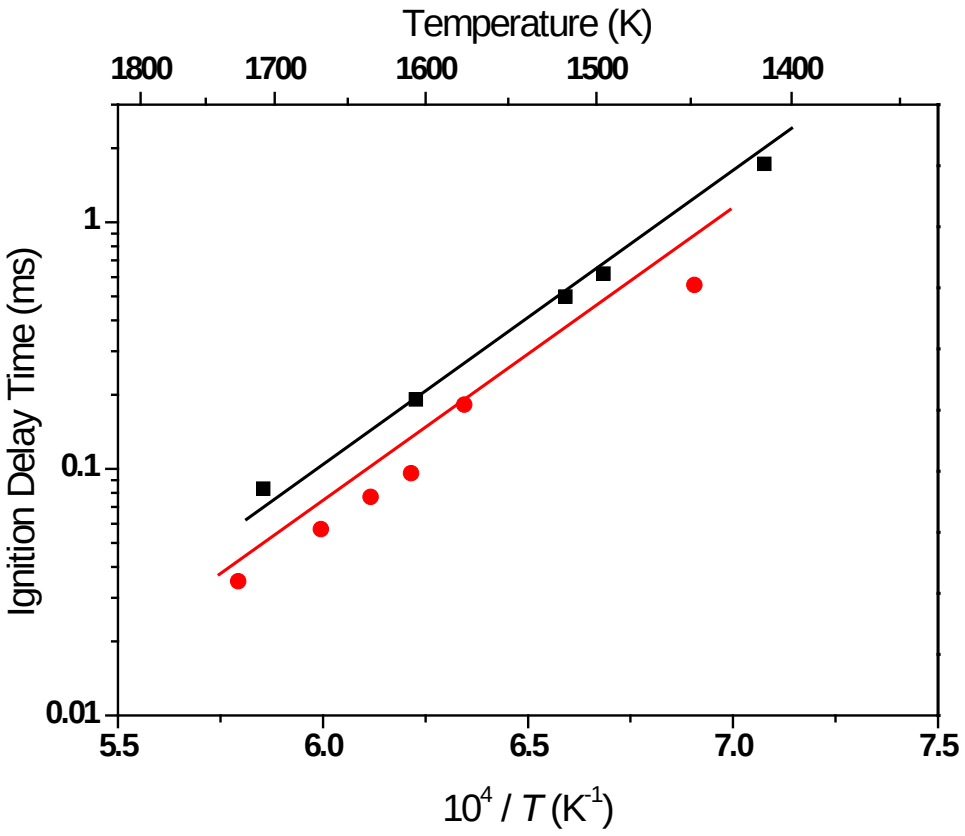

Figure S3. Comparison of experimental and model simulated ignition delay times for 0.1% *iso*-pentane in 0.8% O_2 and argon bath gas, at pressures near ■ – 2 atm, and ● – 5 atm. Symbols represent experimental data and lines refer to model simulations.

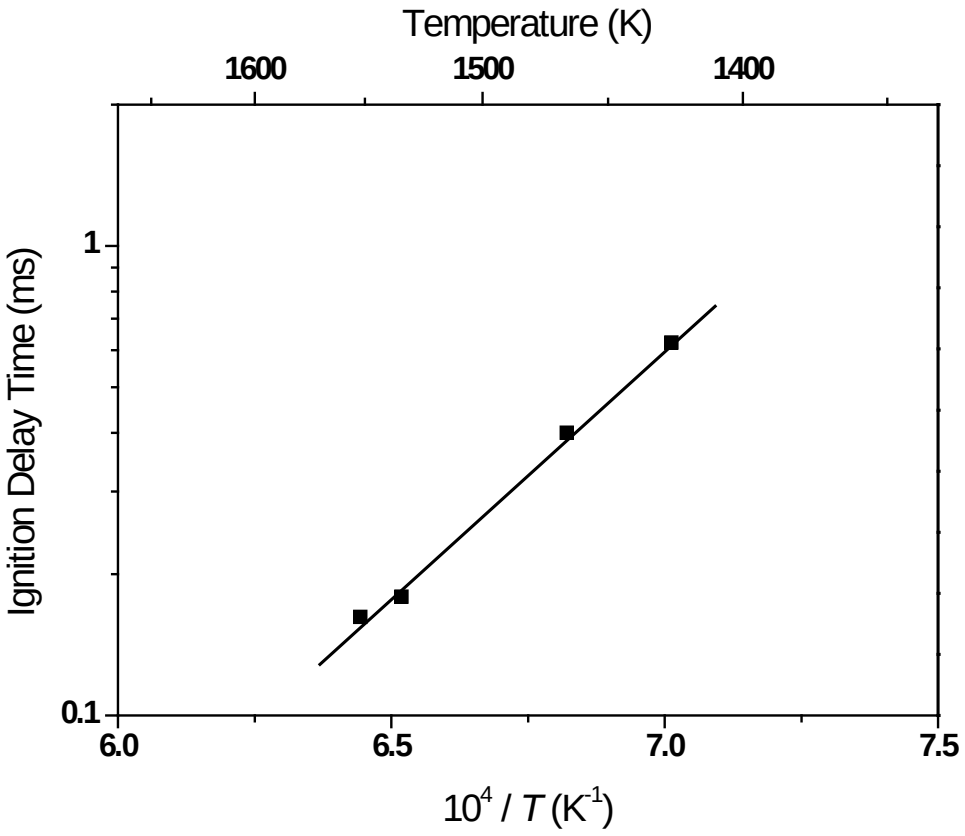

Figure S4. Comparison of experimental and model simulated ignition delay times for 0.5% *iso*-pentane in 4% O_2 and argon bath gas, at pressures near ■ – 2 atm. Symbols represent experimental data and lines refer to model simulations.

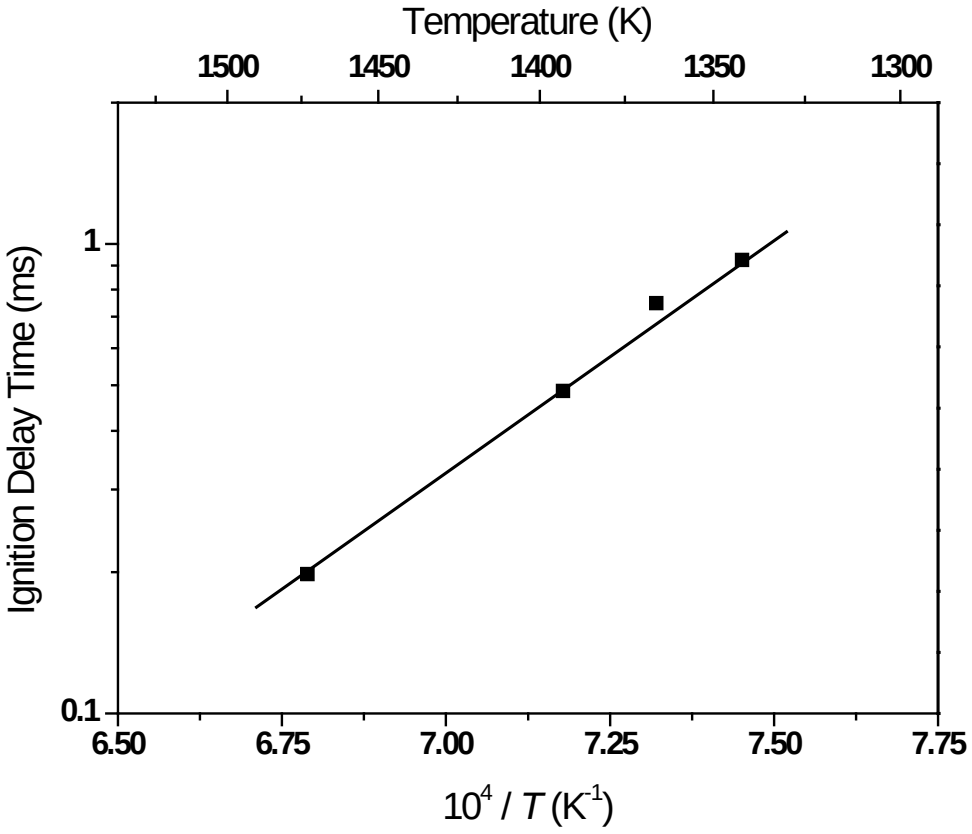

Figure S5. Comparison of experimental and model simulated ignition delay times for 1% *iso*-pentane in 8% O_2 and argon bath gas, at pressures near ■ – 2 atm. Symbols represent experimental data and lines refer to model simulations.

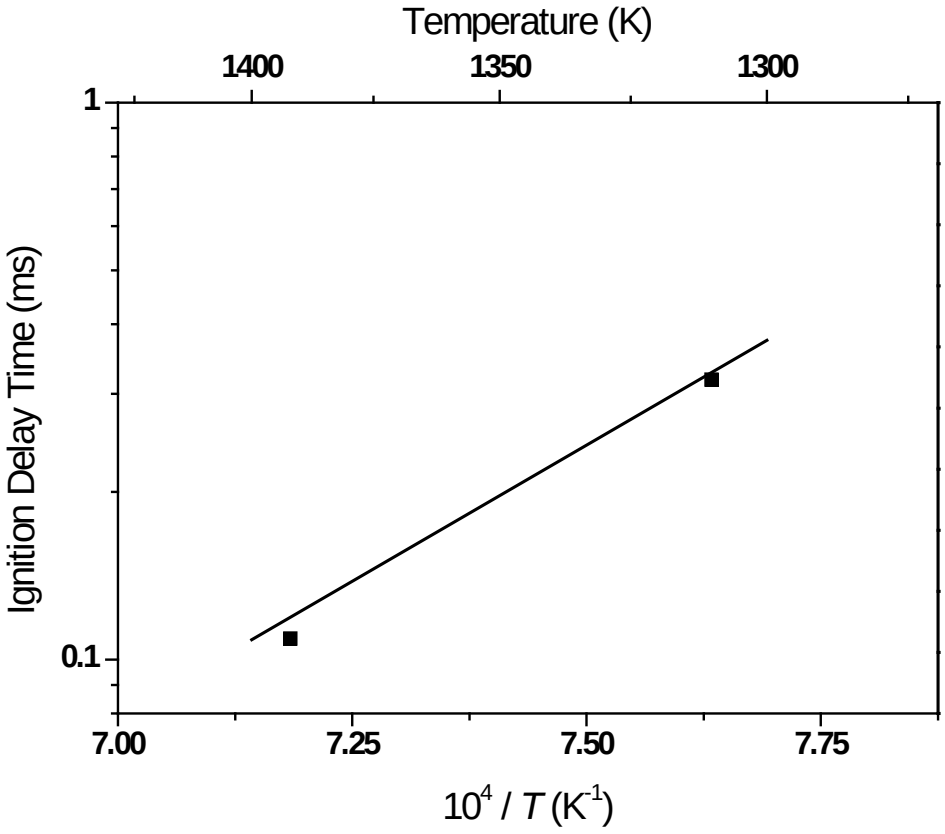

Figure S6. Comparison of experimental and model simulated ignition delay times for 1.25% *iso*-pentane in 20% O_2 and argon bath gas, at pressures near ■ – 2 atm. Symbols represent experimental data and lines refer to model simulations.

A. P. Kelley, A. J. Smallbone, D. L. Zhu, C. K. Law, Laminar flame speeds of C_5 to C_8 *n*-alkanes at elevated pressures: Experimental determination, fuel similarity, and stretch sensitivity, Proc. Combust. Inst. 33 (2011) 963–970.

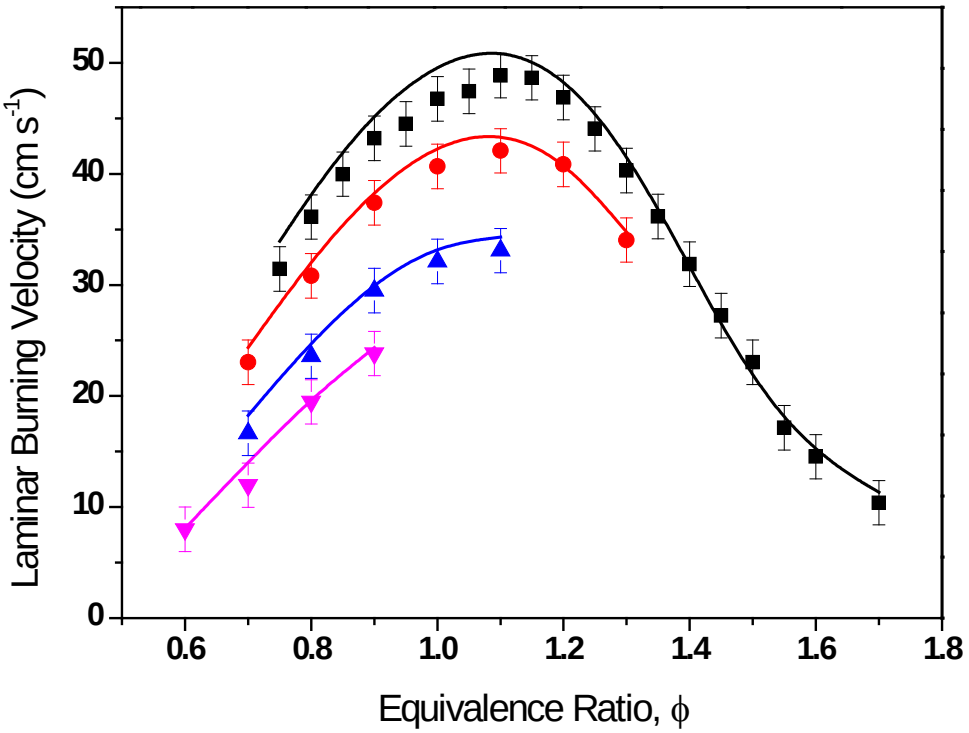

Figure S7. Comparison of experimental and model simulated laminar burning velocities for *n*-pentane in 21/79 O_2/N_2 mixture, at pressures of ■ – 1 atm, ● – 2 atm, ▲ – 5 atm, and ▼ – 10 atm. Symbols represent experimental data and lines refer to model simulations.

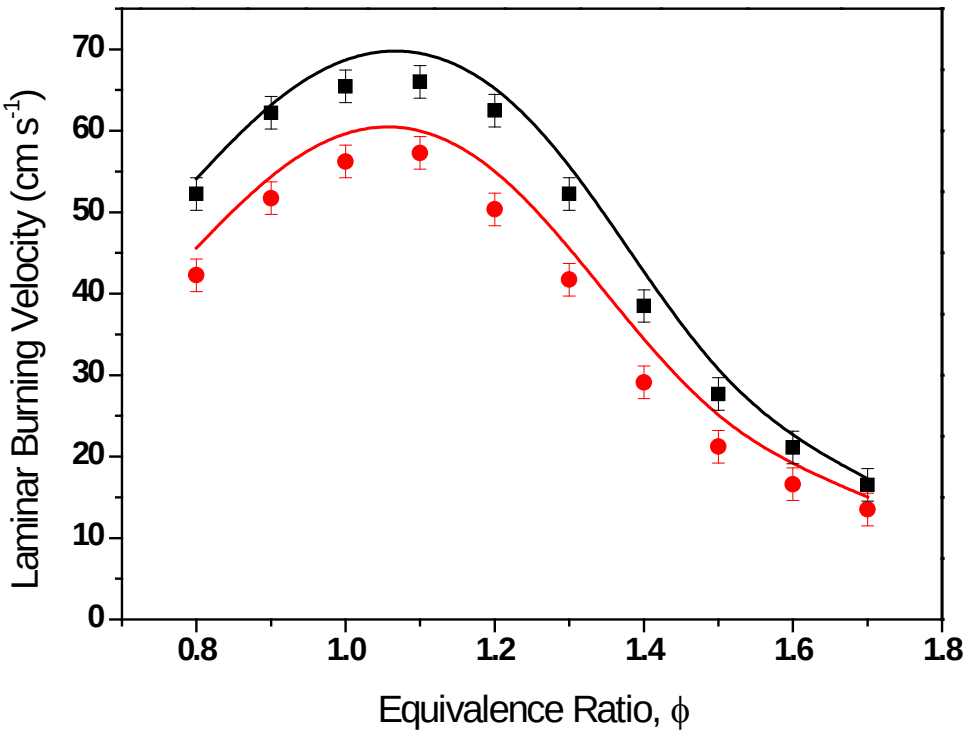

Figure S8. Comparison of experimental and model simulated laminar burning velocities for *n*-pentane in 15/85 O_2/He mixture, at pressures of ■ – 10 atm, ● – 20 atm. Symbols represent experimental data and lines refer to model simulations.

Model comparison

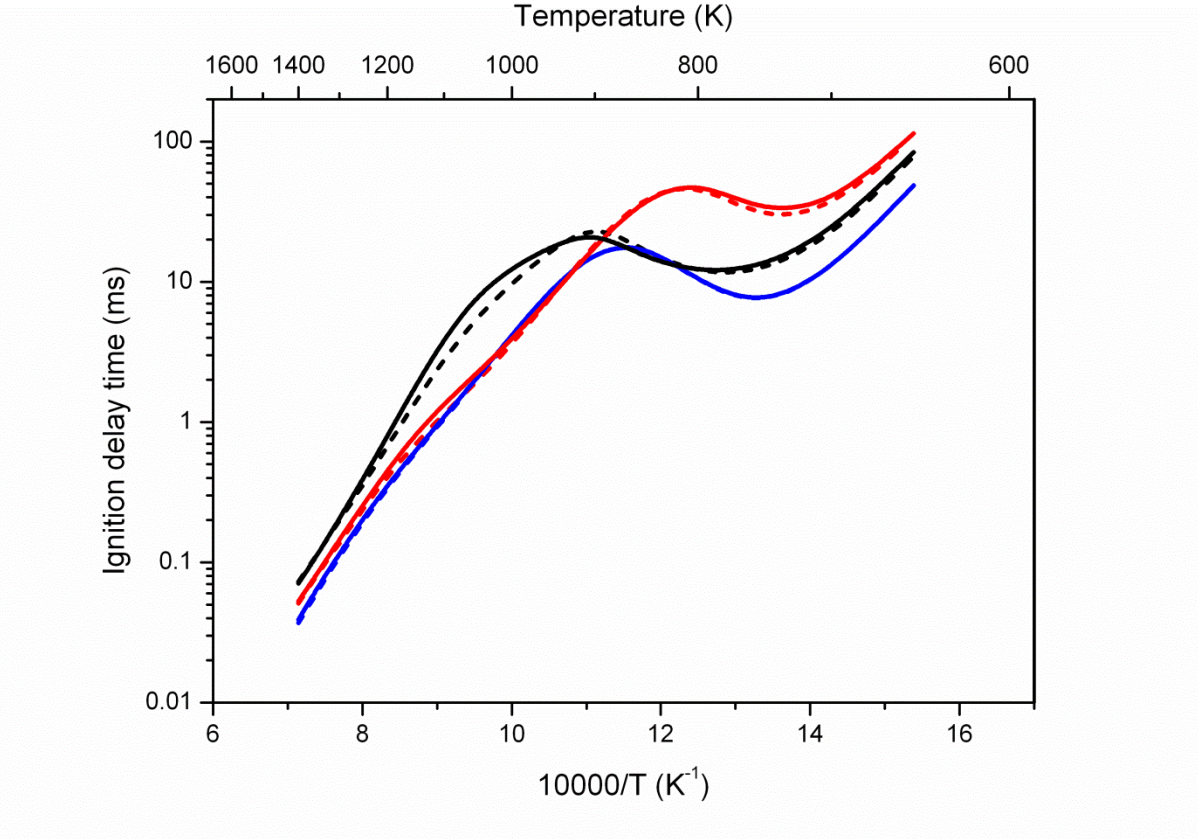

Figure S9. Comparison of model simulated ignition delay times for φ = 1.0 in 'air' at 10 atm. Dashed lines correspond to simulations using the model presented in Ref. 14. Solid lines correspond to simulations using the model presented in this study. Blue – *n*-pentane, red – *iso*-pentane, black – *neo*-pentane.

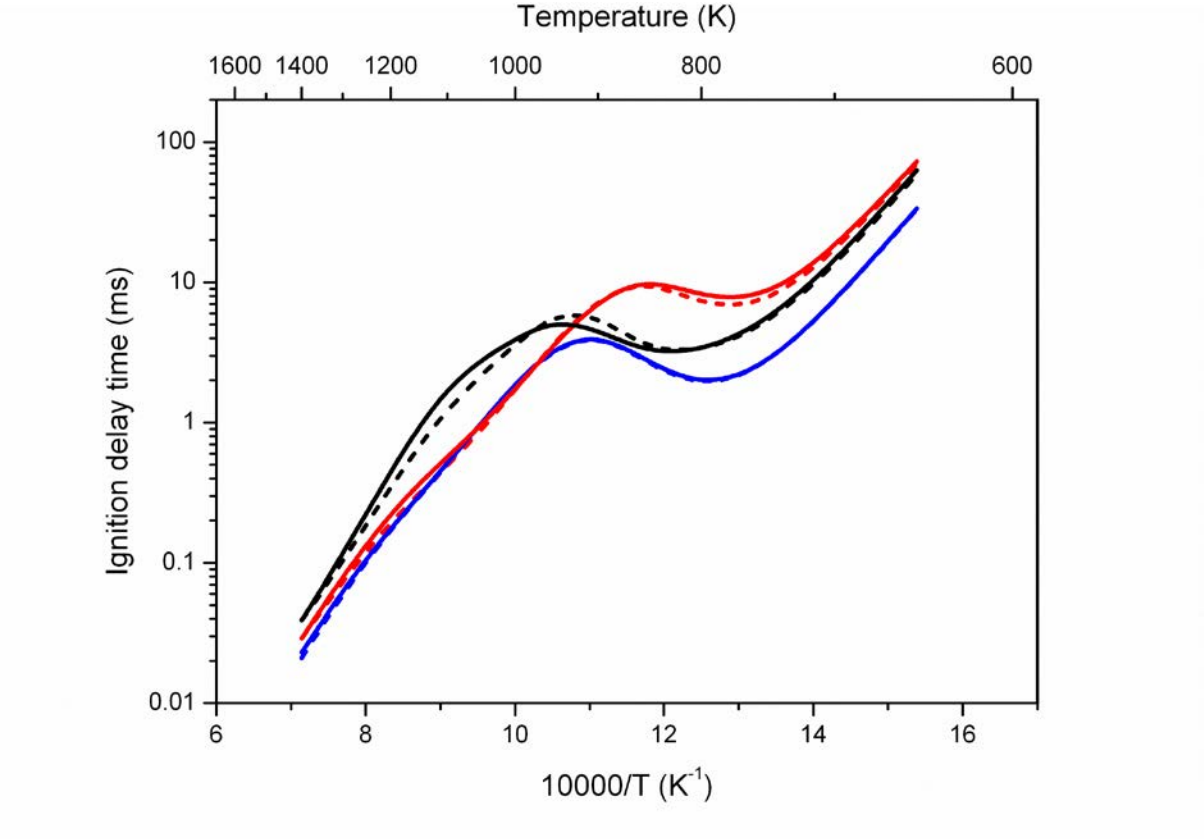

Figure S10. Comparison of model simulated ignition delay times for φ = 1.0 in 'air' at 20 atm. Dashed lines correspond to simulations using the model presented in Ref. 14. Solid lines correspond to simulations using the model presented in this study. Blue – *n*-pentane, red – *iso*-pentane, black – *neo*-pentane.

Effects of making $\dot{R} + O_2 \rightleftarrows R\dot{O}_2$ irreversible

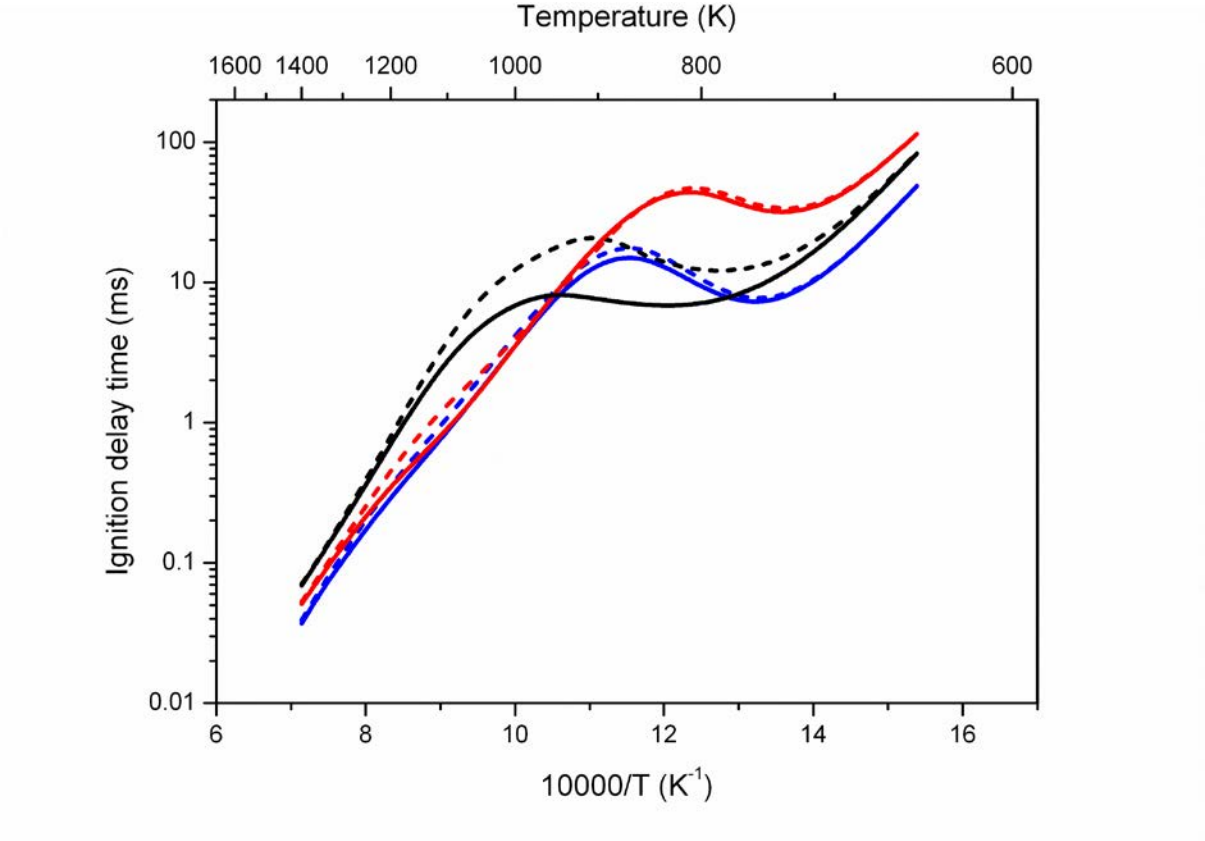

Figure S11. Comparison of model simulated ignition delay times for φ = 1.0 in 'air' at 10 atm. Dashed lines correspond to simulations using the model presented in this study. Solid lines correspond to simulations upon making addition reactions of fuel radicals to O_2 irreversible. Blue – *n*-pentane, red – *iso*-pentane, black – *neo*-pentane.

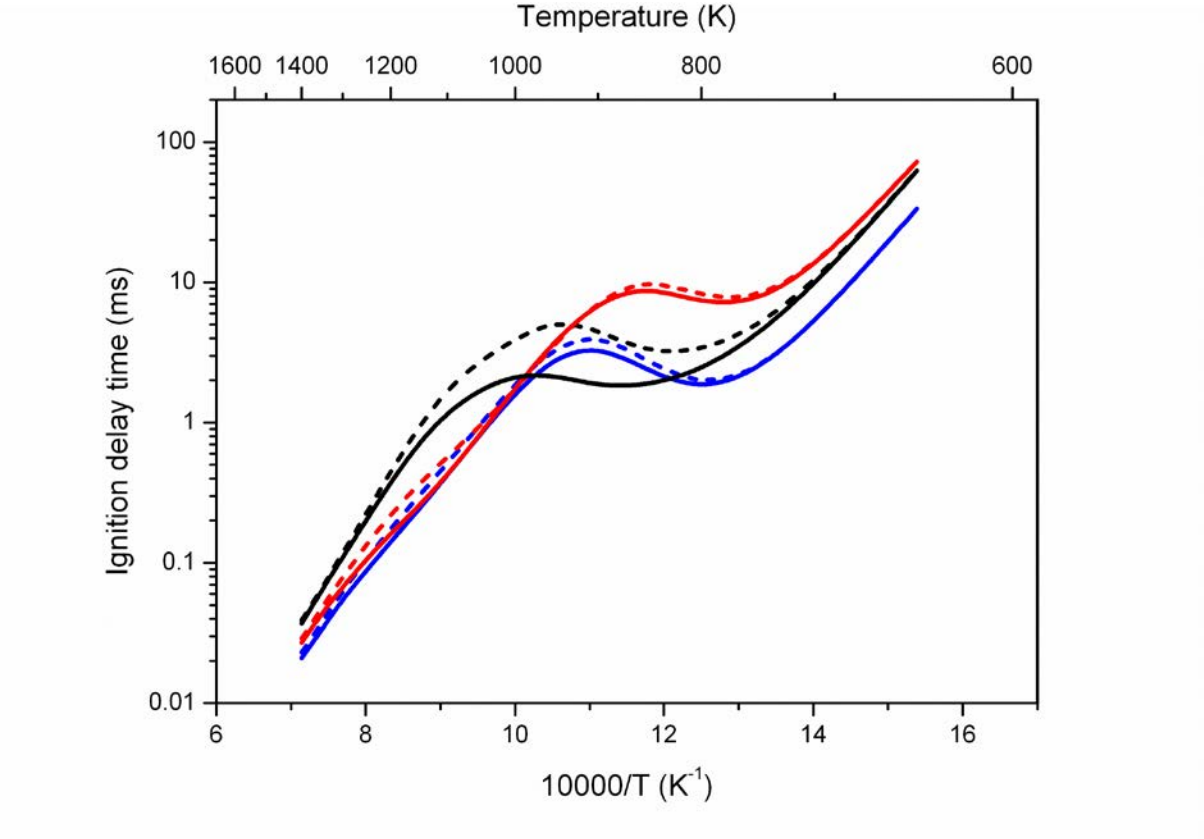

Figure S12. Comparison of model simulated ignition delay times for φ = 1.0 in 'air' at 20 atm. Dashed lines correspond to simulations using the model presented in this study. Solid lines correspond to simulations upon making addition reactions of fuel radicals to O_2 irreversible. Blue – *n*-pentane, red – *iso*-pentane, black – *neo*-pentane.

Ignition delay times obtained in this study

Texas A&M University shock tube data

n-C_5H_{12} in 'air'

Φ	p (atm)	T (K)	τ (μs)
0.3	1.31	1215	937
0.3	1.23	1222	794
0.3	1.32	1230	631
0.3	1.25	1268	357
0.3	1.22	1303	213
0.3	1.19	1308	164
0.3	1.25	1351	98
0.3	1.19	1385	66
0.3	10.38	1140	1091
0.3	9.93	1184	584
0.3	9.73	1199	485
0.3	9.87	1237	299
0.3	9.66	1270	197
0.3	9.17	1303	133
0.3	25.47	1055	1319
0.3	26.78	1083	869
0.3	26.20	1096	803
0.3	25.65	1128	586
0.3	24.96	1167	406
0.3	24.11	1194	283
0.3	20.93	1220	229
0.3	23.83	1255	141
0.5	1.23	1199	2000
0.5	1.23	1209	1579
0.5	1.24	1226	997
0.5	1.19	1232	830
0.5	1.17	1244	750
0.5	1.27	1245	707
0.5	1.14	1262	609
0.5	1.29	1264	553
0.5	1.15	1296	357
0.5	1.05	1302	293
0.5	1.19	1306	305
0.5	1.16	1314	295
0.5	1.18	1314	283
0.5	1.20	1315	254
0.5	1.13	1358	143

0.5	1.08	1360	163
0.5	1.05	1366	139
0.5	1.07	1405	104
0.5	10.29	1124	1132
0.5	9.66	1147	770
0.5	9.66	1171	604
0.5	9.07	1213	407
0.5	9.94	1275	160
0.5	9.63	1280	170
0.5	8.88	1307	142
0.5	9.44	1357	62
0.5	8.93	1363	57
0.5	22.93	1048	1172
0.5	23.09	1067	942
0.5	24.27	1110	590
0.5	23.74	1146	395
0.5	23.07	1164	314
0.5	22.08	1219	164
0.5	21.19	1247	110
0.5	20.26	1309	69
1.0	1.16	1223	1367
1.0	1.13	1229	1269
1.0	1.12	1252	1010
1.0	1.10	1263	876
1.0	1.07	1271	751
1.0	1.16	1280	610
1.0	1.16	1281	580
1.0	1.17	1281	655
1.0	1.03	1298	509
1.0	1.00	1312	419
1.0	1.17	1322	415
1.0	1.15	1327	373
1.0	1.01	1355	273
1.0	1.00	1373	234
1.0	1.03	1383	200
1.0	0.99	1405	176
1.0	0.94	1428	131
1.0	10.82	1102	1011
1.0	10.16	1118	886
1.0	9.79	1135	807
1.0	9.66	1153	666
1.0	9.55	1182	526
1.0	10.01	1217	344
1.0	8.86	1247	271
1.0	10.03	1254	234
1.0	9.71	1277	168

1.0	9.10	1312	121
1.0	8.66	1384	55
1.0	23.55	992	1458
1.0	23.89	1011	1155
1.0	24.44	1068	627
1.0	23.94	1082	522
1.0	22.15	1153	273
1.0	21.63	1185	207
1.0	20.50	1247	115
1.0	19.32	1293	77
2.0	1.06	1276	1429
2.0	1.03	1286	1176
2.0	1.15	1303	818
2.0	1.04	1309	934
2.0	1.13	1312	776
2.0	0.99	1317	876
2.0	1.09	1326	758
2.0	1.11	1335	669
2.0	0.94	1361	504
2.0	1.17	1361	513
2.0	1.09	1368	416
2.0	1.05	1388	365
2.0	0.91	1400	327
2.0	0.86	1406	273
2.0	0.80	1426	211
2.0	1.07	1426	236
2.0	1.06	1428	276
2.0	0.98	1436	211
2.0	1.02	1448	220
2.0	1.11	1474	153
2.0	0.94	1475	183
2.0	0.90	1480	147
2.0	1.03	1491	125
2.0	0.91	1531	119
2.0	0.89	1538	95
2.0	9.84	1080	1419
2.0	9.90	1108	917
2.0	9.85	1123	848
2.0	9.27	1198	429
2.0	8.71	1212	380
2.0	8.63	1216	335
2.0	8.65	1218	360
2.0	8.68	1221	334
2.0	8.37	1248	280
2.0	8.25	1280	195
2.0	7.82	1324	137

2.0	26.09	1009	742
2.0	25.73	1018	723
2.0	27.49	1055	436
2.0	26.49	1116	287
2.0	24.68	1129	254
2.0	23.37	1185	172
2.0	24.45	1192	174
2.0	23.04	1223	143
2.0	22.75	1240	124

iso-C_5H_{12} in ‘air’

Φ	*p* (atm)	*T* (K)	τ (μs)
0.3	1.31	1223	1422
0.3	1.36	1240	770
0.3	1.30	1267	546
0.3	1.25	1282	409
0.3	1.39	1284	359
0.3	1.23	1313	272
0.3	1.24	1326	181
0.3	1.21	1346	150
0.3	1.22	1366	92
0.3	1.20	1374	79
0.3	10.50	1135	1223
0.3	10.32	1176	659
0.3	9.80	1197	534
0.3	9.83	1239	287
0.3	9.52	1246	287
0.3	9.61	1292	133
0.3	9.44	1320	107
0.3	9.12	1334	68
0.3	9.27	1348	63
0.3	25.87	1082	1015
0.3	24.92	1113	754
0.3	24.22	1150	535
0.3	23.79	1184	340
0.3	23.31	1208	266
0.3	22.74	1237	182
0.3	22.25	1277	115
0.5	1.36	1235	881
0.5	1.32	1253	750
0.5	1.29	1255	697
0.5	1.47	1261	616
0.5	1.32	1267	582
0.5	1.41	1280	520
0.5	1.16	1302	422

0.5	1.18	1314	350
0.5	1.26	1315	381
0.5	1.19	1359	168
0.5	1.20	1370	164
0.5	1.27	1380	155
0.5	1.17	1388	127
0.5	10.43	1100	1716
0.5	10.73	1114	1208
0.5	10.41	1141	922
0.5	10.17	1147	770
0.5	9.68	1188	483
0.5	9.38	1191	502
0.5	9.61	1235	338
0.5	9.35	1270	224
0.5	9.32	1310	123
0.5	8.82	1320	115
0.5	8.28	1354	77
0.5	24.88	1063	1053
0.5	23.99	1096	762
0.5	24.06	1104	664
0.5	23.62	1125	582
0.5	24.62	1170	334
0.5	24.21	1187	274
0.5	22.98	1229	176
0.5	21.98	1284	92
1.0	1.22	1258	1180
1.0	1.27	1268	1086
1.0	1.17	1278	1004
1.0	1.25	1325	451
1.0	1.17	1329	451
1.0	1.12	1353	367
1.0	1.15	1355	348
1.0	1.12	1367	334
1.0	1.08	1408	215
1.0	1.12	1432	190
1.0	1.02	1432	170
1.0	0.99	1486	100
1.0	1.03	1487	102
1.0	10.53	1103	1274
1.0	10.45	1113	1233
1.0	10.39	1130	918
1.0	10.19	1138	754
1.0	10.27	1145	803
1.0	9.54	1183	553
1.0	9.68	1209	434
1.0	9.19	1257	262

1.0	8.49	1314	122
1.0	8.11	1348	113
1.0	7.99	1384	72
1.0	8.17	1404	61.5
1.0	27.12	1011	1057
1.0	26.24	1017	1061
1.0	26.11	1075	598
1.0	25.53	1113	414
1.0	23.69	1172	234
1.0	23.91	1181	219
1.0	22.65	1233	127
1.0	21.47	1294	80
2.0	1.27	1271	1404
2.0	1.25	1296	1023
2.0	1.24	1335	755
2.0	1.18	1358	514
2.0	1.13	1370	521
2.0	1.13	1406	336
2.0	1.07	1421	291
2.0	1.11	1435	269
2.0	1.06	1442	280
2.0	1.04	1469	190
2.0	0.96	1551	104
2.0	10.72	1096	1283
2.0	10.62	1129	905
2.0	10.23	1145	837
2.0	9.93	1186	521
2.0	9.36	1215	386
2.0	9.03	1243	254
2.0	8.32	1297	151
2.0	26.51	1006	932
2.0	26.04	1026	734
2.0	25.92	1069	506
2.0	27.91	1072	454
2.0	25.12	1135	297
2.0	24.60	1206	166
2.0	22.89	1231	121

neo-C_5H_{12} in ‘air’

Φ	*p* (atm)	*T* (K)	τ (μs)
0.5	1.56	1249	1395
0.5	1.52	1287	673
0.5	1.45	1309	522
0.5	1.36	1344	384
0.5	1.28	1479	80

0.5	1.22	1549	46
0.5	1.14	1555	44
0.5	0.88	1596	34
0.5	11.2	1182	1200
0.5	10.6	1219	636
0.5	9.7	1251	420
0.5	8.9	1348	118
0.5	8.4	1430	50
0.5	23.4	1125	1293
0.5	23.0	1149	946
0.5	22.6	1198	460
0.5	23.0	1263	206
0.5	21.6	1274	164
1.0	1.21	1287	1179
1.0	1.12	1324	566
1.0	1.29	1373	426
1.0	1.25	1442	231
1.0	1.16	1473	164
1.0	1.10	1536	110
1.0	1.04	1594	69
1.0	10.6	1142	1903
1.0	10.6	1158	1296
1.0	10.4	1205	749
1.0	9.7	1249	400
1.0	9.1	1316	204
1.0	8.8	1384	98
1.0	23.3	1049	1998
1.0	25.0	1168	576
1.0	23.3	1190	482
1.0	22.6	1235	252
1.0	22.6	1293	120
2.0	1.38	1302	1499
2.0	1.23	1327	1410
2.0	1.15	1329	1350
2.0	1.30	1345	971
2.0	1.17	1348	1000
2.0	1.20	1380	753
2.0	1.13	1386	720
2.0	1.08	1398	592
2.0	1.04	1431	475
2.0	1.00	1462	375
2.0	1.09	1475	343
2.0	0.94	1517	245
2.0	1.04	1520	259
2.0	0.90	1525	250
2.0	0.91	1563	172

2.0	0.96	1586	154
2.0	0.78	1619	100
2.0	10.6	1164	1277
2.0	9.9	1169	1251
2.0	10.2	1178	976
2.0	10.3	1196	760
2.0	9.6	1214	681
2.0	10.0	1229	465
2.0	9.3	1238	519
2.0	9.5	1257	325
2.0	9.2	1276	305
2.0	9.0	1276	280
2.0	9.1	1281	250
2.0	7.8	1303	195
2.0	8.8	1332	170
2.0	8.4	1370	120
2.0	26.0	1075	1788
2.0	25.2	1095	1497
2.0	24.0	1113	1123
2.0	25.1	1116	1060
2.0	22.6	1131	933
2.0	24.8	1150	617
2.0	24.2	1180	425
2.0	22.7	1189	355
2.0	22.0	1209	310
2.0	23.0	1210	295
2.0	21.6	1249	185
2.0	20.0	1289	120
2.0	19.1	1312	85

n-C_5H_{12}, 99% Ar

Φ	*p* (atm)	*T* (K)	τ (μs)
1.0	1.92	1340	1777
1.0	1.97	1343	1385
1.0	1.98	1400	769
1.0	1.95	1433	445
1.0	1.93	1470	328
1.0	1.90	1526	136
1.0	1.86	1545	114
1.0	1.80	1555	96
1.0	15.5	1316	1146
1.0	15.1	1363	556
1.0	14.6	1404	362
1.0	14.2	1452	220
1.0	14.0	1488	141

1.0	14.1	1540	60

iso-C_5H_{12}, 99% Ar

Φ	*p* (atm)	*T* (K)	τ (μs)
1.0	1.82	1441	926
1.0	1.99	1453	902
1.0	1.81	1474	747
1.0	1.87	1558	261
1.0	1.91	1561	218
1.0	1.84	1583	184
1.0	1.94	1675	52
1.0	15.1	1338	1600
1.0	15.1	1376	982
1.0	14.9	1430	520
1.0	14.2	1452	442
1.0	14.1	1515	192
1.0	13.5	1569	89
1.0	11.7	1593	53

neo-C_5H_{12}, 99% Ar

Φ	*p* (atm)	*T* (K)	τ (μs)
1.0	1.91	1437	1516
1.0	1.85	1446	1332
1.0	1.84	1470	1120
1.0	1.76	1497	761
1.0	1.84	1519	613
1.0	1.83	1573	357
1.0	1.85	1654	129
1.0	1.78	1675	106
1.0	1.95	1677	100
1.0	1.78	1718	65
1.0	14.7	1390	1296
1.0	14.5	1418	1069
1.0	14.2	1470	562
1.0	13.0	1497	385
1.0	13.4	1576	179
1.0	13.1	1592	135
1.0	12.4	1613	110
1.0	12.9	1635	71

NUIG shock tube data

n-C_5H_{12} in ‘air’

Φ	*p* (atm)	*T* (K)	τ (μs)
1.0	19.88	783	2427
1.0	19.49	796	2373
1.0	19.25	812	2452
1.0	19.33	848	2635
1.0	19.79	859	2677
1.0	19.94	890	2953
1.0	19.72	915	2609
1.0	19.60	942	2332
1.0	19.79	976	1553
2.0	19.08	778	2172
2.0	19.37	784	1993
2.0	19.02	796	2243
2.0	21.81	854	1673
2.0	20.20	873	2099
2.0	20.12	903	2439
2.0	20.52	950	2053
2.0	19.80	984	1423

neo-C_5H_{12} in ‘air’

Φ	*p* (atm)	*T* (K)	τ (μs)
2.0	21.66	786	2645
2.0	21.37	793	2598
2.0	20.98	819	2500
2.0	19.38	828	2737
2.0	19.40	872	2944
2.0	19.42	906	3057
2.0	21.45	1005	2783
2.0	21.33	1024	2493
2.0	21.00	1075	1652

NUIG RCM data

Note: Compressed pressures in tables below are approximate. Experimental compressed pressures are within ±1% of the stated pressure.

n-C_5H_{12} in ‘air’

Φ	p (atm)	T (K)	τ (μs)
0.3	10	674	179900
0.3	10	677	179500
0.3	10	698	97500
0.3	10	700	87240
0.3	10	733	54710
0.3	10	733	52250
0.3	10	751	56600
0.3	10	753	53290
0.3	10	776	56810
0.3	10	778	56460
0.3	10	796	67010
0.3	10	797	67290
0.3	10	816	70440
0.3	10	817	76950
0.3	10	837	79730
0.3	10	838	81310
0.3	10	853	83560
0.3	10	856	83750
0.3	10	878	89070
0.3	10	881	88900
0.3	10	896	86250
0.3	10	897	88370
0.3	10	916	69920
0.3	10	917	70390
0.3	10	947	36290
0.3	10	949	37440
0.3	10	955	36220
0.3	10	978	18230
0.3	10	985	17700
0.3	20	678	68200
0.3	20	678	64190
0.3	20	701	30450
0.3	20	702	29840
0.3	20	737	11460
0.3	20	737	10680
0.3	20	755	8770
0.3	20	756	8620
0.3	20	779	8530
0.3	20	781	8640

0.3	20	804	8370
0.3	20	804	8400
0.3	20	825	9712
0.3	20	826	10030
0.3	20	843	12020
0.3	20	845	11820
0.3	20	862	12840
0.3	20	865	13470
0.3	20	881	13500
0.3	20	883	14950
0.3	20	902	14590
0.3	20	903	14800
0.3	20	923	13040
0.3	20	927	13370
0.3	20	952	7390
0.3	20	953	8020
0.3	20	983	3830
0.3	20	988	4170
0.5	10	709	32390
0.5	10	710	29640
0.5	10	736	15390
0.5	10	737	18930
0.5	10	756	16110
0.5	10	757	17520
0.5	10	779	19510
0.5	10	780	20200
0.5	10	796	25240
0.5	10	799	25990
0.5	10	810	37390
0.5	10	811	37080
0.5	10	830	42370
0.5	10	832	41220
0.5	10	844	47130
0.5	10	847	46640
0.5	10	866	53810
0.5	10	869	53210
0.5	10	888	54010
0.5	10	889	53220
0.5	10	906	45890
0.5	10	909	45240
0.5	10	931	32550
0.5	10	931	31790
0.5	10	953	21220
0.5	10	953	21500
0.5	10	977	10220
0.5	10	977	10010

0.5	10	1009	4810
0.5	10	1009	4530
0.5	20	712	8460
0.5	20	713	8140
0.5	20	741	4500
0.5	20	743	4950
0.5	20	759	3720
0.5	20	761	3980
0.5	20	782	3950
0.5	20	784	4090
0.5	20	802	4180
0.5	20	803	4300
0.5	20	814	4530
0.5	20	814	4640
0.5	20	830	5830
0.5	20	838	5760
0.5	20	857	6410
0.5	20	858	6420
0.5	20	874	8880
0.5	20	875	7980
0.5	20	892	7720
0.5	20	892	7470
0.5	20	912	7310
0.5	20	915	7900
0.5	20	933	5610
0.5	20	935	6320
0.5	20	954	3280
0.5	20	957	3800
0.5	20	989	1790
0.5	20	991	1540
1.0	10	682	32800
1.0	10	684	32050
1.0	10	695	22270
1.0	10	698	21630
1.0	10	715	9820
1.0	10	716	10320
1.0	10	733	7090
1.0	10	734	7150
1.0	10	751	6410
1.0	10	753	6800
1.0	10	771	7760
1.0	10	772	7730
1.0	10	790	9690
1.0	10	792	9910
1.0	10	807	12590
1.0	10	811	12650

1.0	10	825	14880
1.0	10	826	15540
1.0	10	842	18320
1.0	10	843	18020
1.0	10	844	20160
1.0	10	845	18710
1.0	10	860	22540
1.0	10	863	22690
1.0	10	865	18890
1.0	10	865	19230
1.0	10	879	24240
1.0	10	881	23290
1.0	10	903	23190
1.0	10	906	24010
1.0	10	922	22790
1.0	10	922	21060
1.0	10	941	16950
1.0	10	942	17470
1.0	10	967	8400
1.0	10	967	8160
1.0	10	997	3690
1.0	10	999	3680
1.0	20	685	16330
1.0	20	685	16520
1.0	20	700	10240
1.0	20	702	11720
1.0	20	718	4670
1.0	20	720	5280
1.0	20	736	2560
1.0	20	737	2620
1.0	20	755	1620
1.0	20	756	1380
1.0	20	774	1130
1.0	20	776	1310
2.0	10	643	259680
2.0	10	644	301870
2.0	10	660	91920
2.0	10	660	90020
2.0	10	676	37070
2.0	10	677	35900
2.0	10	690	19740
2.0	10	691	20730
2.0	10	705	10610
2.0	10	708	10920
2.0	10	725	6350
2.0	10	726	6360

2.0	10	741	4530
2.0	10	743	4610
2.0	10	748	4270
2.0	10	750	4060
2.0	10	757	3490
2.0	10	757	3420
2.0	10	771	3480
2.0	10	777	3840
2.0	10	788	4240
2.0	10	789	4330
2.0	10	805	5590
2.0	10	808	5800
2.0	10	822	7780
2.0	10	825	7730
2.0	10	840	9780
2.0	10	841	9830
2.0	10	858	11740
2.0	10	862	11910
2.0	10	881	12720
2.0	10	882	12760
2.0	10	894	12560
2.0	10	897	12620
2.0	10	913	10060
2.0	10	913	10320
2.0	10	915	9970
2.0	10	918	10030
2.0	10	941	6400
2.0	10	942	6650
2.0	20	644	99400
2.0	20	644	101430
2.0	20	660	46160
2.0	20	660	44950
2.0	20	678	21400
2.0	20	678	19070
2.0	20	692	11040
2.0	20	693	11400
2.0	20	709	5390
2.0	20	710	5720
2.0	20	726	3160
2.0	20	727	3290
2.0	20	740	1780
2.0	20	744	1910
2.0	20	753	1540
2.0	20	753	1540
2.0	20	758	1040
2.0	20	760	1090

iso-C_5H_{12} in ‘air’

Φ	*p* (atm)	*T* (K)	τ (μs)
0.3	10	889	150200
0.3	10	889	157700
0.3	10	919	68510
0.3	10	926	68300
0.3	10	947	30340
0.3	10	949	29950
0.3	20	747	42040
0.3	20	751	41390
0.3	20	776	43330
0.3	20	777	42310
0.3	20	804	46710
0.3	20	806	46420
0.3	20	833	52300
0.3	20	835	52380
0.3	20	864	44550
0.3	20	864	45900
0.3	20	893	27340
0.3	20	894	28010
0.3	20	926	14590
0.3	20	928	14960
0.3	20	952	7140
0.3	20	953	7270
0.5	10	708	123100
0.5	10	709	132600
0.5	10	733	96230
0.5	10	734	97840
0.5	10	761	122000
0.5	10	762	123900
0.5	10	788	157300
0.5	10	792	157800
0.5	10	817	197200
0.5	10	819	199300
0.5	10	846	182900
0.5	10	846	175200
0.5	10	893	132500
0.5	10	893	134300
0.5	10	921	65240
0.5	10	924	62860
0.5	10	945	30270
0.5	10	947	29480
0.5	20	711	29760
0.5	20	712	25810
0.5	20	735	15150

0.5	20	737	17070
0.5	20	765	15440
0.5	20	767	16390
0.5	20	793	18910
0.5	20	794	18910
0.5	20	823	24790
0.5	20	823	24600
0.5	20	850	27490
0.5	20	851	28040
0.5	20	898	24420
0.5	20	898	21490
0.5	20	927	13860
0.5	20	927	13760
0.5	20	950	7360
0.5	20	950	7230
1.0	10	687	101000
1.0	10	689	84740
1.0	10	689	86910
1.0	10	704	47430
1.0	10	704	47730
1.0	10	722	39160
1.0	10	724	34730
1.0	10	725	34910
1.0	10	740	36440
1.0	10	742	38440
1.0	10	759	44180
1.0	10	761	45180
1.0	10	776	57520
1.0	10	777	58560
1.0	10	806	78470
1.0	10	806	81220
1.0	10	826	90890
1.0	10	828	82440
1.0	10	846	93780
1.0	10	847	98960
1.0	10	872	78320
1.0	10	873	74000
1.0	10	898	43260
1.0	10	900	44440
1.0	10	942	16070
1.0	10	944	16390
1.0	10	974	6010
1.0	10	977	6180
1.0	10	1005	2690
1.0	10	1011	2660
1.0	20	666	131000

1.0	20	666	121900
1.0	20	692	34900
1.0	20	692	31930
1.0	20	707	16380
1.0	20	708	18080
1.0	20	727	8500
1.0	20	728	8620
1.0	20	744	7320
1.0	20	744	6820
1.0	20	762	6330
1.0	20	763	6820
1.0	20	780	7160
1.0	20	780	7100
1.0	20	809	10370
1.0	20	809	10220
1.0	20	830	13170
1.0	20	831	13140
1.0	20	848	14660
1.0	20	848	14730
1.0	20	873	14190
1.0	20	873	13690
1.0	20	917	6030
1.0	20	917	5700
1.0	20	948	2680
1.0	20	949	2680
2.0	10	663	242200
2.0	10	664	237100
2.0	10	688	63110
2.0	10	689	64560
2.0	10	710	27030
2.0	10	710	26610
2.0	10	735	17890
2.0	10	736	17930
2.0	10	758	19600
2.0	10	759	18980
2.0	10	782	24980
2.0	10	783	24580
2.0	10	809	30900
2.0	10	809	32180
2.0	10	832	37970
2.0	10	833	37600
2.0	10	862	34490
2.0	10	864	35550
2.0	10	891	22180
2.0	10	892	22150
2.0	10	915	12050

2.0	10	919	11940
2.0	10	943	6350
2.0	10	943	6300
2.0	20	666	102700
2.0	20	667	98680
2.0	20	689	30490
2.0	20	690	30100
2.0	20	715	11770
2.0	20	715	11900
2.0	20	738	5700
2.0	20	738	5700
2.0	20	762	3690
2.0	20	763	3750
2.0	20	785	3000
2.0	20	786	3440
2.0	20	811	4090
2.0	20	811	4060
2.0	20	838	5790
2.0	20	838	5780
2.0	20	865	5880
2.0	20	865	5890
2.0	20	894	4340
2.0	20	894	4370
2.0	20	918	2490
2.0	20	919	2480

neo-C_5H_{12} in ‘air’

Φ	*p* (atm)	*T* (K)	τ (μs)
0.5	10	700	149900
0.5	10	703	149100
0.5	10	703	153700
0.5	10	727	93000
0.5	10	728	92360
0.5	10	728	97260
0.5	10	752	72140
0.5	10	752	72120
0.5	10	753	65100
0.5	10	753	64900
0.5	10	753	74800
0.5	10	754	66300
0.5	10	784	57490
0.5	10	785	58350
0.5	10	785	56240
0.5	10	818	50680
0.5	10	818	51120

0.5	10	819	51200
0.5	10	845	49680
0.5	10	849	50690
0.5	10	849	49400
0.5	10	876	52010
0.5	10	876	52110
0.5	10	877	53510
0.5	10	886	67810
0.5	10	887	66710
0.5	10	888	67310
0.5	10	906	58900
0.5	10	907	58310
0.5	10	907	59590
0.5	10	916	71520
0.5	10	922	70440
0.5	10	922	69880
0.5	10	949	66280
0.5	10	953	66360
0.5	10	954	64080
0.5	10	991	43990
0.5	10	992	45500
0.5	10	993	44100
0.5	10	1028	21260
0.5	10	1028	21330
0.5	10	1029	21680
0.5	10	1065	11300
0.5	10	1065	10410
0.5	10	1065	11560
0.5	20	651	222700
0.5	20	651	208800
0.5	20	652	202200
0.5	20	676	64050
0.5	20	677	65860
0.5	20	677	65550
0.5	20	704	33310
0.5	20	704	33330
0.5	20	705	33820
0.5	20	729	19210
0.5	20	729	19310
0.5	20	730	19320
0.5	20	755	12250
0.5	20	755	12290
0.5	20	755	12470
0.5	20	757	10080
0.5	20	757	9780
0.5	20	757	9940

1.0	10	672	185700
1.0	10	675	179800
1.0	10	704	44210
1.0	10	705	50520
1.0	10	711	37400
1.0	10	711	37670
1.0	10	712	37600
1.0	10	739	22420
1.0	10	740	22120
1.0	10	740	22610
1.0	10	765	19450
1.0	10	767	19130
1.0	10	768	20040
1.0	10	798	18610
1.0	10	799	18540
1.0	10	800	19220
1.0	10	829	19610
1.0	10	830	20740
1.0	10	830	19720
1.0	10	852	20840
1.0	10	857	22030
1.0	10	857	21430
1.0	10	869	29530
1.0	10	870	29080
1.0	10	870	29010
1.0	10	899	32140
1.0	10	901	32420
1.0	10	902	32570
1.0	10	932	32640
1.0	10	934	31750
1.0	10	934	31590
1.0	10	966	25120
1.0	10	968	24930
1.0	10	968	25560
1.0	10	993	17290
1.0	10	996	15850
1.0	10	1000	16780
1.0	20	678	58560
1.0	20	679	57250
1.0	20	707	14500
1.0	20	708	14790
1.0	20	713	9480
1.0	20	715	9740
1.0	20	715	9510
1.0	20	741	4350
1.0	20	742	4440

1.0	20	743	4500
2.0	10	675	88310
2.0	10	676	83810
2.0	10	676	84040
2.0	10	699	28680
2.0	10	700	27350
2.0	10	700	28150
2.0	10	725	14400
2.0	10	725	13860
2.0	10	727	14120
2.0	10	747	9330
2.0	10	750	9530
2.0	10	750	9600
2.0	10	774	8550
2.0	10	775	8510
2.0	10	776	8290
2.0	10	782	10140
2.0	10	783	11000
2.0	10	783	10490
2.0	10	806	10000
2.0	10	807	10030
2.0	10	808	10130
2.0	10	837	11390
2.0	10	837	11150
2.0	10	837	11300
2.0	10	861	14550
2.0	10	862	14630
2.0	10	865	14610
2.0	10	893	17450
2.0	10	893	17460
2.0	10	893	17370
2.0	10	920	19090
2.0	10	920	19090
2.0	10	921	18490
2.0	20	653	165000
2.0	20	653	158400
2.0	20	654	152600
2.0	20	678	37970
2.0	20	678	37570
2.0	20	678	36910
2.0	20	701	12040
2.0	20	701	12460
2.0	20	701	12020
2.0	20	728	4760
2.0	20	728	4900
2.0	20	728	4780

2.0	20	753	2340
2.0	20	753	2290
2.0	20	753	2360