Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Extinction Measurements for Optical Band Gap Determination of Soot in a Series of Nitrogen-Diluted Ethylene/Air Non-Premixed Flames

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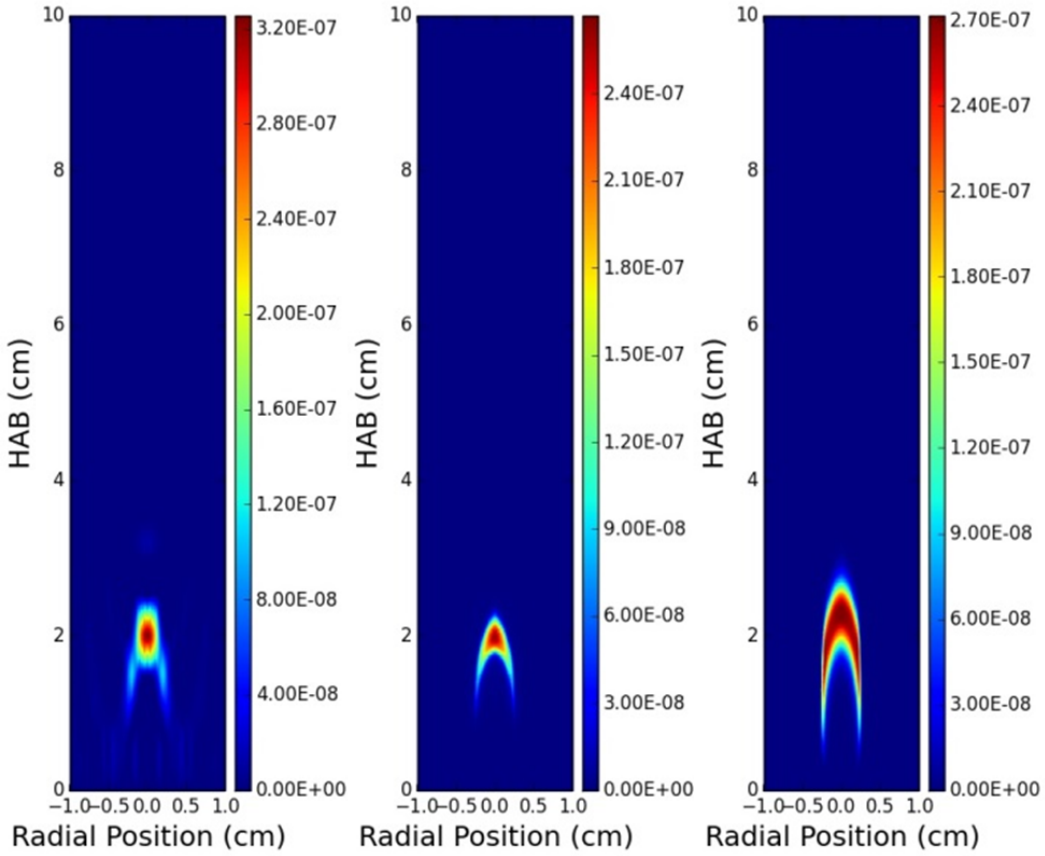
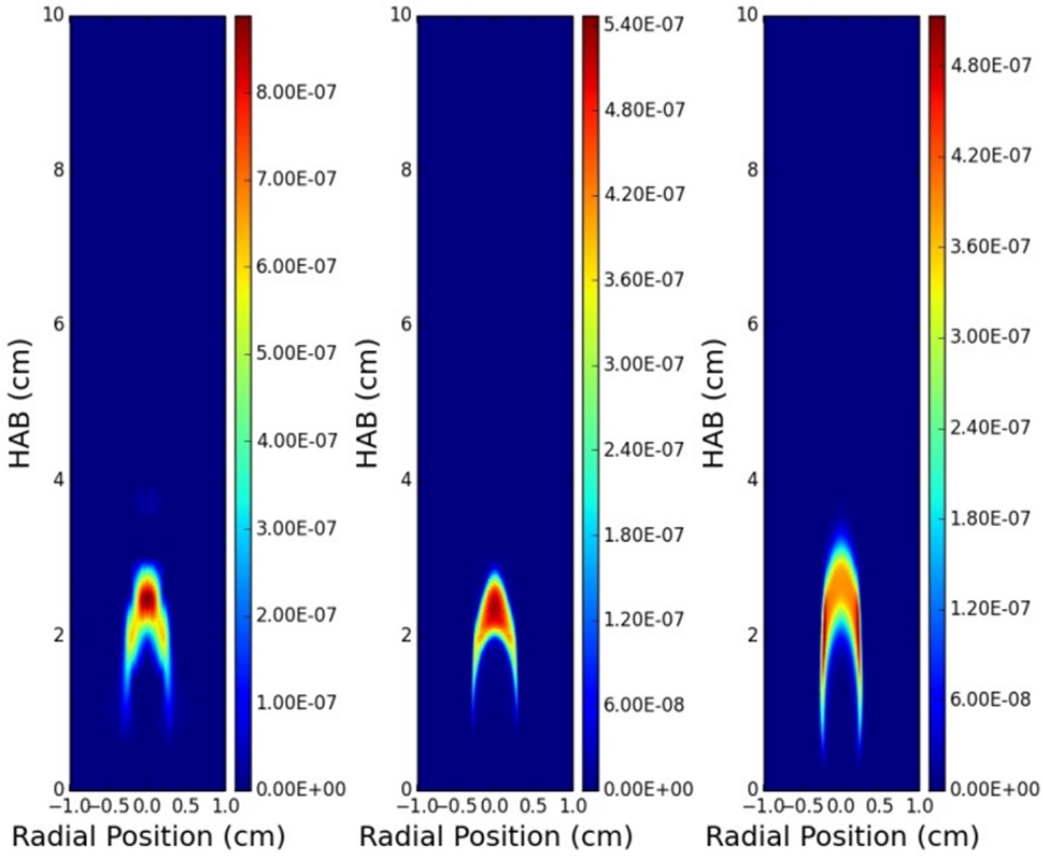
The following supplemental materials include

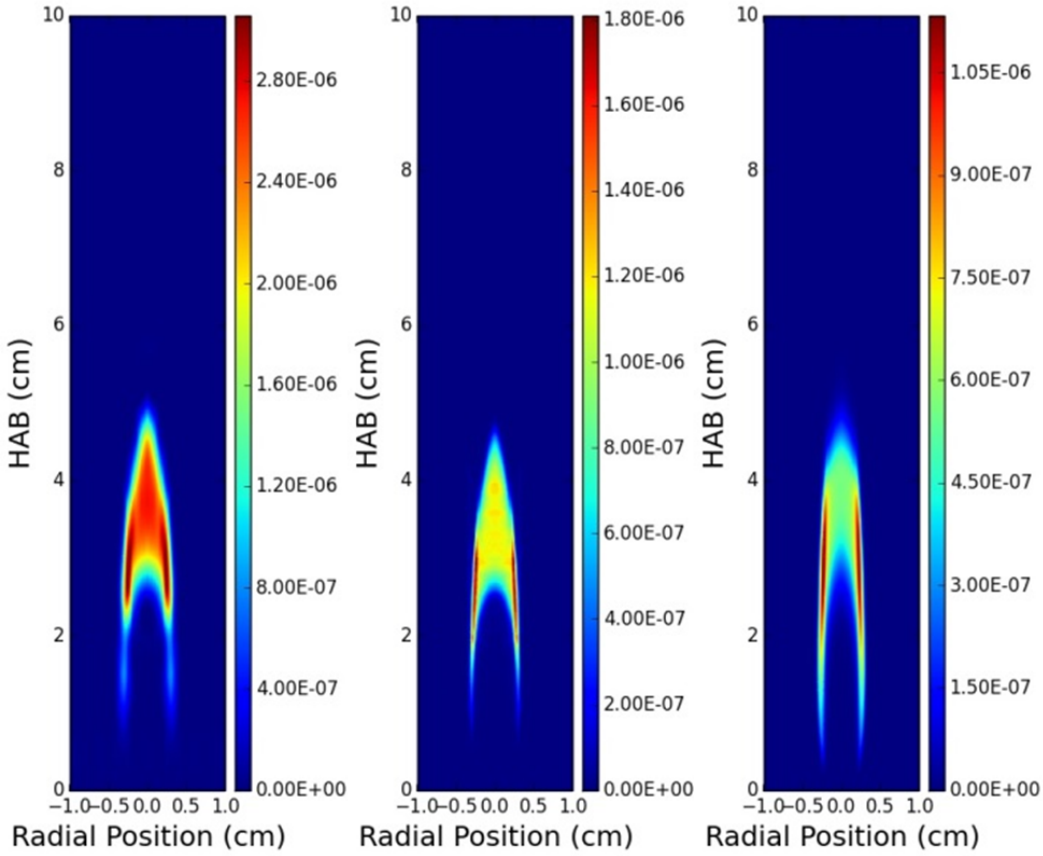
- Comparisons of soot volume fractions from the extinction experiments reported here, LII measurements from the Long Group at Yale, and computations from the Smooke Group at Yale
- Plots of experimentally determined OBG overlaid on contour plots of soot volume fraction calculated by the Smooke group at Yale for the entire flame system
- Comparisons between calculated HOMO-LUMO energy gaps (OBG) with number of aromatic rings and conjugation length for the entire flame system.



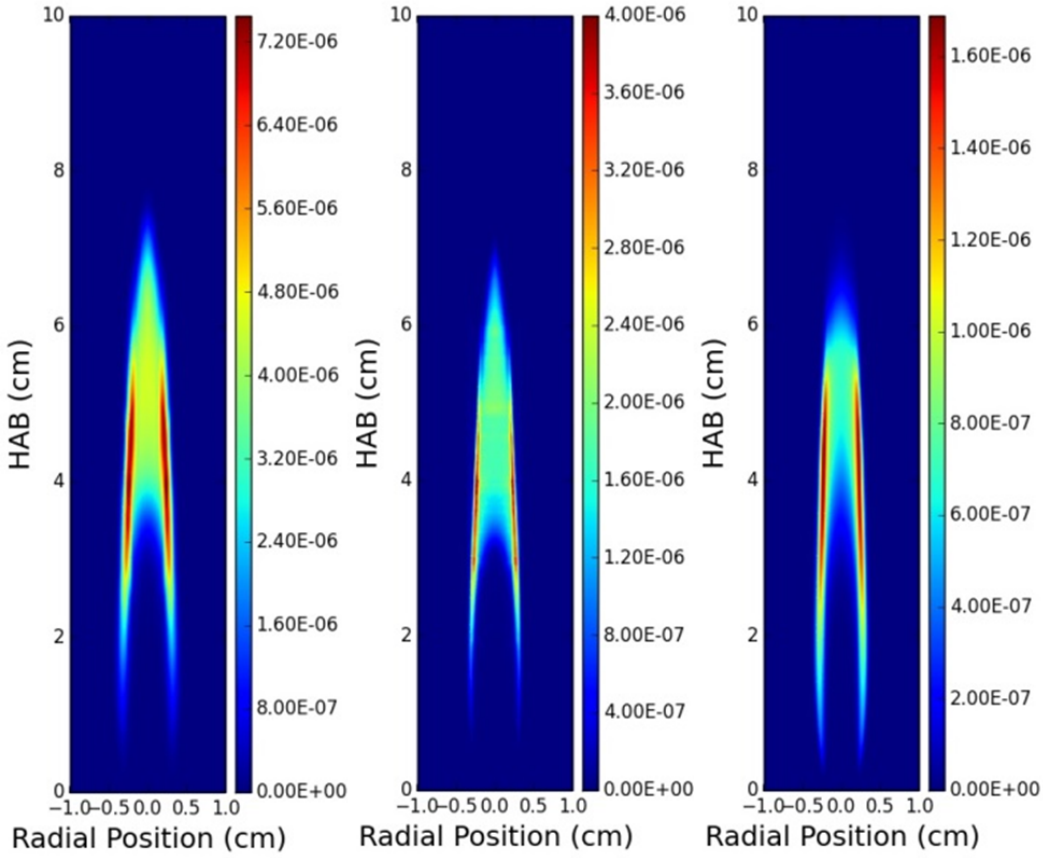
Supplemental Figure 1: 32%-C_2H_4/68%-N_2 flame Left: Calculated SVF from line of sight Extinction data at 500nm. Middle: LII data from Long group at Yale. Right: Computed SVF from Smooke group at Yale. All data sets shown are for the



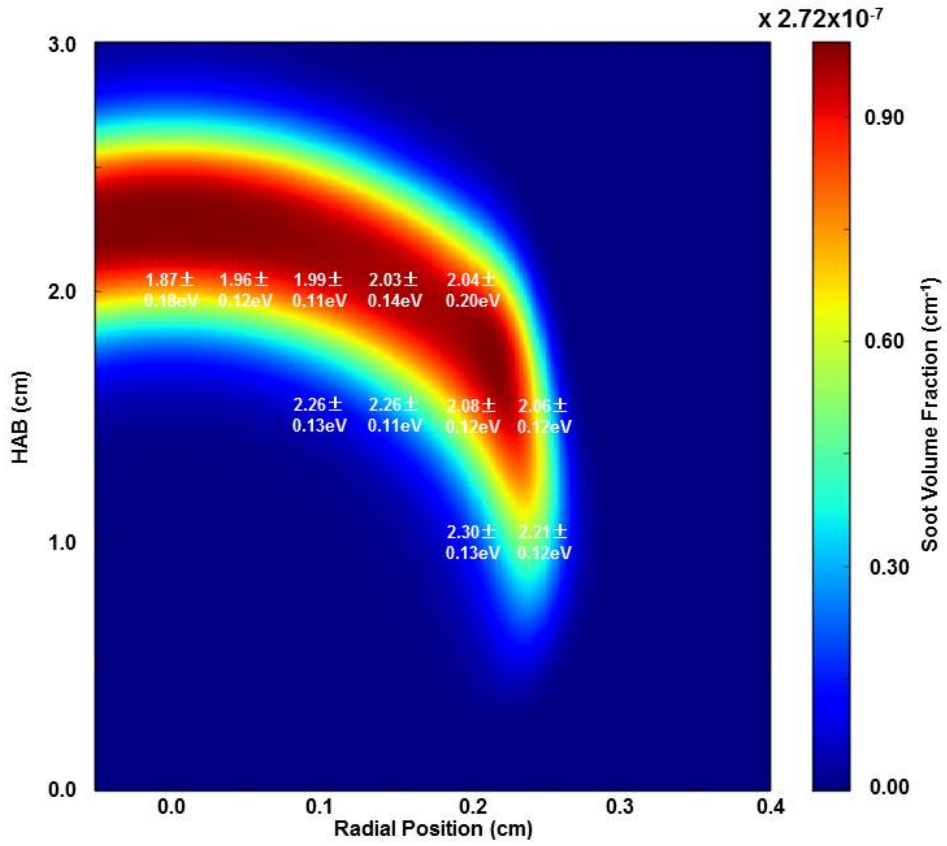
Supplemental Figure 2: 40%-C_2H_4/60%-N_2 flame. Left: Calculated SVF from line of sight Extinction data at 500nm. Middle: LII data from Long group at Yale. Right: Computed SVF from Smooke group at Yale.



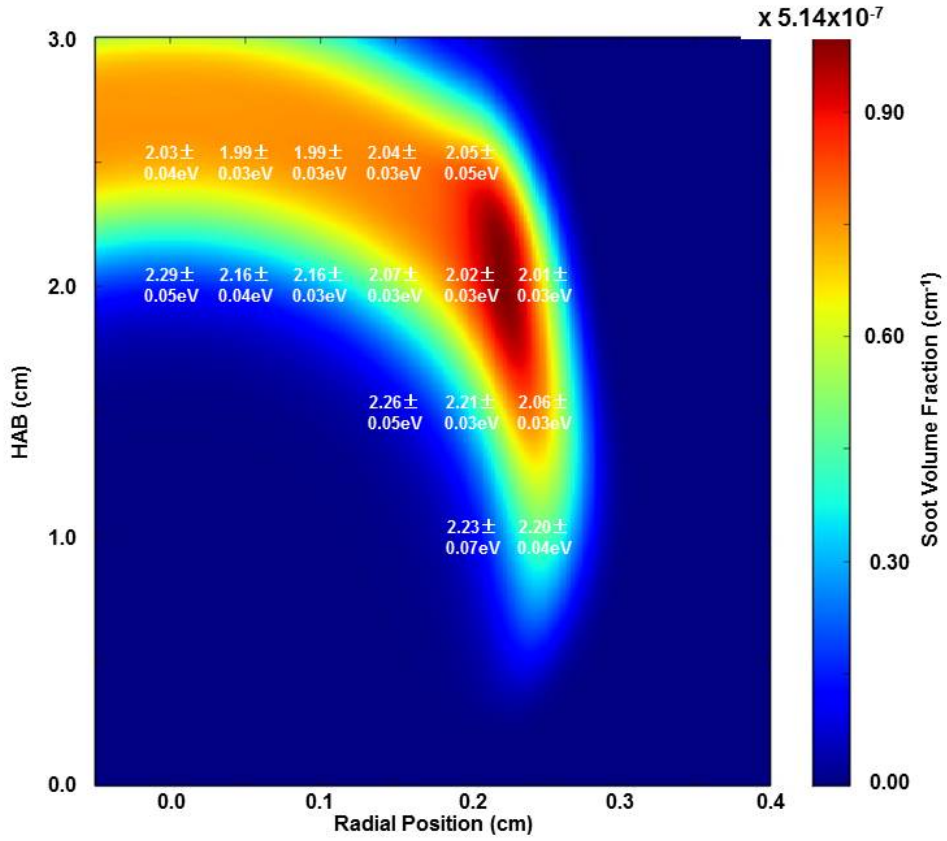
Supplemental Figure 3: 60%-C_2H_4/40%-N_2 flame Left: Calculated SVF from line of sight Extinction data at 500nm. Middle: LII data from Long group at Yale. Right: Computed SVF from Smooke group at Yale.



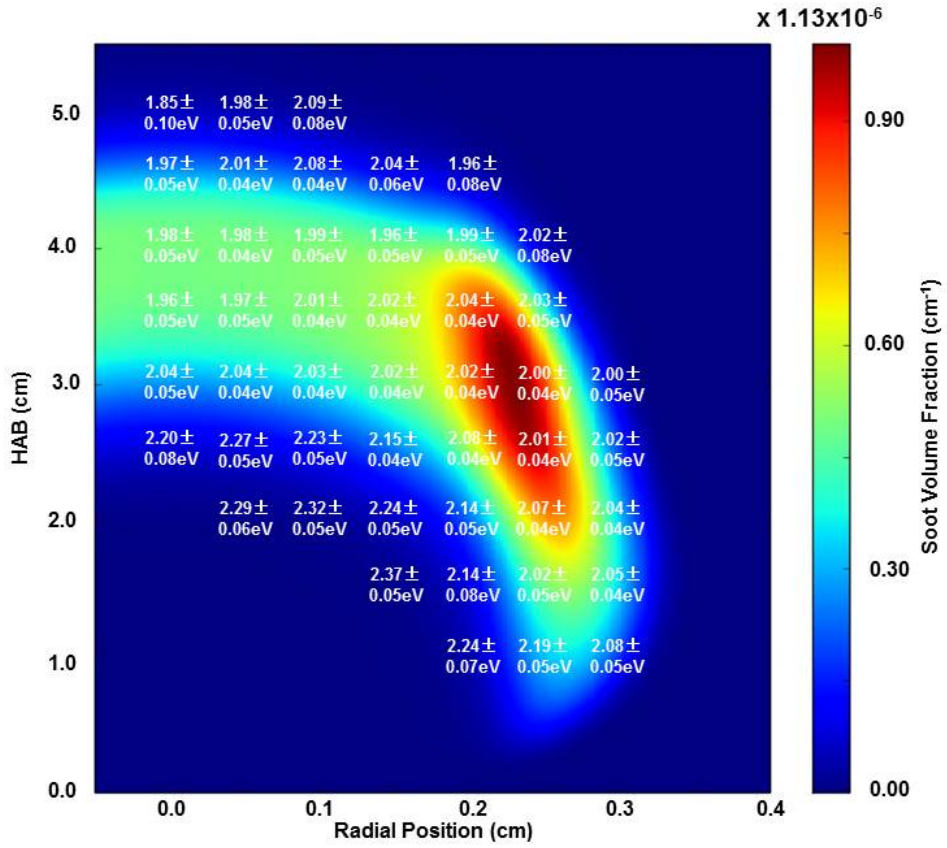
Supplemental Figure 4: 80%-C_2H_4/20%-N_2 flame Left: Calculated SVF from line of sight Extinction data at 500nm. Middle: LII data from Long group at Yale. Right: Computed SVF from Smooke group at Yale.



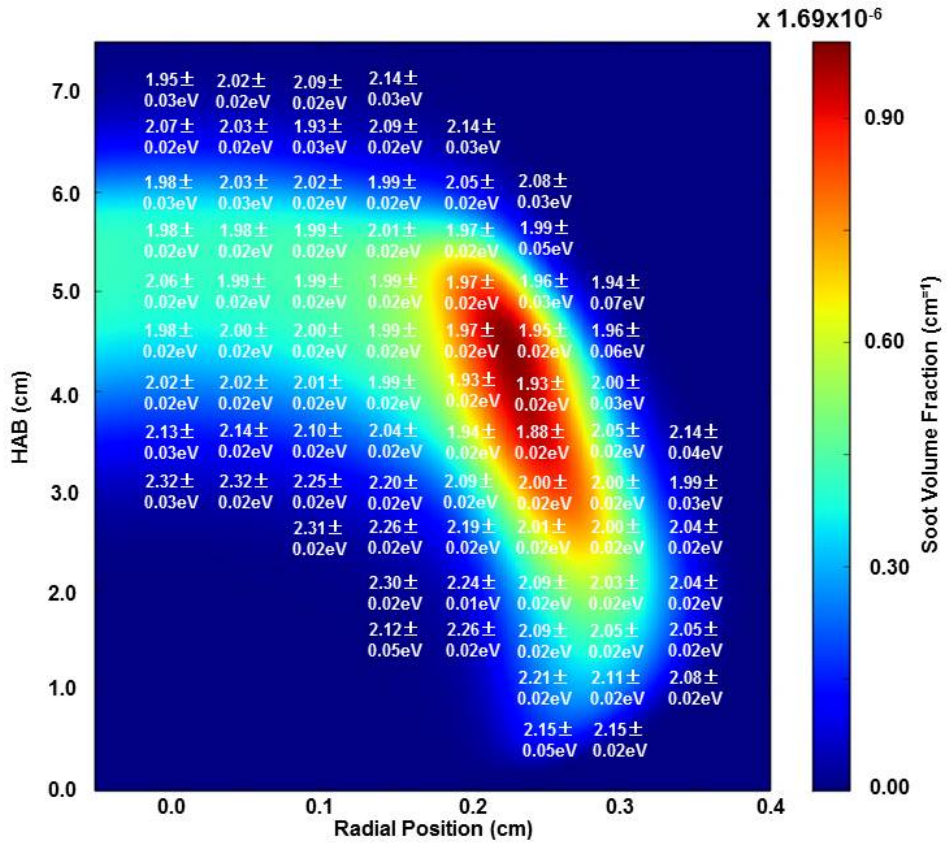
Supplemental Figure 5: Experimentally determined OBG overlaid on contour plots of soot volume fraction calculated by the Smooke group at Yale for the 32%-C_2H_4/68%-N_2 flame



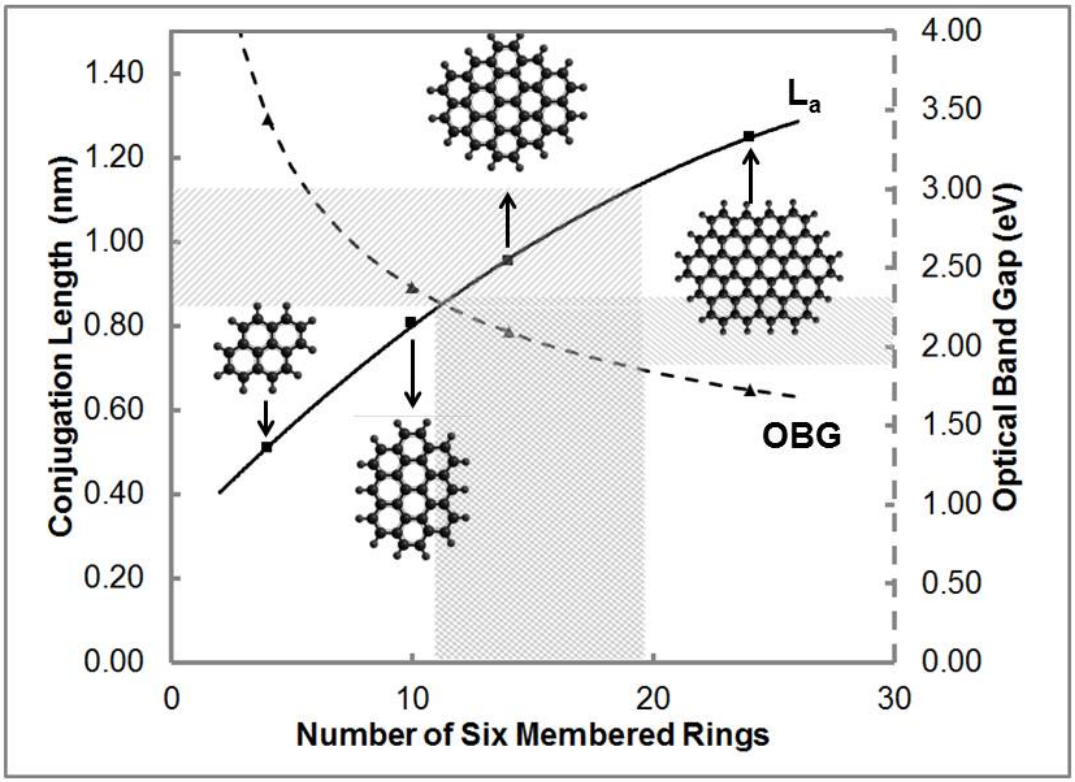
Supplemental Figure 6: Experimentally determined OBG overlaid on contour plots of soot volume fraction calculated by the Smooke group at Yale for the 40%-C_2H_4/60%-N_2 flame



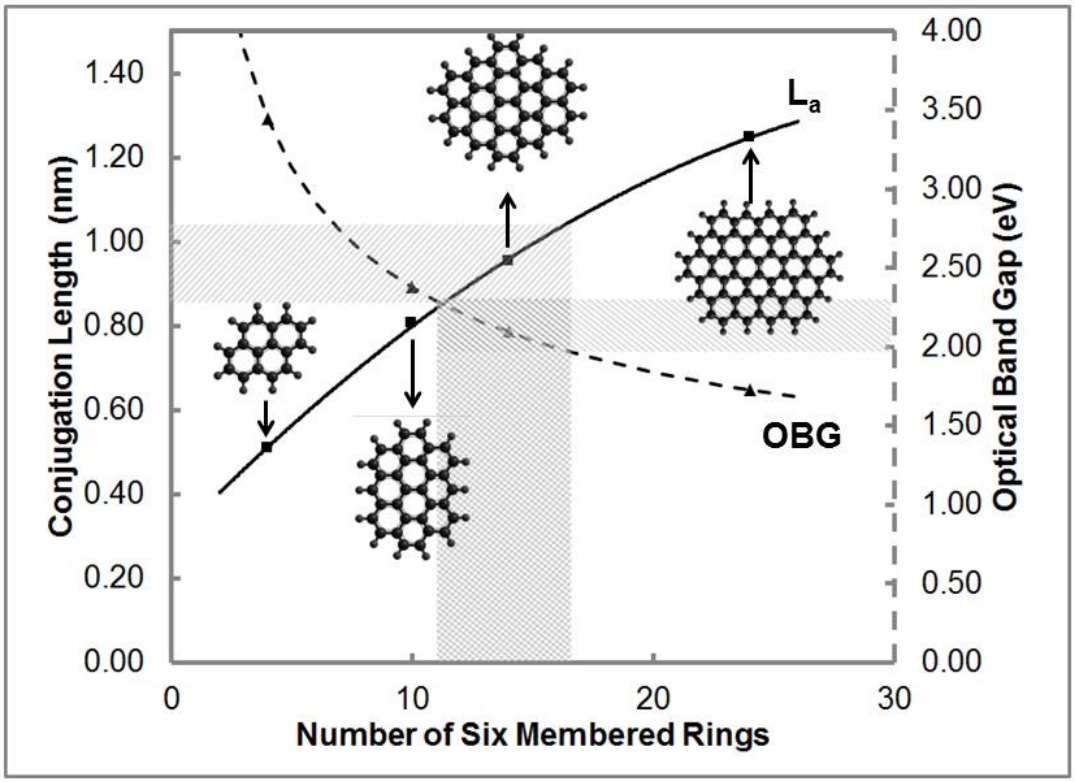
Supplemental Figure 7: Experimentally determined OBG overlaid on contour plots of soot volume fraction calculated by the Smooke group at Yale for the 60%-C_2H_4/40%-N_2 flame



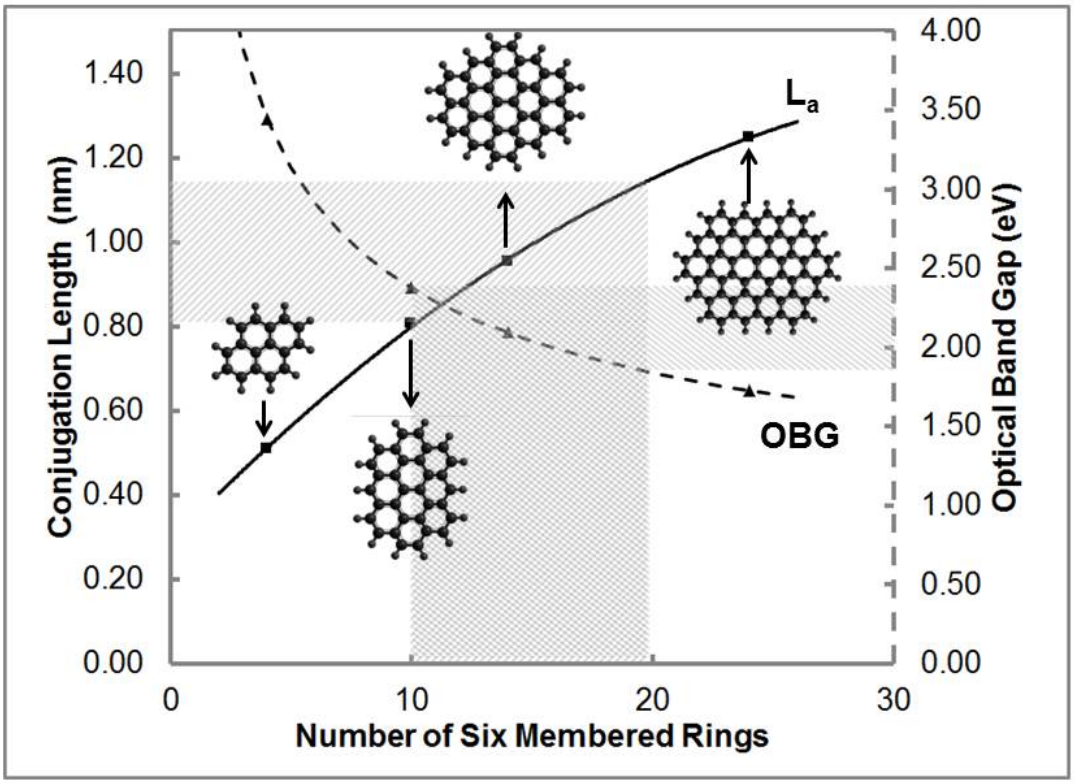
Supplemental Figure 8: Experimentally determined OBG overlaid on contour plots of soot volume fraction calculated by the Smooke group at Yale for the 80%-C_2H_4/20%-N_2 flame



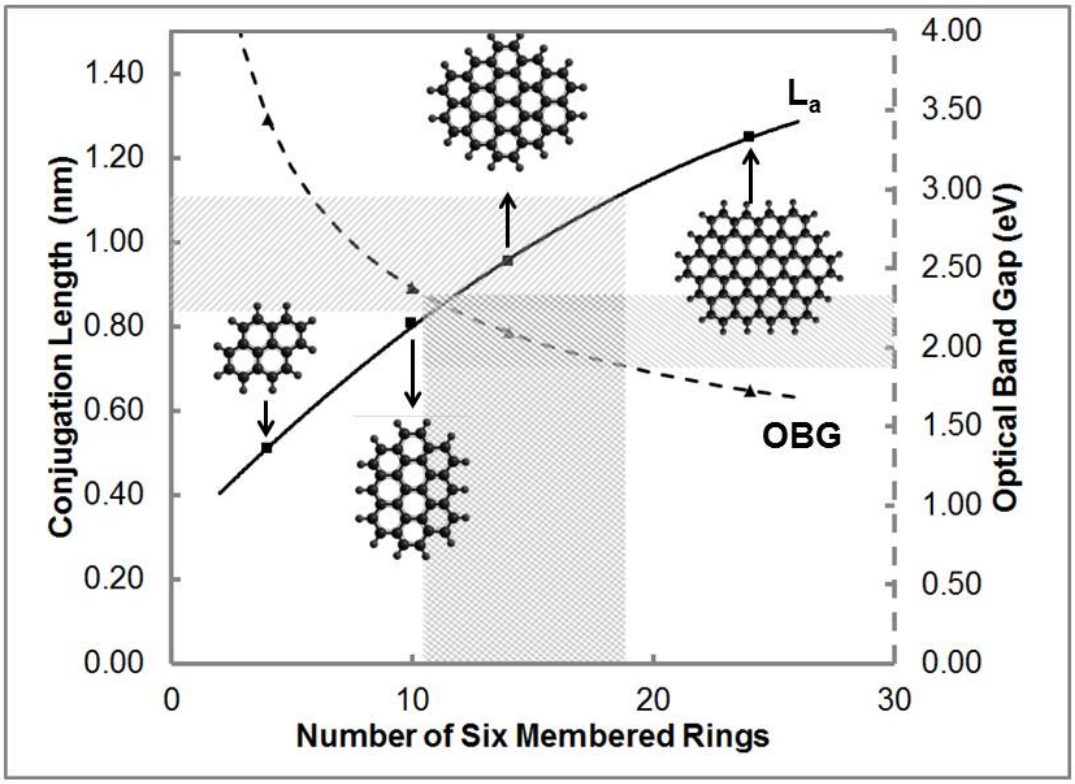
Supplemental Figure 9: Comparison between calculated HOMO-LUMO energy gaps (OBG) with number of aromatic rings and conjugation length. The dashed line and triangle show the relationship between OBG and number of rings. The solid line and squares show the relationship between conjugation length and number of rings. The grey bands depict how the range of OBG observed throughout the 32%-C_2H_4/68%-N_2 flame correlate to physical morphology parameters.



Supplemental Figure 10: Comparison between calculated HOMO-LUMO energy gaps (OBG) with number of aromatic rings and conjugation length. The dashed line and triangle show the relationship between OBG and number of rings. The solid line and squares show the relationship between conjugation length and number of rings. The grey bands depict how the range of OBG observed throughout the 40%-C_2H_4/60%-N_2 flame correlate to physical morphology parameters.



Supplemental Figure 11: Comparison between calculated HOMO-LUMO energy gaps (OBG) with number of aromatic rings and conjugation length. The dashed line and triangle show the relationship between OBG and number of rings. The solid line and squares show the relationship between conjugation length and number of rings. The grey bands depict how the range of OBG observed throughout the 60%-C_2H_4/40%-N_2 flame correlate to physical morphology parameters.



Supplementary Figure 12: Comparison between calculated HOMO-LUMO energy gaps (OBG) with number of aromatic rings and conjugation length. The dashed line and triangle show the relationship between OBG and number of rings. The solid line and squares show the relationship between conjugation length and number of rings. The grey bands depict how the range of OBG observed throughout the 80%-C_2H_4/20%-N_2 flame correlate to physical morphology parameters.