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Electronic supplementary information

Enthalpy formation of fluorene: Is a challenging problem for theory or experiment?

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Table S1 Cartesian coordinates of the compounds studied[a]

Molecule	Coordinates (Å)			Molecule	Coordinates (Å)		
	x	y	z		x	y	z
Reference species							
HNO_2	**O=N-OH**			**H_2**	**H_2**		
	H 1.761014	-0.180405	0.000000		H 0.000000	0.000000	0.371468
	O 0.889711	-0.601107	0.000000		H 0.000000	0.000000	-0.371468
	N 0.000000	0.517994	0.000000				
	O -1.109838	0.170412	0.000000				
H_2O	**H_2O**			**H_2S**	**H_2S**		
	O 0.000000	0.000000	0.117109		S 0.000000	0.000000	0.084007
	H 0.000000	0.761712	-0.468435		H 0.000000	-1.069800	-0.672054
	H 0.000000	-0.761712	-0.468435		H 0.000000	1.069800	-0.672054
H_3N	**NH_3**			**CH_2O**	**$H_2C=O$**		
	N 0.000000	0.000000	0.112912		C 0.000000	0.000000	-0.526109
	H 0.000000	0.940500	-0.263462		O 0.000000	0.000000	0.672793
	H -0.814497	-0.470250	-0.263462		H 0.000000	0.938077	-1.112847
	H 0.814497	-0.470250	-0.263462		H 0.000000	-0.938077	-1.112847
CH_2O_2	**HC(O)OH**			**CH_3NO_2**	**CH_3NO_2**		
	C -0.136367	0.397798	0.000010		C -0.000327	-1.323031	0.000000
	O -1.133269	-0.264132	-0.000003		N 0.009778	0.174277	0.000000
	O 1.116449	-0.088861	-0.000006		O -0.000327	0.729415	1.083589
	H -0.105397	1.493769	0.000044		O -0.000327	0.729415	-1.083589
	H 1.058160	-1.056616	-0.000032		H -1.044918	-1.625956	0.000000
					H 0.491831	-1.663214	-0.903597
					H 0.491831	-1.663214	0.903597
CH_4	**CH_4**			**CH_4O**	**CH_3OH**		
	C 0.000000	0.000000	0.000000		C -0.046455	0.664052	0.000000
	H 0.628376	0.628376	0.628376		O -0.046455	-0.756575	0.000000
	H -0.628376	-0.628376	0.628376		H 0.862206	-1.065981	0.000000
	H -0.628376	0.628376	-0.628376		H -1.088142	0.979286	0.000000
	H 0.628376	-0.628376	-0.628376		H 0.438153	1.077494	0.890390
					H 0.438153	1.077494	-0.890390
CH_4S	**CH_3SH**			**CH_5N**	**CH_3NH_2**		
	C -0.047863	1.156321	0.000000		N -0.049361	-0.757400	0.000000
	S -0.047863	-0.666733	0.000000		C -0.049361	0.705277	0.000000
	H 1.283492	-0.832957	0.000000		H 0.944040	1.172626	0.000000
	H -1.092695	1.459073	0.000000		H -0.587921	1.064444	0.877519
	H 0.431099	1.551842	0.892158		H -0.587921	1.064444	-0.877519
	H 0.431099	1.551842	-0.892158		H 0.436749	-1.115687	-0.812092
					H 0.436749	-1.115687	0.812092
C_2H_2	**CH≡CH**			**C_2H_4**	**$CH_2=CH_2$**		
	C 0.000000	0.000000	0.598321		C 0.000000	0.000000	0.662323
	C 0.000000	0.000000	-0.598321		C 0.000000	0.000000	-0.662323
	H 0.000000	0.000000	-1.660302		H 0.000000	0.920921	1.231436
	H 0.000000	0.000000	1.660302		H 0.000000	-0.920921	1.231436
					H 0.000000	0.920921	-1.231436
					H 0.000000	-0.920921	-1.231436
C_2H_4O	**$CH_3C(O)H$**			**$C_2H_4O_2$**	**$CH_3C(O)OH$**		
	C 0.000000	0.459770	0.000000		C 1.065949	-0.901513	0.000000
	O 1.200901	0.385861	0.000000		C 0.000000	0.155597	0.000000
	C -0.929177	-0.718162	0.000000		O 0.181726	1.344259	0.000000
	H -0.372168	-1.652087	0.000000		O -1.241571	-0.389499	0.000000
	H -0.498741	1.451840	0.000000		H -1.871739	0.344862	0.000000
	H -1.580616	-0.668145	0.876478		H 2.044017	-0.431945	0.000000
	H -1.580616	-0.668145	-0.876478		H 0.955394	-1.537751	0.878108
					H 0.955394	-1.537751	-0.878108
C_2H_6	**CH_3CH_3**			**C_2H_6O**	**CH_3OCH_3**		
	C 0.000000	0.000000	0.763144		O 0.000000	0.000000	0.588067
	C 0.000000	0.000000	-0.763144		C 0.000000	1.171680	-0.194838
	H 0.000000	1.016225	1.160196		C 0.000000	-1.171680	-0.194838
	H -0.880077	-0.508113	1.160196		H 0.000000	2.020283	0.486336

	H	0.880077	-0.508113	1.160196		H	-0.889848	1.226868	-0.834789
	H	0.000000	-1.016225	-1.160196		H	0.889848	1.226868	-0.834789
	H	-0.880077	0.508113	-1.160196		H	0.000000	-2.020283	0.486336
	H	0.880077	0.508113	-1.160196		H	0.889848	-1.226868	-0.834789
						H	-0.889848	-1.226868	-0.834789
C_2H_6O	**CH_3CH_2OH**				**C_2H_6S**	**CH_3SCH_3**			
	O	-1.239580	-0.256437	-0.107447		S	0.000000	0.000000	0.660163
	C	-0.079177	0.556011	0.046867		C	0.000000	1.380330	-0.512308
	C	1.212392	-0.241331	-0.021550		C	0.000000	-1.380330	-0.512308
	H	-1.256934	-0.904437	0.602149		H	0.000000	2.298648	0.071640
	H	-0.127865	1.122230	0.984452		H	-0.890895	1.361412	-1.139550
	H	-0.123863	1.277166	-0.769350		H	0.890895	1.361412	-1.139550
	H	2.078524	0.419214	0.053097		H	0.000000	-2.298648	0.071640
	H	1.274993	-0.790033	-0.961477		H	0.890895	-1.361412	-1.139550
	H	1.272494	-0.960723	0.798802		H	-0.890895	-1.361412	-1.139550
C_2H_7N	**CH_3NHCH_3**				**C_3H_4**	**$H_2C=C=CH_2$**			
	N	0.026594	0.579887	0.000000		C	0.000000	0.000000	1.300144
	H	-0.768683	1.204465	0.000000		H	0.000000	0.925774	1.862483
	C	0.026594	-0.221532	1.212291		H	0.000000	-0.925774	1.862483
	C	0.026594	-0.221532	-1.212291		C	0.000000	0.000000	0.000000
	H	-0.797516	-0.951092	1.265224		C	0.000000	0.000000	-1.300144
	H	-0.033665	0.428244	2.085269		H	-0.925774	0.000000	-1.862483
	H	0.962880	-0.779799	1.277813		H	0.925774	0.000000	-1.862483
	H	-0.797516	-0.951092	-1.265224					
	H	-0.033665	0.428244	-2.085269					
	H	0.962880	-0.779799	-1.277813					
C_3H_4	**$CH{\equiv}CCH_3$**				**C_3H_6**	**$CH_2{=}CHCH_3$**			
	C	0.000000	0.000000	-1.235942		C	1.286807	0.149663	0.000000
	H	0.000000	1.019046	-1.625856		C	0.000000	0.472771	0.000000
	H	-0.882520	-0.509523	-1.625856		H	1.610325	-0.884641	0.000000
	H	0.882520	-0.509523	-1.625856		H	2.061607	0.904383	0.000000
	C	0.000000	0.000000	0.218159		H	-0.275596	1.523543	0.000000
	C	0.000000	0.000000	1.417585		C	-1.133414	-0.503232	0.000000
	H	0.000000	0.000000	2.478754		H	-0.773802	-1.532279	0.000000
						H	-1.771446	-0.363109	0.876431
						H	-1.771446	-0.363109	-0.876431
C_3H_6O	**$CH_3C(O)CH_3$**				**C_3H_8**	**$CH_3CH_2CH_3$**			
	O	0.000000	0.000000	1.394504		C	0.000000	0.000000	0.586254
	C	0.000000	0.000000	0.185703		C	0.000000	1.270906	-0.259369
	C	0.000000	1.285544	-0.611684		C	0.000000	-1.270906	-0.259369
	C	0.000000	-1.285544	-0.611684		H	0.873639	0.000000	1.243452
	H	0.000000	2.140893	0.058339		H	-0.873639	0.000000	1.243452
	H	0.000000	-2.140893	0.058339		H	0.000000	2.167516	0.361993
	H	-0.876840	1.325270	-1.261681		H	-0.880627	1.312177	-0.903996
	H	0.876840	1.325270	-1.261681		H	0.880627	1.312177	-0.903996
	H	0.876840	-1.325270	-1.261681		H	0.000000	-2.167516	0.361993
	H	-0.876840	-1.325270	-1.261681		H	0.880627	-1.312177	-0.903996
						H	-0.880627	-1.312177	-0.903996
C_3H_8O	**$CH_3CH_2CH_2OH$**				**C_4H_4O**	**Furan**			
	C	1.547699	-0.504695	0.119931		O	0.000000	0.000000	1.156375
	H	1.117110	-1.471128	-0.140045		C	0.000000	1.094029	0.346084
	H	1.704850	-0.493269	1.200414		C	0.000000	-1.094029	0.346084
	H	2.523339	-0.425352	-0.360474		C	0.000000	0.716277	-0.955447
	C	0.624905	0.633383	-0.305570		C	0.000000	-0.716277	-0.955447
	H	1.058500	1.597419	-0.023262		H	0.000000	2.047640	0.841341
	H	0.530614	0.651712	-1.396978		H	0.000000	-2.047640	0.841341
	C	-0.766723	0.541846	0.307440		H	0.000000	1.369223	-1.810666
	H	-1.354545	1.427808	0.041526		H	0.000000	-1.369223	-1.810666
	H	-0.695333	0.510823	1.395963					
	O	-1.464779	-0.647280	-0.055173					
	H	-1.601596	-0.642970	-1.006566					
C_4H_4S	**Thiophene**				**C_4H_5N**	**Pyrrole**			
	S	0.000000	0.000000	1.188846		N	0.000000	0.000000	1.118334
	C	0.000000	1.234863	-0.005799		C	0.000000	1.122216	0.330850
	C	0.000000	-1.234863	-0.005799		C	0.000000	-1.122216	0.330850

	C 0.000000 0.711138 -1.266559		C 0.000000 0.710842 -0.980067
	C 0.000000 -0.711138 -1.266559		C 0.000000 -0.710842 -0.980067
	H 0.000000 2.271593 0.284694		H 0.000000 2.107352 0.762214
	H 0.000000 -2.271593 0.284694		H 0.000000 -2.107352 0.762214
	H 0.000000 1.315284 -2.161313		H 0.000000 1.355964 -1.841722
	H 0.000000 -1.315284 -2.161313		H 0.000000 -1.355964 -1.841722
			H 0.000000 0.000000 2.121283
C_4H_6	**H_2C=CHCH=CH_2**	C_4H_8	**CH_3CH=CHCH_3**
	C -0.325120 0.648964 0.000000		C 0.323649 0.579962 0.000000
	C 0.325120 -0.648964 0.000000		H 1.410985 0.568123 0.000000
	C -0.325120 -1.813733 0.000000		C -0.323649 -0.579962 0.000000
	C 0.325120 1.813733 0.000000		C -0.323649 1.928966 0.000000
	H -1.410924 0.643571 0.000000		H -1.410984 1.848261 0.000000
	H 1.410924 -0.643571 0.000000		H -0.026460 2.510884 0.876585
	H -1.407500 -1.854089 0.000000		H -0.026460 2.510884 -0.876585
	H 0.200974 -2.757838 0.000000		H -1.410985 -0.568123 0.000000
	H 1.407500 1.854089 0.000000		C 0.323649 -1.928966 0.000000
	H -0.200974 2.757838 0.000000		H 1.410984 -1.848261 0.000000
			H 0.026460 -2.510884 0.876585
			H 0.026460 -2.510884 -0.876585
C_5H_6	**1,3-Cyclopentadiene**	C_5H_6O	**2-Methylfuran**
	C 0.000000 1.176409 0.280811		O 1.034610 -0.245462 0.000000
	C 0.000000 0.732510 -0.987533		C 0.493460 -1.497971 0.000000
	C 0.000000 -0.732510 -0.987533		C 0.000000 0.648101 0.000000
	C 0.000000 -1.176409 0.280811		C -0.857890 -1.422706 0.000000
	H 0.874921 0.000000 1.872727		C -1.179126 -0.025859 0.000000
	H 0.000000 2.204945 0.606388		H 1.192421 -2.314052 0.000000
	H 0.000000 1.344843 -1.877293		H -1.544323 -2.251480 0.000000
	H 0.000000 -1.344843 -1.877293		H -2.160099 0.416974 0.000000
	H 0.000000 -2.204945 0.606388		C 0.358051 2.085863 0.000000
	C 0.000000 0.000000 1.212836		H 0.947352 2.348419 0.881035
	H -0.874921 0.000000 1.872727		H 0.947352 2.348419 -0.881035
			H -0.546554 2.690853 0.000000
C_5H_7N	**N-Methylpyrrole**	C_5H_8	**Cyclopentene**
	C 0.017211 -0.172888 1.116667		C 0.259901 -1.203519 0.000000
	C 0.017211 -1.486746 0.709800		C -0.066913 -0.325810 1.231638
	C 0.017211 -1.486746 -0.709800		C -0.066913 1.070934 0.664441
	C 0.017211 -0.172888 -1.116667		C -0.066913 1.070934 -0.664441
	N 0.023690 0.622901 0.000000		C -0.066913 -0.325810 -1.231638
	H 0.017356 0.261012 2.101445		H -0.282703 -2.147562 0.000000
	H 0.028426 -2.346978 1.356880		H 0.655377 -0.456779 2.039681
	H 0.028426 -2.346978 -1.356880		H -1.048940 -0.565826 1.653734
	H 0.017356 0.261012 -2.101445		H -0.104012 1.956445 1.284602
	C -0.069368 2.066130 0.000000		H -0.104012 1.956445 -1.284602
	H 0.427211 2.464554 -0.882795		H 0.655377 -0.456779 -2.039681
	H -1.108678 2.401348 0.000000		H -1.048940 -0.565826 -1.653734
	H 0.427211 2.464554 0.882795		H 1.324346 -1.440483 0.000000
$C_6H_5NO_2$	**Nitrobenzene**	C_6H_6	**Benzene**
	C 0.000000 0.000000 0.241467		C 0.000000 1.390514 0.000000
	C 0.000000 0.000000 -2.507740		C 1.204221 0.695257 0.000000
	C 0.000000 1.214691 -0.428152		C 1.204221 -0.695257 0.000000
	C 0.000000 -1.214691 -0.428152		C 0.000000 -1.390514 0.000000
	C 0.000000 -1.206749 -1.815508		C -1.204221 -0.695257 0.000000
	C 0.000000 1.206749 -1.815508		C -1.204221 0.695257 0.000000
	N 0.000000 0.000000 1.716616		H 0.000000 2.472345 0.000000
	O 0.000000 1.081433 2.283336		H 2.141114 1.236173 0.000000
	O 0.000000 -1.081433 2.283336		H 2.141114 -1.236173 0.000000
	H 0.000000 0.000000 -3.589125		H 0.000000 -2.472345 0.000000
	H 0.000000 2.133714 0.136119		H -2.141114 -1.236173 0.000000
	H 0.000000 -2.133714 0.136119		H -2.141114 1.236173 0.000000
	H 0.000000 -2.142999 -2.355620		
	H 0.000000 2.142999 -2.355620		
C_6H_7N	**Aniline**	C_7H_6O	**Benzaldehyde**
	C -0.002913 0.934363 0.000000		C 0.000000 0.570147 0.000000
	C -0.003293 0.220086 1.202828		C -1.041204 -0.361676 0.000000

	C	-0.003293	-1.166938	1.197484	C	-0.753865	-1.715791	0.000000
	C	-0.003354	-1.873754	0.000000	C	0.571841	-2.147937	0.000000
	C	-0.003293	-1.166938	-1.197484	C	1.611433	-1.225278	0.000000
	C	-0.003293	0.220086	-1.202828	C	1.324044	0.132989	0.000000
	N	-0.060345	2.326626	0.000000	C	-0.285036	2.018723	0.000000
	H	-0.008144	0.759135	2.142225	O	-1.389863	2.507484	0.000000
	H	-0.002228	-1.699063	2.139693	H	0.617221	2.663598	0.000000
	H	-0.002683	-2.954511	0.000000	H	-2.060329	-0.000939	0.000000
	H	-0.002228	-1.699063	-2.139693	H	-1.556789	-2.440284	0.000000
	H	-0.008144	0.759135	-2.142225	H	0.792244	-3.207006	0.000000
	H	0.281237	2.773275	-0.835112	H	2.638180	-1.564335	0.000000
	H	0.281237	2.773275	0.835112	H	2.125096	0.862028	0.000000
$C_7H_6O_2$	**Benzoic acid**				C_7H_8	**Toluene**		
	C	0.000000	0.220372	0.000000	C	2.414421	0.000000	0.009211
	C	-1.123369	-0.607641	0.000000	C	0.909826	-0.000002	-0.011484
	C	-0.965598	-1.986360	0.000000	C	0.193931	1.197104	-0.008921
	C	0.309039	-2.542066	0.000000	C	-1.195498	1.200079	0.002001
	C	1.430465	-1.718135	0.000000	C	-1.896359	0.000001	0.008609
	C	1.277702	-0.340654	0.000000	C	-1.195501	-1.200077	0.002000
	C	-0.111571	1.699184	0.000000	C	0.193931	-1.197104	-0.008921
	O	0.822078	2.463680	0.000000	H	2.790787	0.000050	1.035326
	O	-1.394951	2.135939	0.000000	H	2.818481	-0.882946	-0.485755
	H	-1.836298	-2.627599	0.000000	H	2.818480	0.882896	-0.485844
	H	-1.354991	3.101918	0.000000	H	0.731657	2.137116	-0.018061
	H	-2.109769	-0.169419	0.000000	H	-1.730829	2.140356	0.001626
	H	0.428929	-3.617150	0.000000	H	-2.977899	0.000003	0.014179
	H	2.421291	-2.151147	0.000000	H	-1.730832	-2.140354	0.001625
	H	2.133819	0.318253	0.000000	H	0.731651	-2.137120	-0.018060
C_9H_8	**Indene**				C_9H_{10}	**Indane**		
	C	0.000000	0.724111	0.000000	C	1.560644	-1.225379	0.128920
	C	-0.427384	-0.616503	0.000000	C	1.560643	1.225379	0.128921
	C	0.499592	-1.652421	0.000000	C	2.413689	0.000000	-0.266640
	C	1.855285	-1.336071	0.000000	H	2.559907	0.000000	-1.348097
	C	2.276843	-0.008631	0.000000	H	3.398244	0.000000	0.198586
	C	1.347380	1.032382	0.000000	H	1.732126	-2.087247	-0.516442
	C	-1.213016	1.617679	0.000000	H	1.732126	2.087247	-0.516441
	C	-2.352611	0.631786	0.000000	H	1.786973	-1.543549	1.151832
	C	-1.889362	-0.627713	0.000000	H	1.786972	1.543549	1.151832
	H	0.176734	-2.685357	0.000000	C	0.148808	-0.698103	0.052097
	H	2.590852	-2.129350	0.000000	C	0.148808	0.698103	0.052097
	H	3.334699	0.216936	0.000000	C	-1.046513	1.400405	0.004628
	H	1.682950	2.061800	0.000000	C	-2.246941	0.695908	-0.047123
	H	-1.241645	2.273452	0.875930	C	-2.246941	-0.695908	-0.047122
	H	-2.491180	-1.524959	0.000000	C	-1.046513	-1.400405	0.004628
	H	-3.391121	0.926312	0.000000	H	-1.050344	2.483176	0.001220
	H	-1.241645	2.273452	-0.875930	H	-3.184885	1.233076	-0.093076
					H	-3.184885	-1.233076	-0.093076
					H	-1.050344	-2.483176	0.001220
$C_{10}H_8$	**Naphthalene**				$C_{12}H_8$	**Acenaphthylene**		
	C	0.000000	2.422564	0.705670	C	0.000000	2.381355	-0.319758
	C	0.000000	1.239487	1.396714	C	0.000000	1.158171	-0.947609
	C	0.000000	0.000000	0.713624	C	0.000000	0.000000	-0.139586
	C	0.000000	0.000000	-0.713624	C	0.000000	0.000000	1.250818
	C	0.000000	1.239487	-1.396714	C	0.000000	1.277636	1.873311
	C	0.000000	2.422564	-0.705670	C	0.000000	2.419403	1.100451
	C	0.000000	-1.239487	1.396714	H	0.000000	3.309722	-0.876311
	C	0.000000	-1.239487	-1.396714	C	0.000000	-1.158171	-0.947609
	C	0.000000	-2.422564	-0.705670	C	0.000000	-1.277636	1.873311
	C	0.000000	-2.422564	0.705670	H	0.000000	1.354263	2.952918
	H	0.000000	3.363043	1.239977	H	0.000000	3.384399	1.589506
	H	0.000000	1.237020	2.479314	C	0.000000	-2.419403	1.100451
	H	0.000000	1.237020	-2.479314	C	0.000000	-2.381355	-0.319758
	H	0.000000	3.363043	-1.239977	H	0.000000	-1.354263	2.952918
	H	0.000000	-1.237020	-2.479314	H	0.000000	-3.384399	1.589506
	H	0.000000	-3.363043	-1.239977	H	0.000000	-3.309722	-0.876311

	H	0.000000	-3.363043	1.239977		C	0.000000	0.679783	-2.337784
	H	0.000000	-1.237020	2.479314		C	0.000000	-0.679783	-2.337784
						H	0.000000	-1.312947	-3.211478
						H	0.000000	1.312947	-3.211478
$C_{12}H_{10}$	**Acenaphthene**				$C_{14}H_{10}$	**Anthracene**			
	C	0.000000	2.416978	1.181511		C	0.000000	3.643783	0.710490
	C	0.000000	1.270476	1.944179		C	0.000000	2.468515	1.401188
	C	0.000000	0.000000	1.317147		C	0.000000	1.217811	0.719515
	C	0.000000	0.000000	-0.091088		C	0.000000	1.217811	-0.719515
	C	0.000000	1.170797	-0.870414		C	0.000000	2.468515	-1.401188
	C	0.000000	2.386434	-0.236470		C	0.000000	3.643783	-0.710490
	H	0.000000	-1.336455	3.024501		C	0.000000	0.000000	1.398174
	H	0.000000	3.378619	1.677998		C	0.000000	0.000000	-1.398174
	H	0.000000	1.336455	3.024501		C	0.000000	-1.217811	-0.719515
	C	0.000000	-1.270476	1.944179		C	0.000000	-1.217811	0.719515
	C	0.000000	-1.170797	-0.870414		C	0.000000	-2.468515	1.401188
	H	0.000000	3.316090	-0.790658		H	0.000000	-2.466660	2.483691
	C	0.000000	-2.386434	-0.236470		C	0.000000	-3.643783	0.710490
	C	0.000000	-2.416978	1.181511		C	0.000000	-3.643783	-0.710490
	H	0.000000	-3.316090	-0.790658		C	0.000000	-2.468515	-1.401188
	H	0.000000	-3.378619	1.677998		H	0.000000	0.000000	2.481507
	C	0.000000	0.782015	-2.333954		H	0.000000	4.586086	1.241499
	C	0.000000	-0.782015	-2.333954		H	0.000000	2.466660	2.483691
	H	-0.875030	1.180479	-2.849563		H	0.000000	2.466660	-2.483691
	H	-0.875030	-1.180479	-2.849563		H	0.000000	4.586086	-1.241499
	H	0.875030	1.180479	-2.849563		H	0.000000	0.000000	-2.481507
	H	0.875030	-1.180479	-2.849563		H	0.000000	-4.586086	1.241499
						H	0.000000	-4.586086	-1.241499
						H	0.000000	-2.466660	-2.483691
$C_{14}H_{10}$	**Phenanthrene**				$C_{18}H_{12}$	**Triphenylene**			
	C	0.000000	1.416553	0.862984		C	0.697861	3.684706	0.000000
	C	0.000000	0.725456	-0.377758		C	1.378647	2.488036	0.000000
	C	0.000000	-0.725456	-0.377758		C	0.707033	1.251274	0.000000
	C	0.000000	-1.416553	0.862984		C	-0.707033	1.251274	0.000000
	C	0.000000	-0.676577	2.086159		C	-1.378647	2.488036	0.000000
	C	0.000000	0.676577	2.086159		C	-0.697861	3.684706	0.000000
	H	0.000000	-1.226723	3.018368		C	1.437151	-0.013328	0.000000
	H	0.000000	1.226723	3.018368		C	-1.437151	-0.013328	0.000000
	C	0.000000	2.825223	0.874763		C	-0.730118	-1.237946	0.000000
	H	0.000000	3.334997	1.829774		C	0.730118	-1.237946	0.000000
	C	0.000000	1.491202	-1.559996		C	-1.465379	-2.437961	0.000000
	H	0.000000	0.998006	-2.520274		H	-0.949035	-3.384557	0.000000
	C	0.000000	2.867461	-1.523985		C	-2.842119	-2.446719	0.000000
	H	0.000000	3.428264	-2.448862		C	-3.539980	-1.237988	0.000000
	C	0.000000	3.544500	-0.296424		C	-2.844026	-0.050075	0.000000
	H	0.000000	4.625744	-0.273464		H	1.244993	4.617571	0.000000
	C	0.000000	-2.825223	0.874763		H	2.456595	2.514167	0.000000
	H	0.000000	-3.334997	1.829774		H	-2.456595	2.514167	0.000000
	C	0.000000	-1.491202	-1.559996		H	-1.244993	4.617571	0.000000
	H	0.000000	-0.998006	-2.520274		H	-3.376437	-3.386981	0.000000
	C	0.000000	-2.867461	-1.523985		H	-4.621430	-1.230589	0.000000
	H	0.000000	-3.428264	-2.448862		H	-3.405630	0.870390	0.000000
	C	0.000000	-3.544500	-0.296424		C	2.844026	-0.050075	0.000000
	H	0.000000	-4.625744	-0.273464		C	3.539980	-1.237988	0.000000
						C	2.842119	-2.446719	0.000000
						C	1.465379	-2.437961	0.000000
						H	3.405630	0.870390	0.000000
						H	4.621430	-1.230589	0.000000
						H	3.376437	-3.386981	0.000000
						H	0.949035	-3.384557	0.000000
Fluorene and its derivatives									
$C_{12}H_8O$	**Dibenzofuran**				$C_{12}H_8S$	**Dibenzothiophene**			
	C	0.000000	1.099777	0.821770		C	0.000000	-1.251982	0.730333
	O	0.000000	0.000000	1.647254		S	0.000000	0.000000	1.955800

	C	0.000000	-1.099777	0.821770		C	0.000000	1.251982	0.730333
	C	0.000000	0.724261	-0.530630		C	0.000000	-0.724214	-0.576576
	C	0.000000	-0.724261	-0.530630		C	0.000000	0.724214	-0.576576
	C	0.000000	2.415480	1.242384		C	0.000000	-2.624568	0.959031
	C	0.000000	3.389049	0.248766		C	0.000000	-3.478536	-0.132452
	C	0.000000	3.045224	-1.107254		C	0.000000	-2.972090	-1.436080
	C	0.000000	1.716294	-1.508810		C	0.000000	-1.606052	-1.660067
	C	0.000000	-2.415480	1.242384		C	0.000000	2.624568	0.959031
	C	0.000000	-3.389049	0.248766		C	0.000000	3.478536	-0.132452
	C	0.000000	-3.045224	-1.107254		C	0.000000	2.972090	-1.436080
	C	0.000000	-1.716294	-1.508810		C	0.000000	1.606052	-1.660067
	H	0.000000	2.669034	2.292430		H	0.000000	-3.017246	1.966382
	H	0.000000	4.432537	0.532111		H	0.000000	-4.548003	0.027804
	H	0.000000	3.829019	-1.851971		H	0.000000	-3.654318	-2.274891
	H	0.000000	1.457836	-2.558937		H	0.000000	-1.220655	-2.670828
	H	0.000000	-2.669034	2.29243		H	0.000000	3.017246	1.966382
	H	0.000000	-4.432537	0.532111		H	0.000000	4.548003	0.027804
	H	0.000000	-3.829019	-1.851971		H	0.000000	3.654318	-2.274891
	H	0.000000	-1.457836	-2.558937		H	0.000000	1.220655	-2.670828
$C_{12}H_9N$	**Carbazole**				$C_{13}H_8O$	**9-Fluorenone**			
	C	0.000000	0.723135	-0.502096		C	0.000000	3.015398	-1.391361
	C	0.000000	1.690871	-1.505118		C	0.000000	3.453693	-0.070404
	C	0.000000	3.031369	-1.150196		C	0.000000	2.532268	0.977791
	C	0.000000	3.415384	0.196604		C	0.000000	1.187336	0.666254
	C	0.000000	2.473705	1.215805		C	0.000000	0.739380	-0.664582
	C	0.000000	1.130963	0.854585		C	0.000000	1.653288	-1.703206
	C	0.000000	-0.723135	-0.502096		H	0.000000	3.742773	-2.192094
	C	0.000000	-1.690871	-1.505118		H	0.000000	4.513904	0.141737
	C	0.000000	-3.031369	-1.150196		H	0.000000	2.852403	2.010947
	C	0.000000	-3.415384	0.196604		H	0.000000	1.330903	-2.735714
	C	0.000000	-2.473705	1.215805		C	0.000000	0.000000	1.578527
	C	0.000000	-1.130963	0.854585		C	0.000000	-1.187336	0.666254
	H	0.000000	1.400001	-2.547166		C	0.000000	-2.532268	0.977791
	H	0.000000	3.791252	-1.919265		C	0.000000	-3.453693	-0.070404
	H	0.000000	4.467103	0.448864		C	0.000000	-3.015398	-1.391361
	H	0.000000	2.777155	2.254241		C	0.000000	-1.653288	-1.703206
	H	0.000000	-1.400001	-2.547166		C	0.000000	-0.739380	-0.664582
	H	0.000000	-3.791252	-1.919265		H	0.000000	-2.852403	2.010947
	H	0.000000	-4.467103	0.448864		H	0.000000	-4.513904	0.141737
	H	0.000000	-2.777155	2.254241		H	0.000000	-3.742773	-2.192094
	N	0.000000	0.000000	1.651104		H	0.000000	-1.330903	-2.735714
	H	0.000000	0.000000	2.65391		O	0.000000	0.000000	2.788147
$C_{13}H_9NO_2$	**2-Nitrofluorene**				$C_{13}H_{10}$	**Fluorene**			
	C	-2.801927	3.206571	0.000000		C	0.000000	3.003466	-1.207162
	C	-1.488201	2.755335	0.000000		C	0.000000	1.643752	-1.498364
	C	-1.252278	1.384183	0.000000		C	0.000000	0.732221	-0.448300
	C	-2.322412	0.472684	0.000000		C	0.000000	1.180610	0.883731
	C	-3.629332	0.928855	0.000000		C	0.000000	2.535122	1.167824
	C	-3.863360	2.302054	0.000000		C	0.000000	3.447159	0.113832
	H	-3.005282	4.268676	0.000000		H	0.000000	3.724951	-2.013131
	H	-0.667443	3.460029	0.000000		H	0.000000	1.305211	-2.526037
	H	-4.459490	0.234493	0.000000		H	0.000000	2.886569	2.191832
	H	-4.879619	2.671986	0.000000		H	0.000000	4.508523	0.322186
	C	0.000000	0.631855	0.000000		C	0.000000	-0.732221	-0.448300
	C	1.323069	1.065799	0.000000		C	0.000000	-1.643752	-1.498364
	C	2.341543	0.125360	0.000000		C	0.000000	-3.003466	-1.207162
	C	2.019626	-1.227984	0.000000		C	0.000000	-3.447159	0.113832
	C	0.704538	-1.685740	0.000000		C	0.000000	-2.535122	1.167824
	C	-0.302622	-0.743525	0.000000		C	0.000000	-1.180610	0.883731
	H	1.562414	2.120070	0.000000		H	0.000000	-1.305211	-2.526037
	H	3.379572	0.417485	0.000000		H	0.000000	-3.724951	-2.013131
	H	0.509136	-2.747040	0.000000		H	0.000000	-2.886569	2.191832
	C	-1.798628	-0.943084	0.000000		C	0.000000	0.000000	1.825749
	H	-2.133035	-1.503165	0.877026		H	0.877135	0.000000	2.478533
	H	-2.133035	-1.503165	-0.877026		H	-0.877135	0.000000	2.478533

	N	3.108371	-2.213711	0.000000		H	0.000000	-4.508523	0.322186
	O	2.803484	-3.398174	0.000000					
	O	4.257526	-1.796521	0.000000					
$C_{13}H_{10}O$	**9-Fluorenol**				$C_{13}H_{11}N$	**2-Aminofluorene**			
	H	2.017257	-1.326235	0.000000		C	3.461312	1.135791	0.004664
	C	-1.434464	0.096638	3.007321		C	2.111251	1.472279	0.002137
	C	-0.119112	-0.030939	3.447077		C	1.163483	0.454379	-0.000066
	C	0.922972	-0.175002	2.530737		C	1.570872	-0.892082	0.000103
	C	0.624535	-0.182651	1.181532		C	2.914133	-1.220678	0.002577
	C	-0.697661	-0.039431	0.734797		C	3.862700	-0.197904	0.004912
	C	-1.735679	0.093901	1.647690		H	4.208321	1.918415	0.006242
	H	-2.231121	0.203004	3.731339		H	1.808221	2.511127	0.001570
	H	0.094320	-0.020135	4.507299		H	3.230819	-2.256178	0.002535
	H	1.946170	-0.272981	2.868750		H	4.916485	-0.441544	0.006724
	H	-2.759734	0.199438	1.314922		C	-1.190127	1.565401	-0.003120
	C	1.566635	-0.330459	0.000000		C	-2.554301	1.315702	-0.004496
	C	0.624535	-0.182651	-1.181532		C	-3.050280	0.003860	-0.005022
	C	0.922972	-0.175002	-2.530737		C	-2.148460	-1.069503	-0.005650
	C	-0.119112	-0.030939	-3.447077		C	-0.791349	-0.816175	-0.004431
	C	-1.434464	0.096638	-3.007321		C	-0.297872	0.499273	-0.003099
	C	-1.735679	0.093901	-1.64769		H	-0.833237	2.587023	-0.000872
	C	-0.697661	-0.039431	-0.734797		H	-3.253684	2.142430	-0.009817
	H	1.946170	-0.272981	-2.86875		H	-2.524627	-2.085909	-0.011648
	H	0.094320	-0.020135	-4.507299		C	0.359210	-1.795825	-0.003032
	H	-2.231121	0.203004	-3.731339		H	0.335507	-2.449105	0.873352
	H	-2.759734	0.199438	-1.314922		H	0.338412	-2.446694	-0.881282
	O	2.677532	0.559977	0.000000		N	-4.422898	-0.228776	-0.064358
	H	2.336317	1.460326	0.000000		H	-4.725420	-1.126074	0.277584
						H	-5.003950	0.520830	0.273263
$C_{14}H_{10}O$	**2-Fluorenecarboxaldehyde**				$C_{14}H_{10}O_2$	**9-Fluorenecarboxylic acid**			
	H	0.681928	-2.363132	0.876872		C	-3.225760	-1.514597	0.138537
	C	3.741383	1.278991	0.000000		C	-3.520109	-0.194682	-0.197392
	C	4.163545	-0.050018	0.000000		C	-2.497658	0.716982	-0.451403
	C	3.237531	-1.090795	0.000000		C	-1.186698	0.287250	-0.366060
	C	1.887056	-0.786497	0.000000		C	-0.886377	-1.038691	-0.021558
	C	1.460911	0.553156	0.000000		C	-1.907559	-1.947322	0.230422
	C	2.387649	1.591062	0.000000		H	-4.032409	-2.208331	0.333582
	H	4.475900	2.072798	0.000000		H	-4.551260	0.125588	-0.257059
	H	5.221623	-0.274156	0.000000		H	-2.730894	1.744047	-0.697997
	H	3.574099	-2.119501	0.000000		H	-1.685174	-2.972017	0.496451
	H	2.064301	2.623460	0.000000		C	0.087025	1.063475	-0.605379
	C	0.693581	-1.710643	0.000000		H	0.158059	1.403380	-1.642278
	H	0.681928	-2.363132	-0.876872		C	1.168604	0.024313	-0.328657
	C	-0.472637	-0.751415	0.000000		C	2.544309	0.152862	-0.378276
	C	-1.823959	-1.013519	0.000000		C	3.330697	-0.961927	-0.089769
	C	-2.723777	0.061489	0.000000		C	2.741057	-2.179658	0.240500
	C	-2.251372	1.377323	0.000000		C	1.356900	-2.308673	0.289897
	C	-0.890403	1.647057	0.000000		C	0.568569	-1.200096	0.005680
	C	0.000000	0.578289	0.000000		H	3.002126	1.098801	-0.631829
	H	-2.217112	-2.021425	0.000000		H	4.408477	-0.879628	-0.123011
	H	-2.965788	2.191321	0.000000		H	3.366861	-3.033779	0.461402
	H	-0.533136	2.667839	0.000000		H	0.904767	-3.257231	0.546870
	C	-4.175622	-0.180938	0.000000		C	0.249009	2.286823	0.277281
	O	-4.699090	-1.271848	0.000000		O	-0.383799	2.548429	1.262024
	H	-4.794339	0.739463	0.000000		O	1.245881	3.082073	-0.185236
						H	1.330741	3.818788	0.436632
$C_{14}H_{12}O$	**9-Fluorenemethanol**				$C_{16}H_{10}$	**Fluoranthene**			
	C	-3.306641	-1.240369	0.160262		C	0.000000	2.388011	0.738036
	C	-3.550647	0.106980	-0.095260		C	0.000000	1.168438	0.105529
	C	-2.492434	0.990434	-0.305147		C	0.000000	0.000000	0.901881
	C	-1.195671	0.509247	-0.256027		C	0.000000	0.000000	2.298720
	C	-0.949221	-0.849338	0.001833		C	0.000000	1.274422	2.923443
	C	-2.005131	-1.729021	0.210008		C	0.000000	2.419844	2.156258
	H	-4.138590	-1.912900	0.320467		H	0.000000	3.317828	0.184608
	H	-4.568790	0.469922	-0.132310		C	0.000000	-1.168438	0.105529

	H	-2.691799	2.035084	-0.507577		C	0.000000	-1.274422	2.923443
	H	-1.822441	-2.776994	0.407361		H	0.000000	1.345820	4.003353
	C	0.111430	1.254451	-0.433781		H	0.000000	3.382362	2.650248
	H	0.166707	1.686896	-1.439886		C	0.000000	-2.419844	2.156258
	C	1.138474	0.152470	-0.271728		C	0.000000	-2.388011	0.738036
	C	2.520306	0.221457	-0.330543		H	0.000000	-1.345820	4.003353
	C	3.261856	-0.941703	-0.128527		H	0.000000	-3.382362	2.650248
	C	2.627215	-2.155231	0.127280		H	0.000000	-3.317828	0.184608
	C	1.239923	-2.229288	0.189668		C	0.000000	1.409452	-2.490816
	C	0.498065	-1.070931	-0.009543		C	0.000000	0.696047	-3.689377
	H	3.015624	1.163697	-0.514749		C	0.000000	-0.696047	-3.689377
	H	4.341997	-0.901334	-0.169504		C	0.000000	-1.409452	-2.490816
	H	3.219743	-3.047330	0.279878		C	0.000000	-0.711838	-1.294623
	H	0.750855	-3.173451	0.389972		C	0.000000	0.711838	-1.294623
	C	0.267792	2.400043	0.577013		H	0.000000	2.491502	-2.500877
	H	-0.615354	3.045191	0.535993		H	0.000000	1.230206	-4.629844
	H	0.333085	1.988420	1.583412		H	0.000000	-1.230206	-4.629844
	O	1.454884	3.157351	0.384028		H	0.000000	-2.491502	-2.500877
	H	1.377992	3.648784	-0.438323					

[a] Calculated at B3LYP-D3(BJ)/def2-TZVPP level.

Table S2 Enthalpies of formation of reference species used in working reactions and DLPNO-CCSD(T_1)/CBS energies, ZPE and thermal corrections for the compounds studied

Formula	Structural formula or name	Enthalpy of formation		E_e [a]	ZPE correction [b]	Enthalpy correction [b]
		$\Delta_f H^\circ_m$	Reference			$H^\circ_{298} - H^\circ_0$
		kJ mol^{-1}		Hartree	Hartree	Hartree
Reference species						
HNO_2	O=N-OH	-79.149 ± 0.079	1	-205.536585	0.019777	0.004200
H_2	H_2	0	1	-1.174676	0.009837	0.003305
H_2O	H_2O	-241.836 ± 0.027	1	-76.376454	0.020845	0.003780
H_2S	H_2S	-20.6 ± 0.5	2	-398.968127	0.014712	0.003794
H_3N	NH_3	-45.557 ± 0.03	1	-56.505222	0.033487	0.003818
CH_2O	$H_2C=O$	-109.218 ± 0.098	1	-114.390496	0.025954	0.003816
CH_2O_2	HC(O)OH	-378.42 ± 0.220	1	-189.598202	0.032975	0.004134
CH_3NO_2	CH_3NO_2	-71.5 ± 0.4	3	-244.786584	0.048587	0.005375
CH_4	CH_4	-74.526 ± 0.055	1	-40.459037	0.043619	0.003818
CH_4O	CH_3OH	-200.89 ± 0.15	1	-115.612461	0.049974	0.004324
CH_4S	CH_3SH	-22.9 ± 0.6	4	-438.221297	0.044869	0.004588
CH_5N	CH_3NH_2	-21.73 ± 0.310	1	-95.747147	0.062428	0.004411
C_2H_2	CH≡CH	228.26 ± 0.13	1	-77.222784	0.026441	0.003766
C_2H_4	$CH_2=CH_2$	52.36 ± 0.12	1	-78.476121	0.049738	0.004002
C_2H_4O	$CH_3C(O)H$	-165.64 ± 0.26	1	-153.662285	0.054073	0.004864
$C_2H_4O_2$	$CH_3C(O)OH$	-433.00 ± 0.43	1	-228.868214	0.060261	0.005555
C_2H_6	CH_3CH_3	-83.97 ± 0.13	1	-79.714152	0.072814	0.004460
C_2H_6O	CH_3OCH_3	-183.89 ± 0.41	1	-154.856005	0.077701	0.005316
C_2H_6O	CH_3CH_2OH	-235.02 ± 0.22	1	-154.875565	0.078005	0.005292
C_2H_6S	CH_3SCH_3	-37.4 ± 0.6	4	-477.481334	0.073005	0.005670
C_2H_7N	CH_3NHCH_3	-18.10 ± 0.48	1	-134.995366	0.090089	0.005410
C_3H_4	$H_2C=C=CH_2$	189.86 ± 0.25	1	-116.487455	0.053791	0.004774
C_3H_4	$CH≡CCH_3$	185.73 ± 0.24	1	-116.489712	0.054354	0.004917
C_3H_6	$CH_2=CHCH_3$	19.93 ± 0.21	1	-117.738879	0.077747	0.005072
C_3H_6O	$CH_3C(O)CH_3$	-216.90 ± 0.38	1	-192.931964	0.081487	0.006414
C_3H_8	$CH_3CH_2CH_3$	-105.03 ± 0.18	1	-118.972715	0.116825	0.008461
C_3H_8O	$CH_3CH_2CH_2OH$	-255.27 ± 0.25	1	-194.133975	0.106004	0.006492

C_4H_4O	furan	-34.7 ± 0.6	5	-229.744436	0.068410	0.004704
C_4H_4S	Thiophene	115.0 ± 1.0	4	-552.365948	0.065208	0.005059
C_4H_5N	Pyrrole	108.2 ± 0.8	6	-209.893602	0.080684	0.004968
C_4H_6	H_2C=CHCH=CH_2	110.83 ± 0.37	1	-155.768732	0.083186	0.005647
C_4H_8	CH_3CH=$CHCH_3$	-11.18 ± 0.41	1	-157.000950	0.105246	0.006493
C_5H_6	1,3-Cyclopentadiene	133.71 ± 0.66	1	-193.826357	0.090385	0.005158
C_5H_6O	2-Methylfuran	-76.4 ± 1.2	7	-269.010585	0.095380	0.006349
C_5H_7N	*N*-Methylpyrrole	103.1 ± 0.5	6	-249.145417	0.107722	0.006603
C_5H_8	Cyclopentene	35.1 ± 0.5	1	-195.050821	0.113984	0.005662
$C_6H_5NO_2$	Nitrobenzene	-71.5 ± 0.4	3	-436.247135	0.100906	0.007854
C_6H_6	Benzene	83.10 ± 0.23	1	-231.913115	0.098272	0.005409
C_6H_7N	Aniline	87.5 ± 0.8	8	-287.217745	0.114441	0.006850
C_7H_6O	Benzaldehyde	-37.19 ± 0.92	1	-345.126422	0.107399	0.007356
$C_7H_6O_2$	Benzoic acid	-294.5 ± 0.9	9	-420.329527	0.113113	0.008178
C_7H_8	Toluene	50.01 ± 0.34	1	-271.175029	0.124900	0.007281
C_9H_8	Indene	160.7 ± 1.3	10	-347.263978	0.137320	0.007458
C_9H_{10}	Indane	60.9 ± 2.1	11	-348.488859	0.160692	0.007937
$C_{10}H_8$	Naphthalene	150.6 ± 1.5	11	-385.334958	0.144207	0.007892
$C_{12}H_8$	Acenaphthylene	263.2 ± 3.7	11	-461.422195	0.155850	0.008765
$C_{12}H_{10}$	Acenaphthene	156.80 ± 3.10	11	-462.648466	0.178390	0.009442
$C_{14}H_{10}$	Anthracene	229.4 ± 2.9	11	-538.750789	0.189829	0.010578
$C_{18}H_{12}$	Triphenylene	270.1 ± 4.4	11	-692.184327	0.236171	0.013487
Fluorene and its derivatives						
$C_{12}H_8O$	Dibenzofuran			-536.604590	0.160690	0.009632
$C_{12}H_8S$	Dibenzothiophene			-859.223835	0.157856	0.010229
$C_{12}H_9N$	Carbazole			-516.749508	0.172602	0.010086
$C_{13}H_8O$	9-Fluorenone			-574.657976	0.166053	0.010664
$C_{13}H_9NO_2$	2-Nitrofluorene			-705.036606	0.186315	0.012658
$C_{13}H_{10}$	Fluorene			-500.701414	0.183805	0.010048
$C_{13}H_{10}O$	9-Fluorenol			-575.863644	0.188429	0.011337
$C_{13}H_{11}N$	2-Aminofluorene			-556.005632	0.199902	0.011599
$C_{14}H_{10}O$	2-Fluorenecarboxaldehyde			-613.916100	0.192887	0.012106
$C_{14}H_{10}O_2$	9-Fluorenecarboxylic acid			-689.111704	0.198505	0.013018
$C_{14}H_{12}O$	9-Fluorenemethanol			-615.123687	0.216398	0.012703
$C_{16}H_{10}$	Fluoranthene			-614.861091	0.202052	0.011462

[a] DLPNO-CCSD(T_1)/CBS//B3LYP-D3(BJ)/def2-TZVPP single point energy. [b] Calculated at B3LYP-D3(BJ)/def2-TZVPP level; ZPE and $(H^{\circ}_{298} - H^{\circ}_{0})$ corrections are calculated using vibrational frequencies scaled by 0.978.

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Table S3 Enthalpies of formation of fluorene and its derivatives calculated by DLPNO-CCSD(T_1)/CBS method using different working reactions (in kJ mol^{-1})

	Reaction[a]	$\Delta_r H_m^\circ$ [b]	$\Delta_f H_m^\circ$	Exp. – Calc. [c]
	(1) $C_{13}H_{10}$ (fluorene)			
1*	$C_{13}H_{10}$ (fluorene) + 6 H_2 → 3 C_2H_2 + 3 C_2H_4 + CH_4	578.4	189.0	-9.6
2*	$C_{13}H_{10}$ (fluorene) + 11 CH_4 → 9 C_2H_4 + 3 C_2H_6	848.3	190.8	-11.4
3	$C_{13}H_{10}$ (fluorene) + C_2H_4 + C_2H_6 → 2 C_6H_6 + C_5H_8 (cyclopentene)	44.1	188.8	-9.4
4*	$C_{13}H_{10}$ (fluorene) + CH_4 → $C_{10}H_8$ (naphthalene) + CH_2=CHCH=CH_2	148.1	187.9	-8.5
5	$C_{13}H_{10}$ (fluorene) + C_2H_4 → $C_{14}H_{10}$ (anthracene) + CH_4	-84.1	186.6	-7.2
6	$C_{13}H_{10}$ (fluorene) + C_5H_6 (1,3-cyclopentadiene) → 2 C_9H_8 (indene)	-0.1	187.8	-8.4
7	$C_{13}H_{10}$ (fluorene) + C_2H_6 → C_9H_{10} (indane) + C_6H_6	38.8	189.2	-9.8
8	$C_{13}H_{10}$ (fluorene) + CH_4 → $C_{12}H_8$ (acenaphthylene) + C_2H_6	64.9	188.9	-9.5
9	$C_{13}H_{10}$ (fluorene) + CH_4 → $C_{12}H_{10}$ (acenaphthene) + C_2H_4	94.9	188.8	-9.4
10	$C_{13}H_{10}$ (fluorene) + C_6H_6 → $C_{18}H_{12}$ (triphenylene) + CH_4	-76.9	189.3	-9.9
		average	**188.7 ± 2.2** [d]	**-9.3**
	(2) $C_{13}H_8O$ (9-fluorenone)			
1*	$C_{13}H_8O$ (9-fluorenone) + 7 H_2 → 4 C_2H_2 + 2 C_2H_4 + CH_4 + H_2O	613.1	88.3	-1.3
2*	$C_{13}H_8O$ (9-fluorenone) + 13 CH_4 → 10 C_2H_4 + 3 C_2H_6 + H_2O	907.9	90.8	-3.8
3	$C_{13}H_8O$ (9-fluorenone) + C_2H_6 + C_2H_4 + C_3H_8 → 2 C_6H_6 + C_5H_8 (cyclopentene) + $CH_3C(O)CH_3$	33.4	87.6	-0.6
4*	$C_{13}H_8O$ (9-fluorenone) + C_2H_6 → $C_{10}H_8$ (naphthalene) + C_5H_6O(2-methylfuran)	69.4	88.8	-1.8
5	$C_{13}H_8O$ (9-fluorenone) + C_2H_4 → $C_{14}H_{10}$ (anthracene) + HC(O)H	-19.6	87.4	-0.4
6	$C_{13}H_8O$ (9-fluorenone) + C_3H_8 + C_2H_4 → C_9H_8 (indene) + C_6H_6 + $CH_3C(O)CH_3$	-7.2	86.8	0.2
7	$C_{13}H_8O$ (9-fluorenone) + C_3H_8 + C_2H_6 → C_9H_{10} (indane) + C_6H_6 + $CH_3C(O)CH_3$	28.2	87.9	-0.9
8	$C_{13}H_8O$ (9-fluorenone) + C_2H_6 → $C_{12}H_8$ (acenaphthylene) + $CH_3C(O)CH_3$	43.3	87.0	0.0
9*	$C_{13}H_8O$ (9-fluorenone) + 2 CH_4 → $C_{12}H_{10}$ (acenaphthene) + H_2C=C=CH_2 + H_2O	165.7	88.2	-1.2
10	$C_{13}H_8O$ (9-fluorenone) + C_6H_6 → $C_{18}H_{12}$ (triphenylene) + HC(O)H	-12.3	90.1	-3.1
		average	**88.3 ± 2.6** [d]	**-1.3**
	(3) $C_{13}H_{10}O$ (9-fluorenol)			
1*	$C_{13}H_{10}O$ (9-fluorenol) + 7 H_2 → 3 C_2H_2 + 3 C_2H_4 + CH_4 + H_2O	489.2	36.3	5.7
2*	$C_{13}H_{10}O$ (9-fluorenol) + 13 CH_4 → 9 C_2H_4 + 4 C_2H_6 + H_2O	824.2	38.2	3.8
3	$C_{13}H_{10}O$ (9-fluorenol) + CH_4 + C_2H_4 + C_2H_6 → 2 C_6H_6 + C_5H_8 (cyclopentene) + CH_3OH	69.7	36.9	5.1
4	$C_{13}H_{10}O$ (9-fluorenol) + CH_4 + C_2H_4 → $C_{10}H_8$ (naphthalene) + CH_3OH + C_5H_6 (cyclopentadiene)	68.3	37.3	4.7
5	$C_{13}H_{10}O$ (9-fluorenol) + C_2H_4 → $C_{14}H_{10}$ (anthracene) + CH_3OH	-58.5	34.7	7.3

6	$C_{13}H_{10}O$ (9-fluorenol) + CH_4 + C_2H_4 → C_9H_8 (indene) + C_6H_6 + CH_3OH	29.0	36.0	6.0
7*	$C_{13}H_{10}O$ (9-fluorenol) + 2 CH_4 → C_9H_{10} (indane) + C_6H_6 + H_2O	14.7	36.5	5.5
8*	$C_{13}H_{10}O$ (9-fluorenol) + CH_4 → $C_{12}H_8$ (acenaphthylene) + CH_3OCH_3	117.9	35.9	6.1
9	$C_{13}H_{10}O$ (9-fluorenol) + 2 CH_4 → $C_{12}H_{10}$ (acenaphthene) + CH_3OH + C_2H_4	120.5	36.8	5.2
10	$C_{13}H_{10}O$ (9-fluorenol) + $C_6H_5CH_3$ → $C_{18}H_{12}$ (triphenylene) + CH_3CH_2OH	-53.1	38.1	3.9
		average	**36.7 ± 2.1** [d]	**5.3**
	(4) $C_{14}H_{12}O$ (9-fluorenemethanol)			
1*	$C_{14}H_{12}O$ (9-fluorenemethanol) + 7 H_2 → 3 C_2H_2 + 3 C_2H_4 + C_2H_6 + H_2O	503.4	12.6	-3.4
2*	$C_{14}H_{12}O$ (9-fluorenemethanol) + 13 CH_4 → 9 C_2H_4 + 3 C_2H_6 + C_3H_8 + H_2O	827.5	13.8	-4.6
3	$C_{14}H_{12}O$ (9-fluorenemethanol) + CH_4 + C_2H_4 + C_2H_6 → 2 C_6H_6 + C_5H_8 (cyclopentene) + CH_3CH_2OH	60.7	11.7	-2.5
4	$C_{14}H_{12}O$ (9-fluorenemethanol) + CH_4 + C_2H_4 → $C_{10}H_8$ (naphthalene) + CH_3CH_2OH + C_5H_6 (cyclopentadiene)	59.4	12.1	-2.9
5	$C_{14}H_{12}O$ (9-fluorenemethanol) + C_2H_4 → $C_{14}H_{10}$ (anthracene) + CH_3CH_2OH	-67.4	9.5	-0.3
6	$C_{14}H_{12}O$ (9-fluorenemethanol) + CH_4 + C_2H_4 → C_9H_8 (indene) + $C_6H_5CH_3$ + CH_3OH	21.9	10.0	-0.8
7	$C_{14}H_{12}O$ (9-fluorenemethanol) + 2 CH_4 → C_9H_{10} (indane) + C_6H_6 + CH_3OH	78.7	13.5	-4.3
8	$C_{14}H_{12}O$ (9-fluorenemethanol) + CH_4 → $C_{12}H_8$ (acenaphthylene) + $CH_3CH_2CH_2OH$	71.2	11.2	-2.0
9*	$C_{14}H_{12}O$ (9-fluorenemethanol) + CH_4 → $C_{12}H_{10}$ (acenaphthene) + $CH_3C(O)CH_3$	3.9	10.5	-1.3
10	$C_{14}H_{12}O$ (9-fluorenemethanol) + C_6H_6 → $C_{18}H_{12}$ (triphenylene) + CH_3CH_2OH	-60.2	12.1	-2.9
		average	**11.7 ± 2.8** [d]	**-2.5**
	(5) $C_{14}H_{10}O$ (2-fluorenecarboxaldehyde)			
1*	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + 7 H_2 → 3 C_2H_2 + 4 C_2H_4 + H_2O	584.9	67.5	-3.0
2*	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + 14 CH_4 → 10 C_2H_4 + 4 C_2H_6 + H_2O	919.9	69.4	-4.9
3	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + CH_4 + 2 C_2H_4 → 2 C_6H_6 + C_5H_6 (cyclopentadiene) + $CH_3C(O)H$	37.9	66.2	-1.7
4	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + CH_4 + C_2H_6 → $C_{10}H_8$ (naphthalene) + $CH_3C(O)H$ + C_5H_8 (cyclopentene)	110.8	67.7	-3.2
5	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + C_2H_4 + CH_4 → $C_{14}H_{10}$ (anthracene) + C_2H_6 + HC(O)H	-7.6	66.0	-1.5
6	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + C_2H_4 → C_9H_8 (indene) + $C_6H_5C(O)H$	6.9	64.3	0.2
7	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + CH_4 + C_2H_6 → C_9H_{10} (indane) + $C_6H_5CH_3$ + HC(O)H	93.9	66.2	-1.7
8	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + 2 CH_4 → $C_{12}H_8$ (acenaphthylene) + C_2H_6 + $CH_3C(O)H$	95.8	66.8	-2.3
9	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + 2 CH_4 → $C_{12}H_{10}$ (acenaphthene) + $CH_3CH{=}CH_2$ + HC(O)H	149.4	67.2	-2.7
10	$C_{14}H_{10}O$ (2-fluorenecarboxaldehyde) + C_6H_6 → $C_{18}H_{12}$ (triphenylene) + $CH_3C(O)H$	-45.9	67.2	-2.7

		average	**66.9 ± 2.7** [d]	**-2.4**
	(6) $C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid)			
1*	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + 8 H_2 → 3 C_2H_2 + 4 C_2H_4 + 2 H_2O	581.7	-171.1	-1.0
2*	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + 16 CH_4 → 10 C_2H_4 + 5 C_2H_6 + 2 H_2O	981.8	-169.3	-2.8
3	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + 2 CH_4 + C_2H_2 → 2 C_6H_6 + C_5H_6 (cyclopentadiene) + HC(O)OH	13.6	-171.3	-0.8
4	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + CH_4 + C_2H_6 → $C_{10}H_8$ (naphthalene) + $CH_3C(O)OH$ + C_5H_8 (cyclopentene)	84.6	-173.4	1.3
5	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + CH_4 + C_2H_4 → $C_{14}H_{10}$ (anthracene) + HC(O)OH + C_2H_6	-37.3	-173.6	1.5
6	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + C_2H_4 → C_9H_8 (indene) + $C_6H_5C(O)OH$	-12.8	-173.4	1.3
7	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + CH_4 + C_2H_6 → C_9H_{10} (indane) + C_6H_6 + $CH_3C(O)OH$	43.6	-174.1	2.0
8	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + 2 CH_4 → $C_{12}H_8$ (acenaphthylene) + C_2H_6 + $CH_3C(O)OH$	69.6	-174.4	2.3
9	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + 2 CH_4 → $C_{12}H_8$ (acenaphthylene) + C_3H_8 + HC(O)OH	100.8	-172.0	-0.1
10	$C_{14}H_{10}O_2$ (9-fluorenecarboxylic acid) + C_6H_6 + CH_4 → $C_{18}H_{12}$ (triphenylene) + C_2H_6 + HC(O)OH	-30.0	-170.9	-1.2
		average	**-172.3 ± 3.3** [d]	**0.2**
	(7) $C_{13}H_{11}N$ (2-aminofluorene)			
1*	$C_{13}H_{11}N$ (2-aminofluorene) + 7 H_2 → 3 C_2H_2 + 3 C_2H_4 + CH_4 + NH_3	526.4	195.4	-1.8
2*	$C_{13}H_{11}N$ (2-aminofluorene) + 12 CH_4 → 9 C_2H_4 + 3 C_2H_6 + CH_3NH_2	895.2	196.7	-3.1
3*	$C_{13}H_{11}N$ (2-aminofluorene) + 2 CH_4 + C_2H_2 → 2 C_6H_6 + C_5H_6 (cyclopentadiene) + NH_3	-20.2	195.3	-1.7
4	$C_{13}H_{11}N$ (2-aminofluorene) + CH_4 + C_2H_4 → $C_{10}H_8$ (naphthalene) + CH_3NH_2 + C_5H_6 (cyclopentadiene)	89.6	195.1	-1.5
5	$C_{13}H_{11}N$ (2-aminofluorene) + C_2H_4 → $C_{14}H_{10}$ (anthracene) + CH_3NH_2	-37.2	192.5	1.1
6	$C_{13}H_{11}N$ (2-aminofluorene) + C_2H_4 → C_9H_8 (indene) + $C_6H_5NH_2$	2.3	193.6	0.0
7*	$C_{13}H_{11}N$ (2-aminofluorene) + CH_4 + C_2H_6 → C_9H_{10} (indane) + $C_6H_5CH_3$ + NH_3	30.5	193.4	0.2
8*	$C_{13}H_{11}N$ (2-aminofluorene) + CH_4 → $C_{12}H_8$ (acenaphthylene) + CH_3NHCH_3	126.8	192.9	0.7
9	$C_{13}H_{11}N$ (2-aminofluorene) + 2 CH_4 → $C_{12}H_{10}$ (acenaphthene) + CH_3NH2 + C_2H_4	141.8	194.7	-1.1
10	$C_{13}H_{11}N$ (2-aminofluorene) + C_6H_6 → $C_{18}H_{12}$ (triphenylene) + CH_3NH_2	-30.0	195.2	-1.6
		average	**194.5 ± 2.7** [d]	**-0.9**
	(8) $C_{13}H_9NO_2$ (2-nitrofluorene)			
1*	$C_{13}H_9NO_2$ (2-nitrofluorene) + 9 H_2 → 4 C_2H_2 + 2 C_2H_4 + CH_4 + NH_3 + 2 H_2O	244.7	169.3	-4.9
2*	$C_{13}H_9NO_2$ (2-nitrofluorene) + 13 CH_4 → 9 C_2H_4 + 4 C_2H_6 + HNO_2	858.3	166.8	-2.4
3	$C_{13}H_9NO_2$ (2-nitrofluorene) + CH_4 + 2 C_2H_4 → 2 C_6H_6 + C_5H_6 (cyclopentadiene) + CH_3NO_2	30.7	167.5	-3.1
4	$C_{13}H_9NO_2$ (2-nitrofluorene) + $CH{\equiv}CCH_3$ → $C_{10}H_8$ (naphthalene) + $C_6H_5NO_2$	-139.6	170.0	-5.6
5	$C_{13}H_9NO_2$ (2-nitrofluorene) + C_2H_4 → $C_{14}H_{10}$ (anthracene) + CH_3NO_2	-60.4	165.9	-1.5

6	$C_{13}H_9NO_2$ (2-nitrofluorene) + $C_2H_4 \rightarrow C_9H_8$ (indene) + $C_6H_5NO_2$	6.4	167.5	-3.1
7	$C_{13}H_9NO_2$ (2-nitrofluorene) + CH_4 + $C_2H_6 \rightarrow C_9H_{10}$ (indane) + C_6H_6 + CH_3NO_2	62.6	168.4	-4.0
8	$C_{13}H_9NO_2$ (2-nitrofluorene) + C_6H_6 + $CH_4 \rightarrow C_{12}H_8$ (acenaphthylene) + $C_6H_5NO_2$ + C_2H_6	67.8	168.4	-4.0
9	$C_{13}H_9NO_2$ (2-nitrofluorene) + 2 $CH_4 \rightarrow C_{12}H_{10}$ (acenaphthene) + CH_3NO_2 + C_2H_4	118.7	168.0	-3.6
10	$C_{13}H_9NO_2$ (2-nitrofluorene) + $C_6H_6 \rightarrow C_{18}H_{12}$ (triphenylene) + CH_3NO_2	-53.1	168.6	-4.2
		average	**168.1 ± 2.4** [d]	**-3.7**
	(9) $C_{12}H_8O$ (dibenzofuran)			
1*	$C_{12}H_8O$ (dibenzofuran) + 6 $H_2 \rightarrow$ 3 C_2H_2 + 3 C_2H_4 + H_2O	542.9	57.1	-2.1
2*	$C_{12}H_8O$ (dibenzofuran) + 12 $CH_4 \rightarrow$ 9 C_2H_4 + 3 C_2H_6 + H_2O	812.8	59.0	-4.0
3	$C_{12}H_8O$ (dibenzofuran) + 3 C_2H_4 + $C_3H_8 \rightarrow$ 3 C_6H_6 + CH_4 + CH_3OCH_3	-118.6	57.4	-2.4
4	$C_{12}H_8O$ (dibenzofuran) + $C_2H_4 \rightarrow C_{10}H_8$ (naphthalene) + C_4H_4O (furan)	6.5	57.1	-2.1
5	$C_{12}H_8O$ (dibenzofuran) + $CH_3CH{=}CHCH_3 \rightarrow C_{14}H_{10}$ (anthracene) + CH_3OCH_3	0.3	56.4	-1.4
6*	$C_{12}H_8O$ (dibenzofuran) + CH_4 + $C_2H_4 \rightarrow C_9H_8$ (indene) + C_6H_6 + H_2O	-32.1	56.2	-1.2
7	$C_{12}H_8O$ (dibenzofuran) + CH_4 + $C_2H_6 \rightarrow C_9H_{10}$ (indane) + C_4H_4O (furan) + C_2H_4	180.7	56.4	-1.4
8	$C_{12}H_8O$ (dibenzofuran) + C_5H_6 (cyclopentadiene) $\rightarrow C_{12}H_8$ (acenaphthylene) + C_5H_6O (2-methylfuran)	-3.6	56.6	-1.6
9*	$C_{12}H_8O$ (dibenzofuran) + $CH_4 \rightarrow C_{12}H_{10}$ (acenaphthene) + HC(O)H	64.3	57.8	-2.8
10	$C_{12}H_8O$ (dibenzofuran) + $C_{10}H_8$ (naphthalene) $\rightarrow C_{18}H_{12}$ (triphenylene) + C_4H_4O (furan)	29.2	55.6	-0.6
		average	**57.0 ± 1.9** [d]	**-2.0**
	(10) $C_{12}H_9N$ (carbazole)			
1*	$C_{12}H_9N$ (carbazole) + 6 $H_2 \rightarrow$ 3 C_2H_2 + 3 C_2H_4 + NH_3	586.1	210.2	-4.2
2*	$C_{12}H_9N$ (carbazole) + 11 $CH_4 \rightarrow$ 9 C_2H_4 + 2 C_2H_6 + CH_3NH_2	889.9	211.5	-5.5
3	$C_{12}H_9N$ (carbazole) + 3 C_2H_4 + $C_3H_8 \rightarrow$ 3 C_6H_6 + CH_4 + CH_3NHCH_3	-103.7	208.3	-2.3
4*	$C_{12}H_9N$ (carbazole) + C_2H_6 + $C_2H_4 \rightarrow C_{10}H_8$ (naphthalene) + C_5H_6 (cyclopentadiene) + CH_3NH_2	84.3	209.9	-3.9
5	$C_{12}H_9N$ (carbazole) + $C_6H_6 \rightarrow C_{14}H_{10}$ (anthracene) + C_4H_5N (pyrrole)	47.1	207.4	-1.4
6	$C_{12}H_9N$ (carbazole) + C_3H_8 + $C_2H_4 \rightarrow C_9H_8$ (indene) + C_6H_6 + CH_3NHCH_3	70.9	207.4	-1.4
7	$C_{12}H_9N$ (carbazole) + CH_4 + $C_2H_6 \rightarrow C_9H_{10}$ (indane) + C_4H_5N (pyrrole) + C_2H_4	170.0	210.0	-4.0
8*	$C_{12}H_9N$ (carbazole) + C_5H_6 (cyclopentadiene) $\rightarrow C_{12}H_8$ (acenaphthylene) + C_5H_7N (N-methylpyrrole)	23.5	209.1	-3.1
9*	$C_{12}H_9N$ (carbazole) + $CH_2{=}CHCH{=}CH_2 \rightarrow C_{12}H_{10}$ (acenaphthene) + C_4H_5N (pyrrole)	-57.4	211.6	-5.6
10	$C_{12}H_9N$ (carbazole) + C_6H_6 + $C_3H_8 \rightarrow C_{18}H_{12}$ (triphenylene) + CH_4 + CH_3NHCH_3	-9.4	208.8	-2.8
		average	**209.4 ± 3.0** [d]	**-3.4**
	(11) $C_{12}H_8S$ (dibenzothiophene)			
1*	$C_{12}H_8S$ (dibenzothiophene) + 6 $H_2 \rightarrow$ 3 C_2H_2 + 3 C_2H_4 + H_2S	605.1	216.2	-4.9

2*	$C_{12}H_8S$ (dibenzothiophene) + 11 CH_4 → 9 C_2H_4 + 2 C_2H_6 + CH_3SH	883.0	217.1	-5.8
3	$C_{12}H_8S$ (dibenzothiophene) + 2 C_2H_4 → 2 C_6H_6 + C_4H_4S (thiophene)	-36.9	213.3	-2.0
4	$C_{12}H_8S$ (dibenzothiophene) + C_3H_8 + C_2H_4 → $C_{10}H_8$ (naphthalene) + C_5H_6 (cyclopentadiene) + CH_3SCH_3	83.4	216.2	-4.9
5	$C_{12}H_8S$ (dibenzothiophene) + C_6H_6 → $C_{14}H_{10}$ (anthracene) + C_4H_4S (thiophene)	50.2	211.1	0.2
6*	$C_{12}H_8S$ (dibenzothiophene) + CH_4 + C_2H_4 → C_9H_8 (indene) + C_6H_6 + H_2S	30.1	215.2	-3.9
7	$C_{12}H_8S$ (dibenzothiophene) + CH_4 + C_2H_6 → C_9H_{10} (indane) + C_4H_4S (thiophene) + C_2H_4	173.1	213.6	-2.3
8	$C_{12}H_8S$ (dibenzothiophene) + C_2H_6 → $C_{12}H_8$ (acenaphthylene) + CH_3SCH_3	94.6	215.1	-3.8
9*	$C_{12}H_8S$ (dibenzothiophene) + C_2H_6 + CH_4 → $C_{12}H_{10}$ (acenaphthene) + CH_3SH + C_2H_4	129.6	215.1	-3.8
10	$C_{12}H_8S$ (dibenzothiophene) + $C_{10}H_8$ (naphthalene) → $C_{18}H_{12}$ (triphenylene) + C_4H_4S (thiophene)	21.7	212.8	-1.5
		average	**214.6 ± 3.7** [d]	**-3.3**
	(12) $C_{16}H_{10}$ (fluoranthene)			
1*	$C_{16}H_{10}$ (fluoranthene) + 7 H_2 → 4 C_2H_2 + 4 C_2H_4	836.2	286.3	-3.9
2*	$C_{16}H_{10}$ (fluoranthene) + 14 CH_4 → 12 C_2H_4 + 3 C_2H_6	1131.0	288.8	-6.4
3*	$C_{16}H_{10}$ (fluoranthene) + 2 CH_4 → 3 C_6H_6	111.5	286.8	-4.4
4	$C_{16}H_{10}$ (fluoranthene) + $CH_3CH{=}CH_2$ + C_2H_4 → $C_{10}H_8$ (naphthalene) + C_6H_6 + C_5H_6 (cyclopentadiene)	7.6	287.5	-5.1
5	$C_{16}H_{10}$ (fluoranthene) + $CH_3CH{=}CH_2$ → $C_{14}H_{10}$ (anthracene) + C_5H_6 (cyclopentadiene)	58.9	284.3	-1.9
6	$C_{16}H_{10}$ (fluoranthene) + $CH_3CH{=}CH_2$ + C_2H_4 → C_9H_8 (indene) + 2 C_6H_6	-31.6	286.2	-3.8
7	$C_{16}H_{10}$ (fluoranthene) + C_3H_8 + C_2H_4 → C_9H_{10} (indane) + 2 C_6H_6	-7.4	287.2	-4.8
8	$C_{16}H_{10}$ (fluoranthene) + C_2H_4 → $C_{12}H_8$ (acenaphthylene) + C_6H_6	7.7	286.2	-3.8
9	$C_{16}H_{10}$ (fluoranthene) + C_2H_6 → $C_{12}H_{10}$ (acenaphthene) + C_6H_6	37.8	286.1	-3.7
10	$C_{16}H_{10}$ (fluoranthene) + $C_6H_5CH_3$ → $C_{18}H_{12}$ (triphenylene) + C_5H_6 (cyclopentadiene)	65.5	288.3	-5.9
		average	**286.8 ± 2.5** [d]	**-4.4**

[a] Isogyric reactions are marked with an asterisk, the remaining reactions are isodesmic. [b] Enthalpy of reaction. [c] Experimental values of enthalpy of formation are given in Table 3. [d] Uncertainties of calculated values are estimated as 2σ, where σ is the standard deviation of the mean.