SUPPORTING INFORMATION

Tables of experimental data

All data are sorted by reaction temperature T5. All reagent mixtures were 1,5-hexadiyne as given in the tables, 150 ppm xenon with the balance argon

Key

15HD, 1,5-hexadiyne;

34DMCB, 3,4-dimethylenecyclobutene;

13HD5Y, 1,3-hexadiene-5-yne;

2E13BD, 2-ethynyl-1,3-butadiene.

Table 1. Reaction conditions and post shock data of 1,5-hexadiyne pyroplysis at **25 bar.**

Shock No.	T_5 (K)	P_5 (bar)	Reaction time (sec.)	$[15HD]_0$ (ppm)	Post Shock Product Distributions (ppm)						
					15HD	34DMCB	Fulvene	Benzene	*cis*-13HD5Y	*trans*-13HD5Y	2E13BD
9	801.17	24.13793	0.001714	42	38.05693	3.33533	0	0	0	0	0
8	824.73	24.13793	0.001693	42	35.42998	5.69849	0.24288	0	0	0	0
5	844.54	23.7931	0.001717	42	32.03847	8.72068	0	0	0	0	0
6	849.01	25.51724	0.001699	42	29.34784	11.78198	0	0	0	0	0
7	857.61	26.55172	0.001783	42	27.27305	14.30458	0.15798	0	0	0	0
4	873.83	25.51724	0.001775	42	25.17354	15.45069	0.34663	0.3372	0	0	0
37	891.31	25.17241	0.00176	42	20.19692	22.9394	0.46446	0.33096	0	0	0
11	913.78	23.44828	0.001725	42	10.6396	29.03132	0.73468	0	0	0	0
2	916.04	25.86207	0.001781	42	11.99708	29.36902	0.5178	0	0	0	0
3	927.24	26.55172	0.001778	42	9.88708	31.48729	0.90933	0	0	0	0
13	949.22	23.44828	0.001675	42	5.05475	33.72957	1.75789	0.29281	0	0	0
12	973.37	26.2069	0.001693	42	2.68445	33.08688	2.81303	0.18005	0.50539	0.05111	0
14	992.4	26.55172	0.001755	42	1.21803	31.0464	6.5202	0.40353	1.16135	0.53612	0
17	1011.06	25.51724	0.001744	42	0.66857	25.4679	9.97272	0.7619	1.57714	1.05965	0.05253
22	1029.7	24.48276	0.001803	42	0.51793	20.22039	14.75277	1.42609	2.41725	1.87542	0.14185

19	1047.75	23.44828	0.001803	42	0.46116	14.59555	15.72991	1.89166	2.73334	2.04422	0.22541
18	1055.56	25.17241	0.001831	42	0.36858	15.07578	17.22602	2.15188	2.53767	1.84789	0.18769
20	1076.21	23.7931	0.001818	42	0.46625	10.12949	20.4328	3.81747	2.59959	2.08151	0.38231
21	1109.91	24.13793	0.00187	42	0.16762	2.59696	23.36473	9.25013	1.93592	1.55907	0.68864
23	1149.01	25.17241	0.001872	42	0.175	1.2251	19.49178	16.16992	1.23091	1.00653	0.72094
24	1168.75	25.17241	0.00188	42	0.19288	0.68363	19.08789	18.44081	0.87419	0.61788	0.88703
25	1199.11	24.48276	0.00188	42	0.30204	0.34602	17.06252	20.50709	0.31816	0.12417	1.03097
26	1221.53	24.62069	0.001849	42	0.19306	0.229	16.50662	22.0383	0.36306	0.13186	0.94118
27	1236.76	24.13793	0.001833	42	0.46998	0.76274	10.92853	21.47495	0.2286	0	0.71533
32	1266.05	23.7931	0.001741	42	0.08855	0.1031	9.31747	26.22212	0.06558	0	0.58244
33	1307.35	24.13793	0.001727	42	0.41614	0.283	6.19339	30.64189	0	0	0
29	1348.39	25.17241	0.001721	42	0.34577	0.44358	4.11956	32.2577	0	0	0.22523

Table 2. Reaction conditions and post shock data of 1,5-hexadiyne pyroplysis at **50 bar.**

Shock No.	T_5 (K)	P_5 (bar)	Reaction time (sec.)	$[15HD]_0$ (ppm)	Post Shock Product Distributions (ppm)						
					15HD	34DMCB	Fulvene	Benzene	*cis*-13HD5Y	*trans*-13HD5Y	2E13BD
17	793.9	56.89655	0.001618	42	39.8924	3.70905	0	0	0	0	0
19	818.24	56.55172	0.001627	42	35.55882	6.20313	0	0	0	0	0
20	840.8	56.2069	0.00159	42	32.92206	10.01102	0	0	0	0	0
21	867.41	57.93103	0.001635	42	25.40965	17.94969	0	0	0	0	0
22	885.37	57.58621	0.00162	42	19.31174	22.8199	0	0	0	0	0
23	894.21	56.2069	0.001659	42	13.58843	26.5825	0.43218	0	0	0	0
28	895.21	51.72414	0.001652	42	15.40367	28.35042	0.47862	0	0	0	0
25	899.77	51.72414	0.001689	42	12.97772	27.99247	0.54249	0	0	0	0
29	907.59	46.89655	0.001693	42	9.73845	31.30703	0.75974	0	0	0	0
26	930.48	53.10345	0.001686	42	5.55365	35.5287	1.65077	0	0	0	0
30	930.69	44.82759	0.001699	42	5.27655	35.09125	1.42627	0	0	0	0
27	954.79	52.75862	0.001724	42	2.04407	35.63495	3.86271	0	0.58479	0	0
31	967.8	45.51724	0.001718	42	1.85806	34.61453	4.11949	0	0.68273	0	0
34	992.96	44.82759	0.001748	42	1.19432	31.06352	7.14376	0.46261	1.30356	0.54045	0
32	1003.4	45.51724	0.001712	42	0.98084	32.28554	7.95842	0.51409	1.46616	0.71987	0
35	1024.29	47.24138	0.001792	42	0.59824	20.58108	14.79256	1.31581	2.32387	1.60532	0.13604

33	1044.72	48.27586	0.001777	42	0.49428	14.46628	18.43965	2.18509	2.72646	2.1558	0.26683
36	1066.89	45.51724	0.00189	42	0.33556	8.63593	21.16073	4.25902	2.69564	2.3072	0.42131
43	1096.74	48.27586	0.001853	42	0.25905	4.17884	24.58114	8.32925	2.49614	2.17051	0.65536
41	1130.15	51.03448	0.001905	42	0.5017	1.57854	21.77732	12.4037	1.37401	0.94005	0.73544
40	1140.08	50.68966	0.00188	42	0.20086	0.7386	21.27378	15.58319	0.90277	0.59902	0.85353
39	1171.28	51.03448	0.001849	42	0.18087	0.39931	17.92137	20.64929	0.48745	0.28444	0.87644
38	1208.95	51.72414	0.001834	42	0.07524	0.17344	13.70972	24.75254	0.21535	0	0.78776
47	1258.58	50	0.001743	42	0.08424	0.11481	10.44854	26.8824	0.11396	0	0.71105
45	1261.71	50.68966	0.001794	42	0.15062	0.13519	8.21175	28.31281	0	0	0.49472
49	1270.61	51.72414	0.001762	42	0.19348	0.14314	7.88346	28.08674	0	0	0.49994
52	1280.42	49.65517	0.001676	42	0.05539	0.08554	6.48544	27.40491	0	0	0.41949
50	1343.22	52.75862	0.001663	42	0	0.05749	2.81666	33.96694	0	0	0.14135
48	1365.86	51.72414	0.001647	42	0	0.0751	1.39656	35.1672	0	0	0

Table 3. Reaction conditions and post shock data of 1,5-hexadiyne pyroplysis at **300 bar**

Shock No.	T_5 (K)	P_5 (bar)	Reaction time (sec.)	$[15HD]_0$ (ppm)	Post Shock Product Distributions (ppm)						
					15HD	34DMCB	Fulvene	Benzene	*cis*-13HD5Y	*trans*-13HD5Y	2E13BD
23	807.3	341.3793	0.001135	40	36.10194	5.64092	0	0	0	0	0
28	824.2	386.2069	0.0012	40	37.22347	7.15077	0	0	0	0	0
20	836.5	344.8276	0.001152	40	31.63669	8.73581	0	0	0	0	0
16	872.9	362.069	0.00115	40	19.73638	16.25834	0	0	0	0	0
19	889.6	355.1724	0.001122	40	14.81905	18.38822	0	0	0	0	0
26	906.2	379.3103	0.001125	40	11.57428	20.2114	0	0	0	0	0
25	926.4	389.6552	0.00112	40	8.25166	22.93464	0	0	0	0	0
21	949.5	372.4138	0.001136	40	4.1233	31.80369	1.07809	0	0	0	0
5	964.1567	334.4828	0.00102	46	0.89828	36.54754	6.91738	0.28149	0.90501	0.08161	0
6	967.6036	320.6897	0.001184	46	0.65826	33.17636	9.0184	0.36183	1.33491	0.27629	0
21	999	310.3448	0.001194	46	0.40778	23.89918	14.6466	1.34104	2.25376	1.53334	0
19	1012.3	303.4483	0.001194	46	0.25823	18.4621	18.66476	1.73797	2.21261	1.65706	0.26817
7	1017.064	317.2414	0.001209	46	0.25128	15.43098	20.12986	1.83563	2.54151	1.4894	0.21417
8	1054.35	318.6207	0.001235	46	0	7.80548	25.60968	5.12948	3.20864	2.44459	0.48584
9	1074.704	313.7931	0.001253	46	0	3.30048	26.5267	9.3252	2.27208	1.72927	0.79302
10	1115.002	324.1379	0.001308	46	0	0.82885	22.43906	16.13657	0.97611	0.5489	0.93981

11	1119.387	310.3448	0.001337	46	0	0.62215	21.66544	17.51123	0.80998	0.40499	0.91179
12	1130.575	293.1034	0.001348	46	0	0.42527	21.00188	20.71291	0.64246	0	0.91989
18	1140.8	297.931	0.00137	46	0	0.29868	17.1736	21.15055	0	0	0.93407
13	1187.355	289.6552	0.001451	46	0	0.18847	13.47768	27.70429	0	0	0.80979
17	1208.6	293.1034	0.001536	46	0	0	11.45101	29.77732	0	0	0.72516
14	1247.964	296.5517	0.0015	46	0	0	7.63089	35.92051	0	0	0.47762
15	1279.805	293.1034	0.001531	46	0	0	3.87862	35.67026	0	0	0
16	1322.641	293.1034	0.001529	46	0	0	1.52591	38.65671	0	0	0
20	1369.6	286.2069	0.001504	46	0	0	0.47643	38.24803	0	0	0

Table 4. Reaction conditions and post shock data of 1,5-hexadiyne pyroplysis at **500 bar.**

Shock No.	T_5 (K)	P_5 (bar)	Reaction time (sec.)	$[15HD]_0$ (ppm)	Post Shock Product Distributions (ppm)						
					15HD	34DMCB	Fulvene	Benzene	*cis*-13HD5Y	*trans*-13HD5Y	2E13BD
29	814.2419	641.3793	0.001196	55	46.83779	11.02532	0	0	0	0	0
19	850	648.2759	0.001196	55	42.71865	17.2561	0	0	0	0	0
28	852.0947	662.069	0.001192	55	39.50623	19.59058	0	0	0	0	0
27	865.9387	655.1724	0.001191	55	33.94908	22.91298	0	0	0	0	0
14	893.2	655.1724	0.001212	55	24.56388	31.29604	0	0	0	0	0
13	901.3	655.1724	0.001205	55	15.93515	34.32153	0	0	0	0	0
20	933.2	662.069	0.00121	55	6.10684	42.8483	1.33742	0	0	0	0
2	987.017	541.3793	0.001167	48	0.14608	32.54402	10.14243	1.00147	0.89551	0	0
21	998.5	620.6897	0.00121	55	1.42102	39.85178	9.24431	0	0	0	0
33	1008.379	620.6897	0.001216	55	1.37823	31.10014	11.85089	0	1.46581	0	0
11	1014.677	531.0345	0.001007	48	0.19091	29.69688	12.96479	1.14002	1.60319	1.07377	0
14	1040.588	513.7931	0.001112	48	0.16967	22.41563	18.30911	1.94379	2.06413	1.7685	0.18033
13	1072.256	500	0.001111	48	0	9.75493	22.60785	4.21439	2.12156	2.07334	0.45103
5	1098.859	510.3448	0.001282	48	0	1.98276	24.70073	12.552	1.13594	0	0.72112
9	1117.631	496.5517	0.001156	48	0	0.97712	23.52906	14.94425	0.89398	0.45435	0.94272
6	1133.117	503.4483	0.001164	48	0	0.42346	20.19642	18.25248	0.36969	0	0.86553

15	1143.499	475.8621	0.001229	48	0	0.63239	20.10636	20.85357	0.29348	0	0.87571
8	1181.269	482.7586	0.001186	48	0	0.21595	15.58049	26.19294	0	0	0.9078
22	1232.439	475.8621	0.001264	48	0	0	10.23303	29.62659	0	0	0.68016
18	1260.572	482.7586	0.001282	48	0	0.1282	6.18075	33.21093	0	0	0.35936
23	1285	472.4138	0.00136	48	0	0	4.61484	33.67163	0	0	0.25864
25	1302.5	468.9655	0.00138	48	0	0	3.52857	34.90592	0	0	0
19	1345.187	468.9655	0.001399	48	0	0	0.32039	37.90906	0	0	0