Species name in mechanism	***Cas number***	***Detailed formula***	***Detailed/usual name***
non cyclic molecules			
AR	7440-37-1	AR	argon
N2	7727-37-9	N2	nitrogen molecule
H	12385-13-6	H	hydrogen radical
O	17778-80-2	O	oxygen radical
OH	3352-57-6	OH	hydroxyl radical
O2	7782-44-7	O2	molecular oxygen
H2	1333-74-0	H2	hydrogen molecule
H2O	7732-18-5	H-O-H	water
HO2	3170-83-0	HO=O*	hydroperoxy radical
H2O2	7722-84-1	HO-OH	hydrogen peroxide
C	7440-44-0	C	carbon
CO	630-08-0	CO	carbon monoxyde
CO2	124-38-9	CO2	carbon dioxyde
CH	3315-37-5	CH	methylidyne
HCO	2597-44-6	HCO	formyl radical
1-CH2	2465-56-7	CH2	singlet methylene radical
3-CH2	2465-56-7	CH2	triplet methylene radical
CH2O	50-00-0	CH2=O	formaldehyde
CH3	2229-07-4	CH3*	methyl radical
CH2OH	2597-43-5	CH2*-OH	hydroxymethyl radical
CH3O	2143-68-2	CH3-O*	methoxy radical
CH3O2	2143-58-0	CH3-O-O*	methylperoxyde radical
CH4	74-82-8	CH4	methane
CH3OH	67-56-1	CH3-OH	methanol
C2O	12071-23-7	C=C=O	dicarbon monoxyde
C2H	2122-48-7	CH≡C*	ethynyl radical
HCCO	51095-15-9	HC*=CO	ketyl radical
C2H2	74-86-2	CH≡CH	acetylene
H2C2	2143-69-3	CH2=C*	vinylidene radical
CH2CO	436-51-4	CH2=CO	ketene
HCCOH	32038-79-2	HC≡C-OH	ethynol
C2H3	2669-89-8	CH2=CH*	vinyl radical
CH2CHO	6912-06-7	CH2=CHO*	vinyl oxy radical

C2H4	74-85-1	CH2=CH2	ethylene
CH3CHO	75-07-0	CH3-CHO	acetaldehyde
C2H5	2025-56-1	CH3-CH2*	ethyl radical
C2H5O	2154-50-9	CH3-CH2-O*	ethyl oxide radical
C2H6	74-84-0	CH3-CH3	ethane
C3H2	67152-18-5	*HC=C=CH*	prop-2-vinylidene
C3H2O	624-67-9	CH≡CCHO	2-propynal
C3H3	2932-78-7	*CH2-CCH	propargyl radical
A-C3H4	463-49-0	CH2=C=CH2	allene
P-C3H4	74-99-7	CH3-C≡CH	propyne
C2H3CHO	107-02-8	CH2=CH-CHO	propenal
A-C3H5	1981-80-2	CH2=CH-CH2*	symmetric allyl radical
S-C3H5	6067-68-1	CH3-CH=CH*	secondary allyl radical
T-C3H5	15552-77-9	CH2=C*CH3	tertiary allyl radical
C3H5O		CH2=CH-CH2-O*	propanal radical
C3H6	115-07-1	CH2=CH-CH3	propylene
CH3COCH3	67-64-1	CH3-CO-CH3	acetone
N-C3H7	2143-61-5	CH3-CH2-CH2*	n-propyl radical
N-C3H7O	16499-18-6	CH3-CH2-CH2-O*	n-propoxy radical
C3H8	74-98-6	CH3-CH2-CH3	propane
C4H	53561-65-2	HC≡C-C≡C*	butadiynyl radical
C4H2	460-12-8	HC≡C-C≡CH	butadiyne
I-C4H3	63707-54-0	HC≡C-C*=CH2	i-1-butene-3-yne-2-yl radical
N-C4H3	2810-61-9	HC≡C-CH=CH*	e-1-butene-3-yne-1-yl radical
C4H4	687-97-4	HC≡C-CH=CH2	1-buten-3-yne
C4H4O	50888-73-8	CH2=CH-CH=CO	vinyl-ketene
N-C4H5	86181-68-2	CH2=CH-CH=CH*	e-1,3-butadiene-1-yl radical
I-C4H5	108179-96-0	CH2=CH-C*=CH2	i-1,3-Butadiene-2-yl radical
13-C4H6	106-99-0	CH2=CH-CH=CH2	1,3-butadiene
C6H2	3161-99-7	CH≡C-C≡C-C≡CH	hexatriene
C8H2	6165-96-4	CH≡C-C≡C-C≡C-C≡C-CH	octatetrayne
molecules from LLNL mech for heptane			
C4H7	2154-62-3	CH2*-CH2-CH=CH2	trans-3-buten-1-yl radical
C4H7O		CH3-CHO*-CH=CH2	butyl oxy radical
1-C4H8	106-98-9	CH3-CH2-CH=CH2	1-butene
N-C3H7CHO	123-72-8	CH3-CH2-CH2-CHO	butanal

P-C4H9	2492-36-6 2348-55-2	CH3-CH2-CH2-CH2* CH3-CH2-CH*-CH3	butyl radical (lumped)
C5H9	 130825-72-8	CH2*-CH2-CH2-CH=CH2 CH3-CH2-CH*-CH=CH2	pentenyl radical (lumped)
1-C5H10	109-67-1	CH3-CH2-CH2-CH=CH2	1-pentene
1-C5H11	2672-01-7 2492-34-4	CH3-CH2-CH2-CH2-CH2* CH3-CH2-CH2-CH*-CH3	pentyl radical (lumped)
C7H13		CH3-CH2-CH*-CH2-CH2-CH=CH2 CH3-CH*-CH2-CH2-CH2-CH=CH2	heptenyl radical (lumped)
3-C7H14	592-76-7 14686-13-6	CH3-CH2-CH2-CH2-CH2-CH=CH2 CH3-CH2-CH2-CH2-CH=CH-CH3	heptene (lumped)
2-C7H15	3356-67-0 3474-30-4	CH3-CH2-CH2-CH2-CH2-CH2-CH2* CH3-CH2-CH2-CH2-CH2-CH*-CH3 CH3-CH2-CH2-CH2-CH*-CH2-CH3 CH3-CH2-CH2-CH*-CH2-CH2-CH3	heptyl radical (lumped)
1-C7H15O		CH3-CH2-CH2-CHO*-CH2-CH2-CH3 CH3-CH2-CHO*-CH2-CH2-CH2-CH3 CH3-CHO*-CH2-CH2-CH2-CH2-CH3	heptanoxy radical (lumped)
N-C7H16	142-82-5	CH3-CH2-CH2-CH2-CH2-CH2-CH3	n-heptane
molecules from LLNL mech for iso-octane			
I-C3H5CHO	4170-30-3	CH3-(C-CHO)=CH2	2-butenal
I-C3H7	2025-55-0	CH3-CH*-CH3	iso-propyl radical
I-C4H7O	309966-76-5	CH2=C(CH3)-CH2O*	2-methyl allyl oxy radical
I-C4H7	15157-95-6	(CH2)2-C-CH3	2-methyl-allyl radical
I-C4H8	115-11-7	(CH3)2-C=CH2	isobutene
T-C4H9	1605-73-8	(CH3)3-C*	t-butyl radical
T-C4H9O	3141-58-0 26397-42-2	(CH3)3-CO* (CH3)2-CH-CH2O*	butoxy radical (lumped)
X-C7H13		(CH3)2-CH-CH=C(CH3)CH2*	heptenyl radical (lumped)
Y-C7H14	2213-32-3 762-62-9 625-65-0	(CH3)2-CH-CH2-C(CH3)=CH2 (CH3)3-C-CH2-CH=CH2 (CH3)2-CH-CH=C(CH3)2	2,4-dimethyl-1-pentene (lumped) 2,2-dimethyl-4-pentene 2,4-dimethyl-2-pentene
Y-C7H15		(CH3)2-CH-CH2-C*-(CH3)2 CH3-CH*-CH2-C-(CH3)3	heptyl radical (lumped)
C-C8H17		(CH3)2-CH-CH2-C-(CH3)2(CH3) (CH3)(CH2)-CH-CH2-C-(CH3)3	octyl radical (lumped)
D-C8H17O		(CH3)3-C-CH2-CH(CH3)-CH2O*	iso-octyl oxy radical
I-C8H18	540-84-1	(CH3)2-CH-CH2-C-(CH3)3	iso-octane
5-member ring			
C5H4O	3177-38-3	C5H4=O	cyclopentadiene-1-one

C5H5	2143-53-5	-CH-CH-CH-CH-CH-	cyclopentadienyl radical
13-C5H5O	136936-20-4	-CH2-CH-CH-CH-CO*-	1-oxyl-1,3-cyclopentadiene radical
24-C5H5O	136936-19-1	-CH-CH-CH-CH-CHO*-	1-oxyl-1,4-cyclopentadiene radical
C5H6	542-92-7	Cy-C5H6	cyclopentadiene
C5H4CH	304524-27-6	Cy-C5H4=CH*	5-methylenyl-Cy-1,3-pentadiene-6-yl
C5H4CH2	497-20-1	Cy-C5H4=CH2	fulvene
1 aromatic ring			
O-C6H4	462-80-6	Cy-C6H4	o-benzyne
OC6H4O	106-51-4	O=C6H4=O	1,4-benzoquinone
A1-	2396-01-2	A1-	Phenyl radical
C-C6H5O	2122-46-5	A1-O*	Phenoxy radical
A1	71-43-2	A1	Benzene
A1OH	108-95-2	A1-OH	Phenol
A1CHO	100-52-7	A1-CHO	benzaldehyde
A1CH2	2154-56-5	A1-CH2*	benzyl radical
A1CH2O	26397-37-5	A1-CH2O*	benzyl alcohol radical
OA1CH3	3174-48-9	O*-A1-CH3	4-methyl-phenoxy radical
A1CH3	108-88-3	A1-CH3	toluene
A1CH2OH	100-51-6	A1-CH2OH	Benzyl alcohol
HOA1CH3	108-39-4	OH-A1-CH3	Cresol
A1C2H*		A1*-C≡CH	2-ethynylphenyl radical
A1C2H	536-74-3	A1-C≡CH	ethynylbenzene
A1C2H2	23065-05-6	A1-CH=CH*	n-stryryl radical
A1C2H3*	126716-67-4	A1*-CH=CH2	o-stryryl radical
A1C2H3	100-42-5	A1-CH=CH3	styrene
A1C2H4		A1-CH2-CH2*	N-phenyl ethyl radical
A1C2H5	100-41-4	A1-CH2-CH3	Ethyl Benzene
1 aromatic ring + 5 member ring			
C9H6O			indenone
C9H7	71551-80-9		indenyl radical
C9H8	95-13-6		indene
2 aromatic rings			
A2-		A2*	1-naphthyl radical

A2*	10237-50-0	A2*	2-naphthyl radical
A2	91-20-3	A2	naphthalene
A2O	33490-95-8	A2-O*	naphthoxy radical
A2OH	135-19-3	A2-OH	naphthol
A2CH2	7419-60-5	A2-CH2*	1-naphtyl-methylene radical
A2CH3	90-12-0	A2-CH3	1-methyl-naphthalene
A2C2HA*		A2*-C≡CH	1-ethynyl-naphthyl radical
A2C2HB*		A2*-C≡CH	2-ethynyl-naphthyl radical
A2C2HA	15727-65-8	A2-C≡CH	1-ethynyl-naphthalene
A2C2HB		A2-C≡CH	2-ethynyl-naphthalene
A2C2H2A	444160-65-0	A2-CH=CH*	1-naphthylvinyl radical
A2C2H2B		A2-CH-CH*	2-naphthylvinyl radical
P2-	3474-38-2	P2*	o-biphenyl radical
P2	92-52-4	P2	biphenyl
2 aromatic rings + 5-member ring			
A2R5-	943317-46-2	A2R5*	acenaphthyl radical
A2R5	208-96-8	A2R5	acenaphthylene
A2R5C2H*		A2R5*-C≡CH	1-ethynyl-acenaphthyl radical
A2R5C2H		A2R5-C≡CH	1-ethynyl-acenaphthylene
A2R5C2H2		A2R5-CH=CH*	acenaphthylvinyl
3 (and more) aromatic rings			
A3-	61062-79-1	A3*	1-phenathryl radical
A3*	61062-83-7	A3*	4-phenathryl radical
A3	85-01-8	A3	phenanthrene
A3R5-		A3R5*	acephenathryl radical
A4-	61062-85-9	A4*	pyrenyl radical
A3R5		A3R5	acephenanthrene
A4	129-00-0	A4	pyrene
FLTN	206-44-0		fluoranthene
A4R5	27208-37-3	A4R5	cyclopenta[cd]pyrene

Species whose name are in *italic* corresponds to lumped species.