

## Supporting information

**Table 1** – Main observed pyrolysis mechanisms for  $C_2H_2$  and  $C_6H_6$  and their relative occurrence. All observed processes are also described in literature, as indicated by the references

	pyrolysis mechanisms	Rel. occurrence (%)	Literature
$C_2H_2$ pyrolysis	$C_2H_2 \rightarrow C_2H + H$	50	[51, 52]
	$C_2H_2 \rightarrow 2CH$	17	[52]
	$C_2H_2 + H \rightarrow C_2H_3 \rightarrow C_2H + 2H$	16	[51, 52, 58]
	$C_2H_2 \rightarrow C_2 + 2H$	6	[52]
	other reactions, see Table 2	11	[51-53, 55]
$C_6H_6$ pyrolysis	$C_6H_6 \rightarrow C_6H_5 + H \rightarrow C_6H_4 + 2H \rightarrow C_4H_3 + C_2H_2 + H$	33	[54]
	$C_6H_6 \rightarrow 3C_2H_2$	13	[57]
	$C_6H_6 + H \rightarrow C_6H_7 \rightarrow C_6H_5 + 2H$	12	[54]
	$C_6H_6 \rightarrow 2C_3H_3$	7	[56]
	other reactions, see Table 2	35	[54-57]

**Table 2** – Additional pyrolysis mechanisms observed for  $C_2H_2$  and  $C_6H_6$ , besides the ones listed in Table 1, with lower frequency of occurrence. The superscript *des* indicates a desorbed molecule.

	Reactions
$C_2H_2$ pyrolysis	$C_2H_2 + H_2 \rightarrow C_2H_4$ $C_2H_2 + CH_2 \rightarrow C_3H_4$ (not propyne) $C_2H_2 + C_2H \rightarrow C_2 + C_2H_3$ $C_2H + H \rightarrow C_2H_2$ $C_2H \rightarrow CH + H$ $C_2H \rightarrow CH_2 + H$ $CH + H \rightarrow CH_2$ $CH + 2H \rightarrow CH_3$ or $CH_2 + H \rightarrow CH_3$ $CH + 3H \rightarrow CH_4$ or $CH_3 + H \rightarrow CH_4$ $CH_3 \rightarrow CH_2 + H$ $CH \rightarrow C + H$ $C_4H_5^{des} + C_2H \rightarrow C_6H_6$ (not benzene)
$C_6H_6$ pyrolysis	$C_6H_5 + H \rightarrow C_6H_6$ $C_6H_6 \rightarrow C_5H_3 + CH_2 + H \rightarrow C_3H + CH_2 + C_2 + 3H$ $C_6H_7 \rightarrow C_6H_6 + H$ $C_6H_7 \rightarrow C_6H_5 + H_2$ $C_4H_4 \rightarrow 2C_2H_2$ $C_2H_2 + C_2H_2 \rightarrow C_4H_4 \rightarrow C_4H_3 + H \rightarrow C_4H_2 + 2H \rightarrow C_4H + 3H \rightarrow C_4 + 4H$ $C_6H_6 \rightarrow C_5H_4 + CH + H \rightarrow C_5H_3 + CH + 2H \rightarrow C_3H_2 + C_2H + CH + 2H \rightarrow C_2 + CH_2 + C_2H$  <p>Note that all aforementioned reactions for <math>C_2H_2</math> pyrolysis may occur in this case as well</p>