COMPILATION OF MEASURED YIELD SOOTING INDICES (YSI'S)

This table lists yield sooting indices measured by our group from 2007 to 2015[1 – 4]. The YSI of a given test compound is defined by the relation

$$YSI = A f_{v,max} + B$$

where $f_{v,max}$ is the maximum soot volume fraction measured in a methane/air nonpremixed coflow flame whose fuel is doped with the compound, and A and B are constants chosen so that the YSI's of two endpoint species will have specific values. For this data, the test compound and endpoints are doped into the flame at a fixed MOLE fraction. Given the very wide range of sooting tendencies for the compounds in the database – which range from small oxygenated hydrocarbons to 4-ring PAH – two different sets of endpoints have been used. The table provides a separate listing for each set. For the low sooting tendency species the uncertainties are ± 2 YSI units, while for the high sooting tendency species they are ± 3 %. The table includes the CAS Registry number for each test compound; these tags uniquely identify a given substance and were taken from the NIST Chemistry Webbook [5]. Finally, the table lists the paper where each measurement was originally reported.

References

[1] C.S. McEnally, L.D. Pfefferle. "Improved sooting tendency measurements for aromatic hydrocarbons and their implications for naphthalene formation pathways." Comb Flame 148 (2007) 210-222.

[2] C.S. McEnally, L.D. Pfefferle. "Sooting tendencies of nonvolatile aromatic hydrocarbons." Proc Comb Inst 32 (2009) 673-679.

[3] C.S. McEnally, L.D. Pfefferle. "Sooting tendencies of oxygenated hydrocarbons in laboratory-scale flames." Env Sci Technol 45 (2011) 2498-2503.

[4] D.D. Das, C.S. McEnally, L.D. Pfefferle. "Sooting tendencies of unsaturated esters in nonpremixed flames." Comb Flame 162 (2015) 1489-1497.

[5] NIST Chemistry Webbook. NIST Standard Reference Database Number 69. http://webbook.nist.gov/chemistry/.