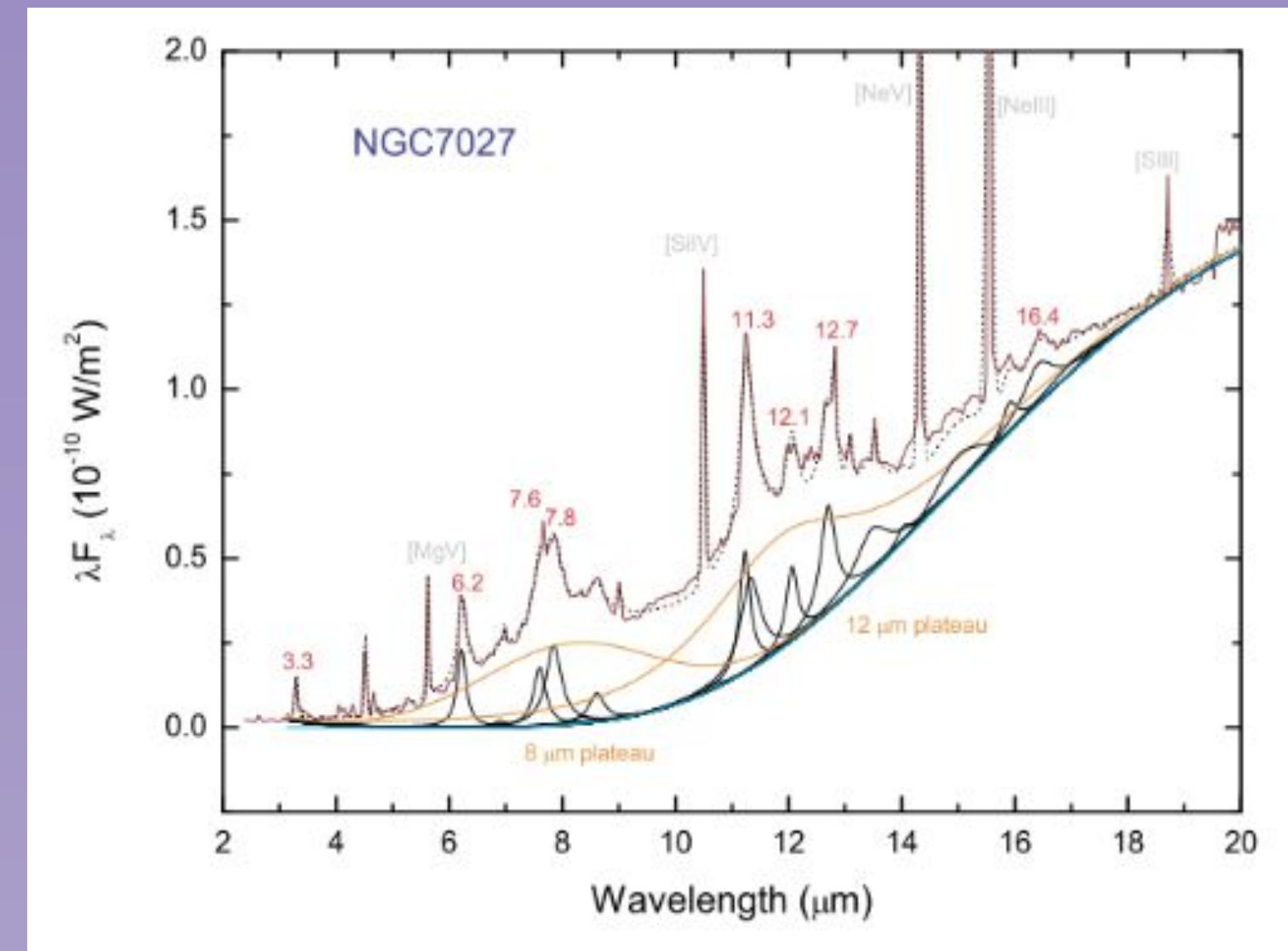


BACKGROUND

- Unidentified Infrared Emission (UIE) bands are seen NGC 7027, a planetary nebula
- I studied proposed Polycyclic Aromatic Hydrocarbons (PAHs) with 5 different heteroatom substitutions
- Previous work showed that 3- and 4-ring systems produced some of the UIE peaks



METHODS

- Computational Program: Gaussian 09
- Visualization Program: GaussView
- B3LYP exchange-correlation functional/6-31G(d,p) basis set
- IR frequencies scaled to better match experimental results

RESULTS

Molecule (# of rings)	Oxygen	Sulfur	Silicon	Phosphorus	Nitrogen
Benzene (1)	1.157 (1)	0.882 (1)	0.481 (1-H)	-0.185 (1)	-0.0174 (1)
Naphthalene (2)	0.715 (2)	0.608 (2)	0.211 (2-H2)	-0.178 (1)	-0.0682 (2)
Anthracene (3)	0.174 (1)	0.244 (4)	-0.199 (4-H2)	-0.191 (1)	-0.123 (4)
Tetracene (4)	-0.0797 (4)	0.000189 (4)	-0.454 (4-H2)	-0.197 (1)	-0.122 (4)

Table 1: Formation energies of the most stable configurations of each heteroatom substitution type and structure type. Numbers in parentheses relate to the position of the heteroatom substitution. (see Figure 1)

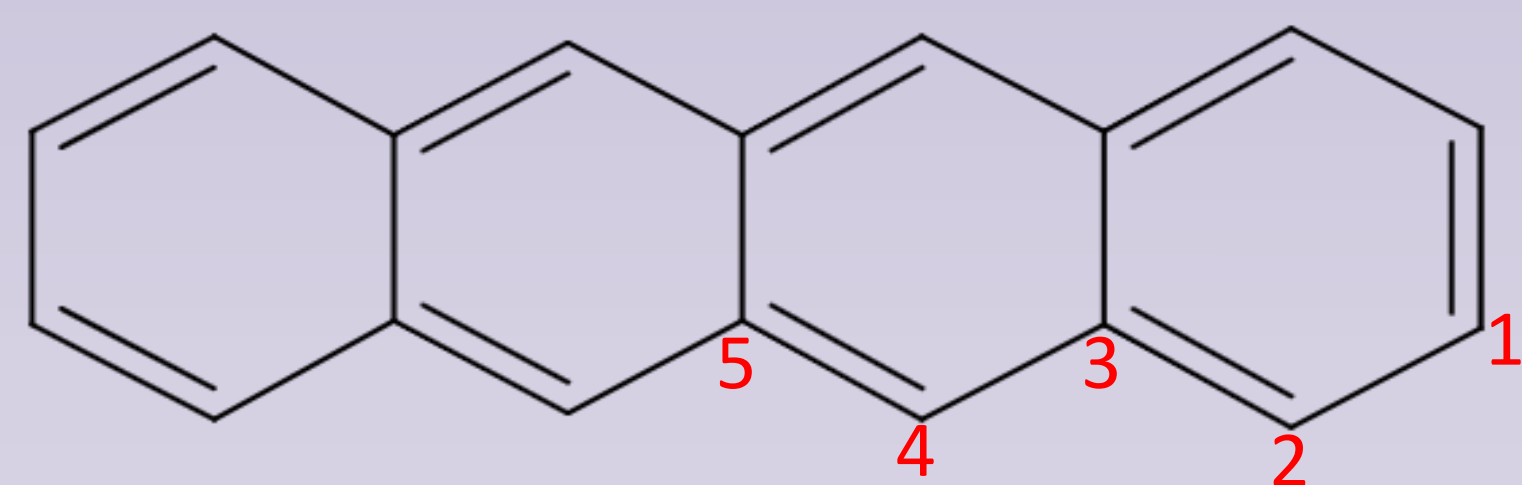


Figure 1: Tetracene with heteroatom substitution positions labeled.

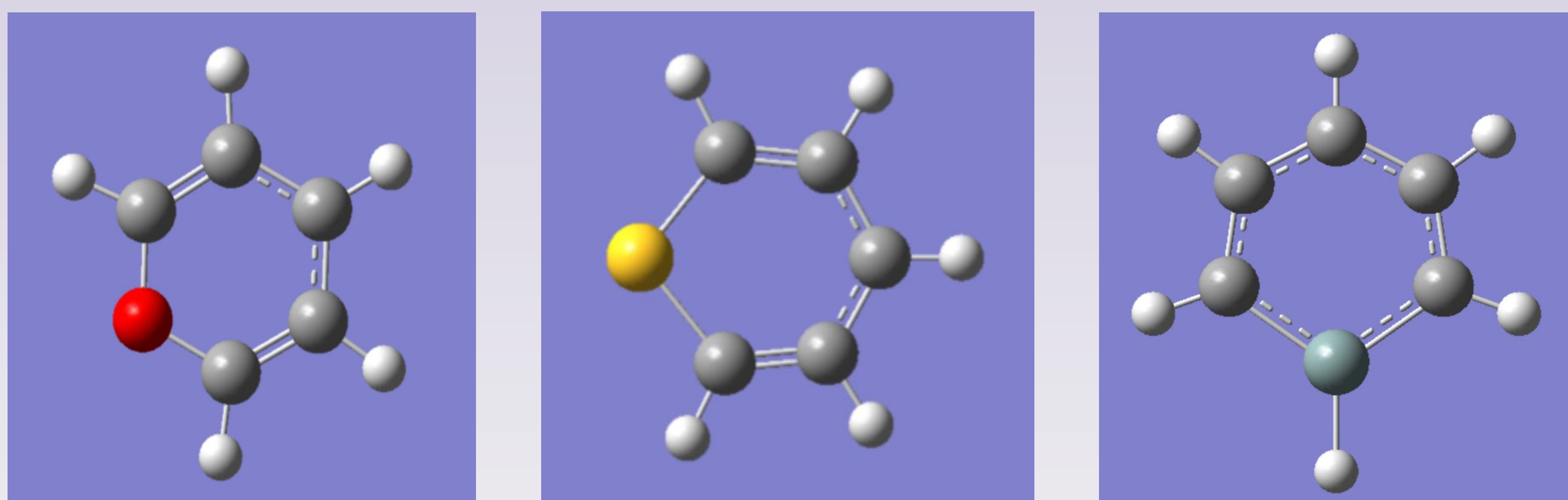


Figure 2: Three benzene structures with different heteroatom substitutions. Leftmost image has an oxygen substitution, middle image has a sulfur substitution, and rightmost image has a silicon substitution along with an additional hydrogen attached to the silicon.

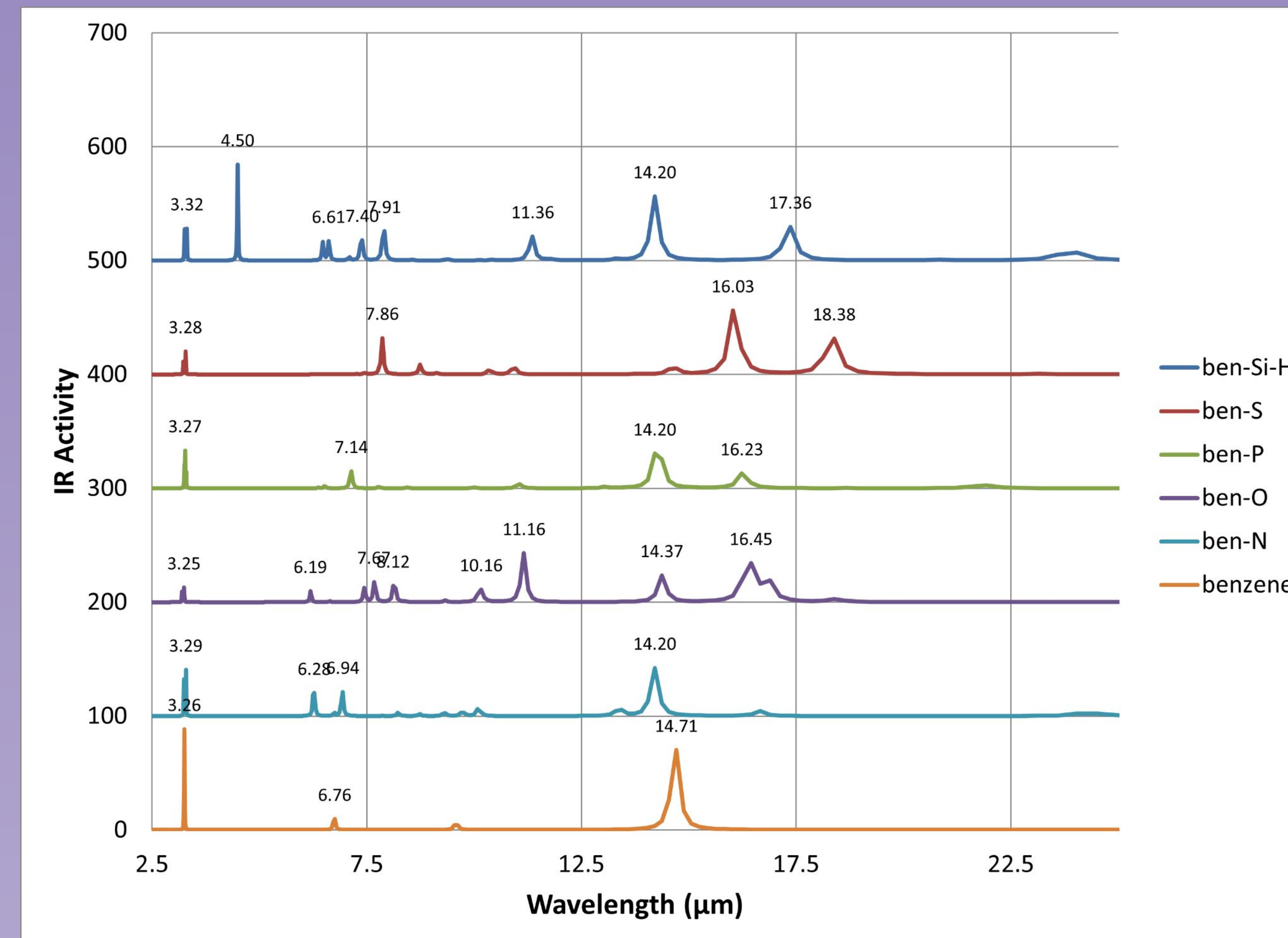


Figure 3: Comparison of IR spectra for heteroatom substitution in benzene.

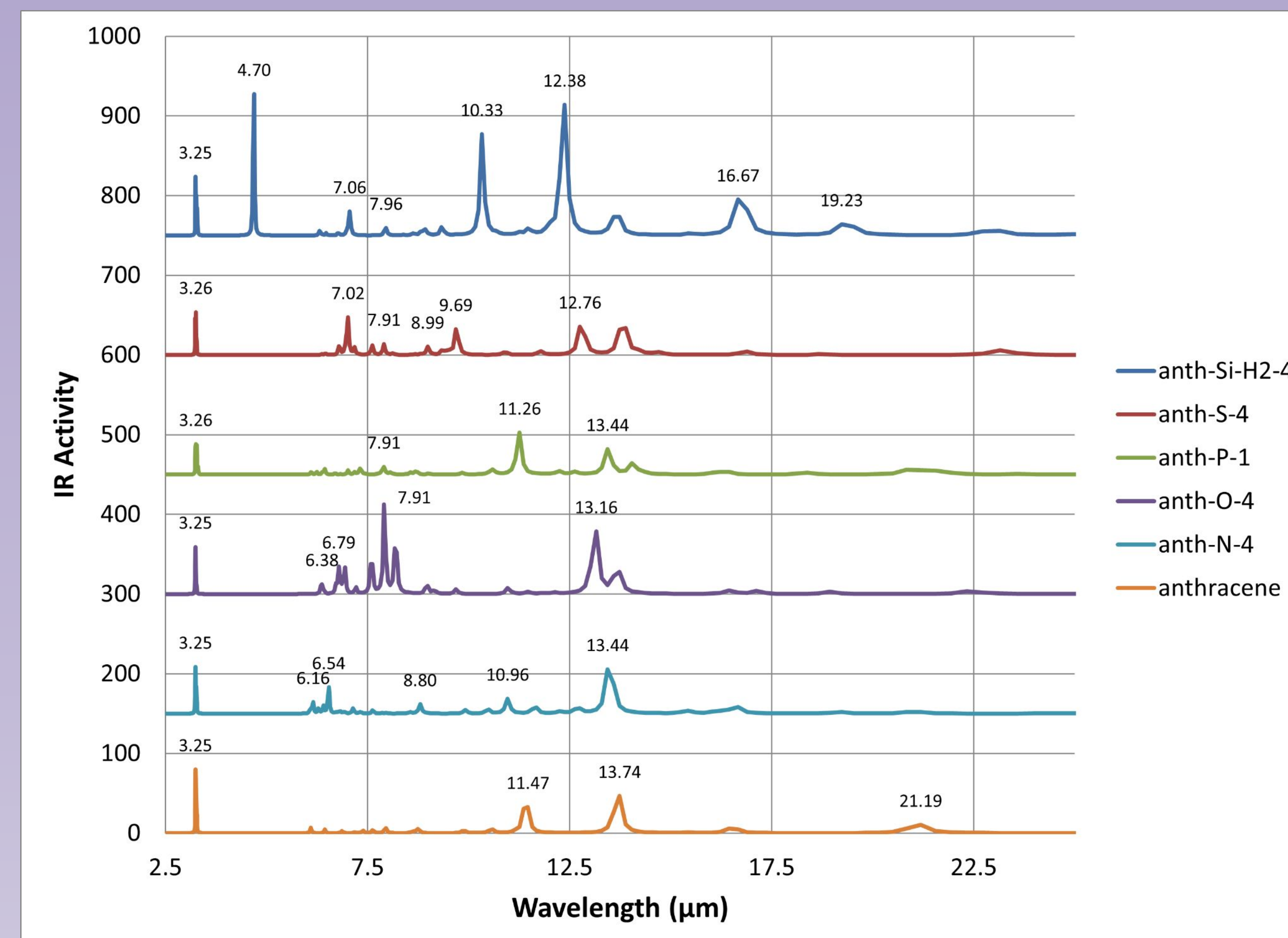


Figure 5: Comparison of IR spectra for heteroatom substitution in anthracene.

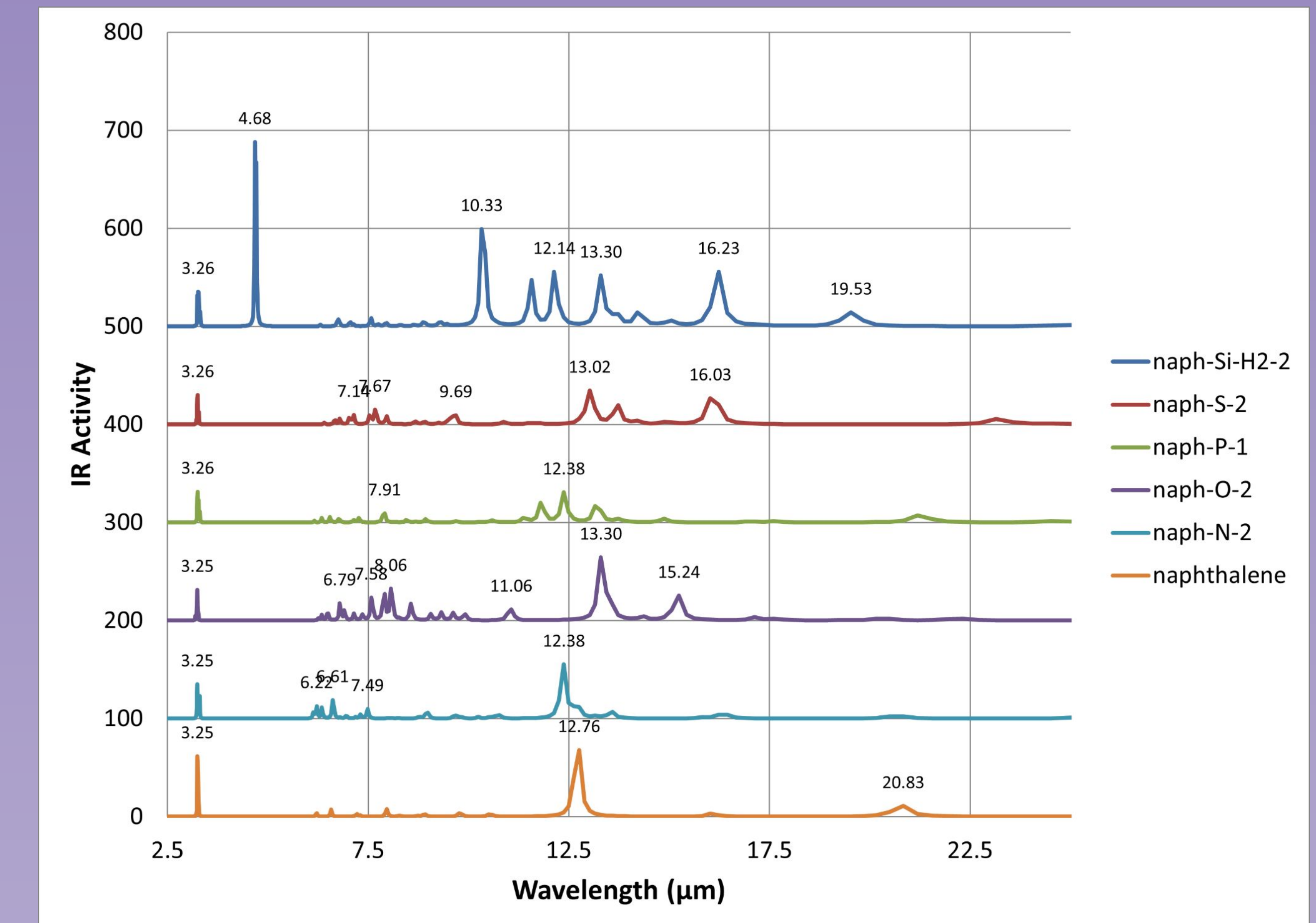


Figure 4: Comparison of IR spectra for heteroatom substitution in naphthalene.

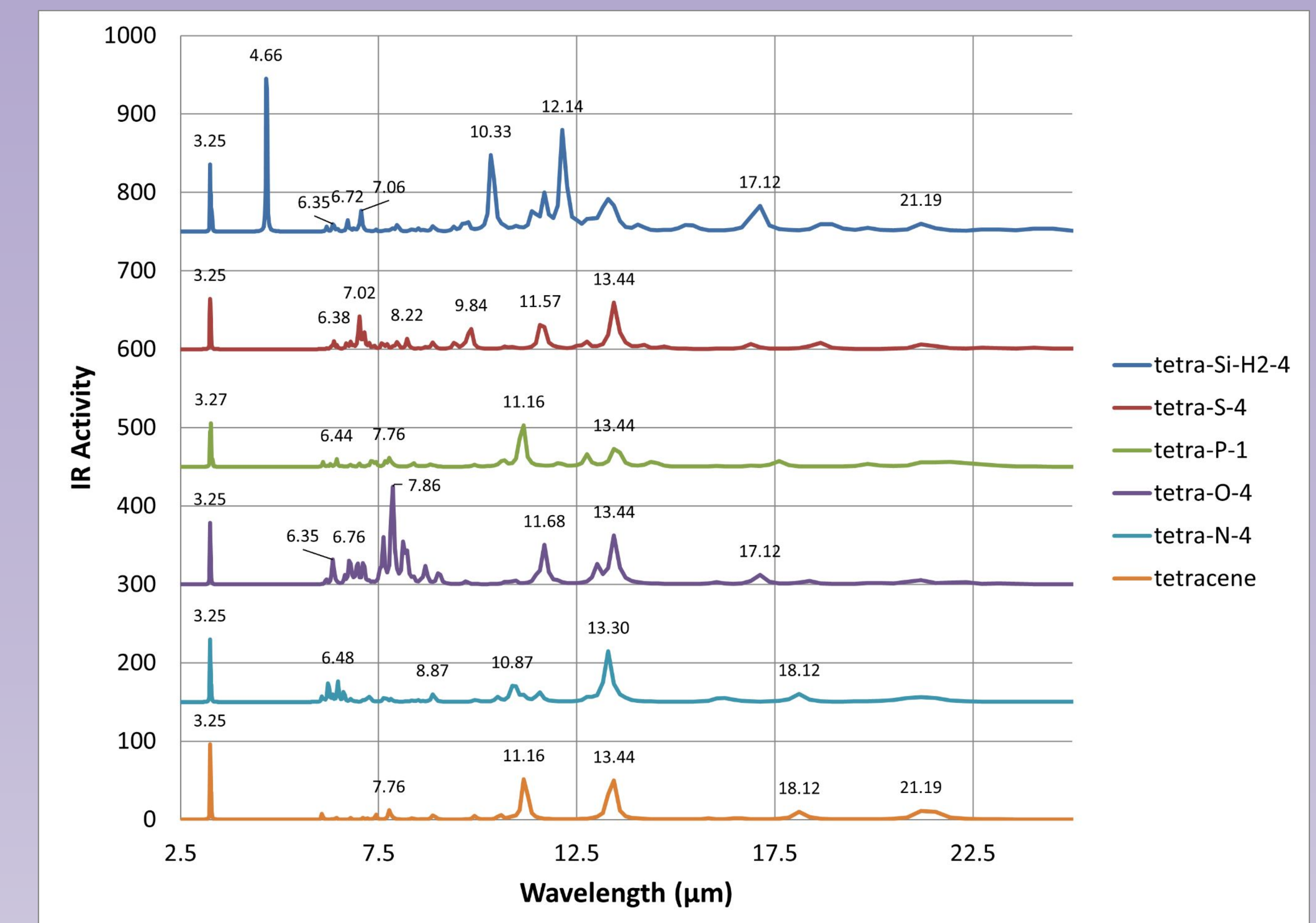


Figure 6: Comparison of IR spectra for heteroatom substitution in tetracene.

CONCLUSIONS

- For anthracene and tetracene, most substitutions prefer the 4 substitution location.
- The formation energy decreases as the number of rings increases.
- The addition of oxygen creates a region of C-H bending modes from 6.0 - 8.0 μm .
- The ~ 4.5 , 10.3, and 12.4 μm peaks in the Si-H and Si-H2 lines are unique to Si-H bonds
 - Eliminates Si-H as a candidate
- Oxygen substitution is a promising candidate.
 - Tetracene with an oxygen substitution has peaks that closely match 4 different UIE peaks (6.2, 7.6-7.8, 11.3, and 12.7)

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