## SUPPORTING INFORMATION: Species Nomenclature.

## H-abstraction Reactions by OH, HO2, O, O2 and Benzyl Radical Addition to O2 and Their Implications for Kinetic Modelling of Toluene Oxidation.

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TableS1 lists nomenclature within the kinetic mechanism, name and formula of relevant species in the toluene model.

Table S1: A list of the C5 and larger species relevant for toluene kinetic model

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| **Formula** | **Name** | **Nomenclature** |
| C7H8 | Toluene | C7H8 |
| C7H7 | Benzyl radical | C7H7 |
| C7H7 | Methlyphenyl radical | CH3C6H4 |
| C7H6 | Fulvenallene | C7H6 |
| C7H5 | Fulvenallenyl | C7H5 |
| C6H4 | Benzyne | C6H4 |
| C6H6 | Benzene | C6H6 |
| C6H6 | Fulvene | FULVENE |
| C6H5 | Phenyl radical | C6H5 |
| C6H5O2 | Phenyl peroxy radical | C6H5O2 |
| C6H5O1 | Phenoxy radical | C6H5OH |
| C6H6O1 | Phenol | C6H5OH |
| C5H6 | Cyclopentadiene | C5H6 |
| C5H5 | Cyclopentadienyl | C5H5 |
| C5H4 | Cyclopentadienylidene | CYC5H4 |
| C7H8O2 | Benzyl hydroperoxide | BZCOOH |
| C7H7O1 | Benzoxyl radical | C6H5CH2O |
| C7H6O1 | Benzaldehyde | C6H5CHO |
| C7H5O1 | Benzoyl radical | C6H5CO |
| C7H7O2 | Benzyl peroxy radical | C7H7O2 |
| C7H7O2 | Methylphenyl peroxy radical | O2C6H4CH3 |
| C7H6O1 | Quinone methide | OC6H4CH2 |
| C7H8O1 | Benzyl Alcohol | C6H5CH2OH |
| C7H8O1 | Cresol | CRESOL |
| C7H7O1 | Methyl phenoxy radicals | RCRESOLO |
| C7H7O1 | hydroxy-benzyl radicals | RCRESOLC |
| C6H4O2 | Benzoquinone | C6H4O2 |
| C8H10 | Ethylbenzene | C6H5C2H5 |
| C8H8 | Styrene | C6H5C2H3 |
| C8H6 | Phenylacetylene | C6H5C2H |
| C6H8 | Methycyclopentadiene | MCPTD |
| C9H8 | Indene | INDENE |
| C9H7 | Indenyl resonance stab radical | INDENYL |
| C10H8 | Napthalene | C10H8 |
| C12H8 | Acenaphthylene | C12H8 |
| C12H10 | Biphenyl | BIPHENYL |
| C13H10 | Fluorene | FLUORENE |
| C13H12 | Diphenylmethane | C13H12 |
| C14H14 | Bibenzyl | C6H5C2H4C6H5 |
| C14H13 | Bibenzyl radical (Ph-CH2CH\*-Ph) | RBBENZ |
| C14H12 | Stilbene | STILB |
| C14H10 | Phenantrene | C14H10 |
| C16H10 | Pyrene | C16H10 |