

## Supporting information

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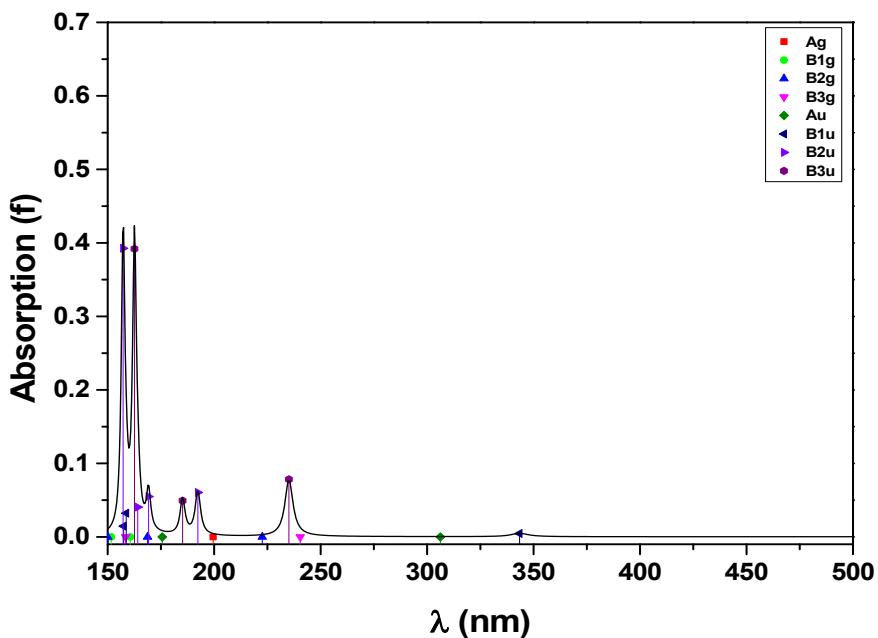
**Part 1.** The absorption spectrum of pyrazine.

**Part 2.** Molecular orbitals of complexes in different electronic transitions.

**Part 3.** The Raman spectra of pyrazine excited at the different incident lights.

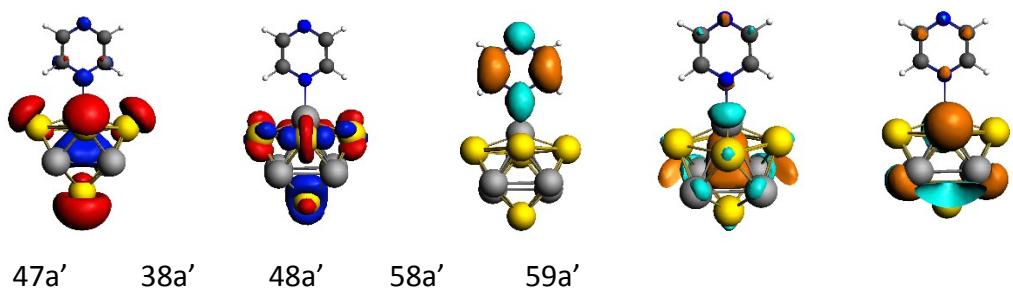
**Part 4.** Vibrational motions and frequencies of normal modes for pyrazine.

**Part 1.** The absorption spectrum of pyrazine.

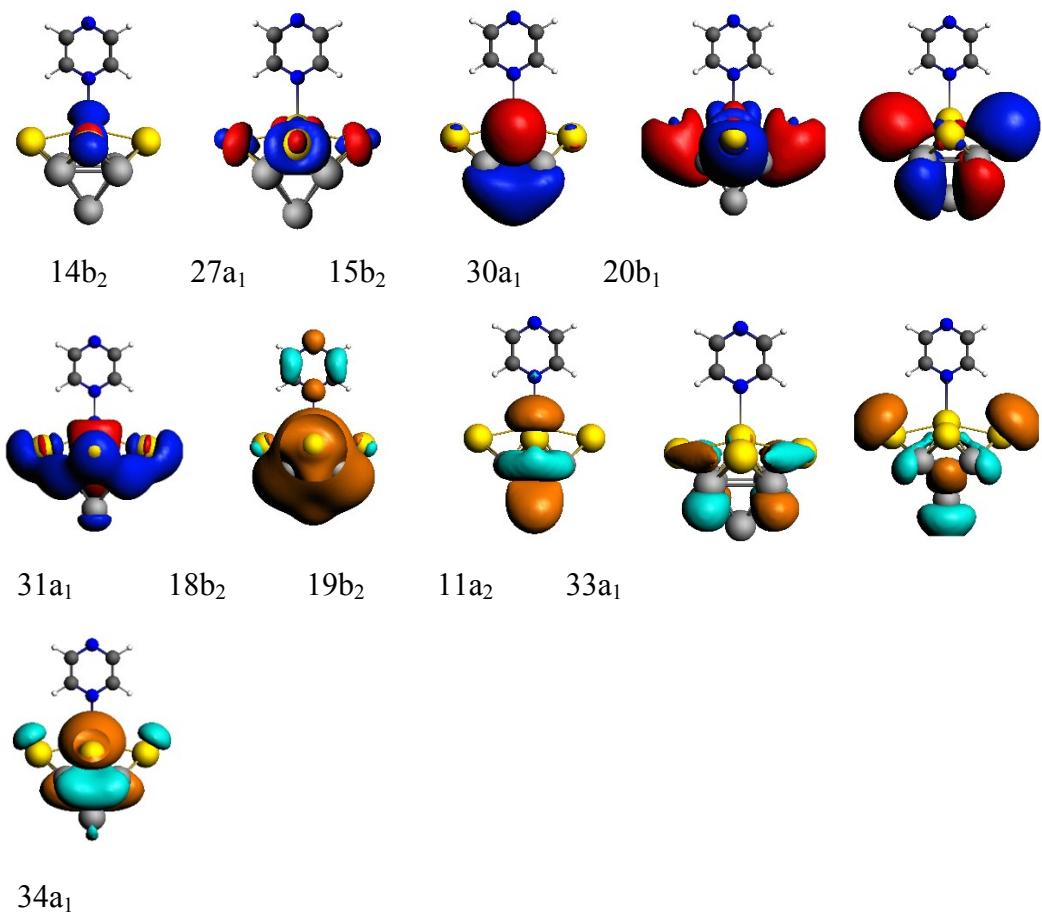


**Figure S1.** Electronic transitions of pyrazine. Absorption coefficients are given as the oscillator strength in a.u. Spectra have been broadened by a Lorentzian having a width of 0.1 eV.

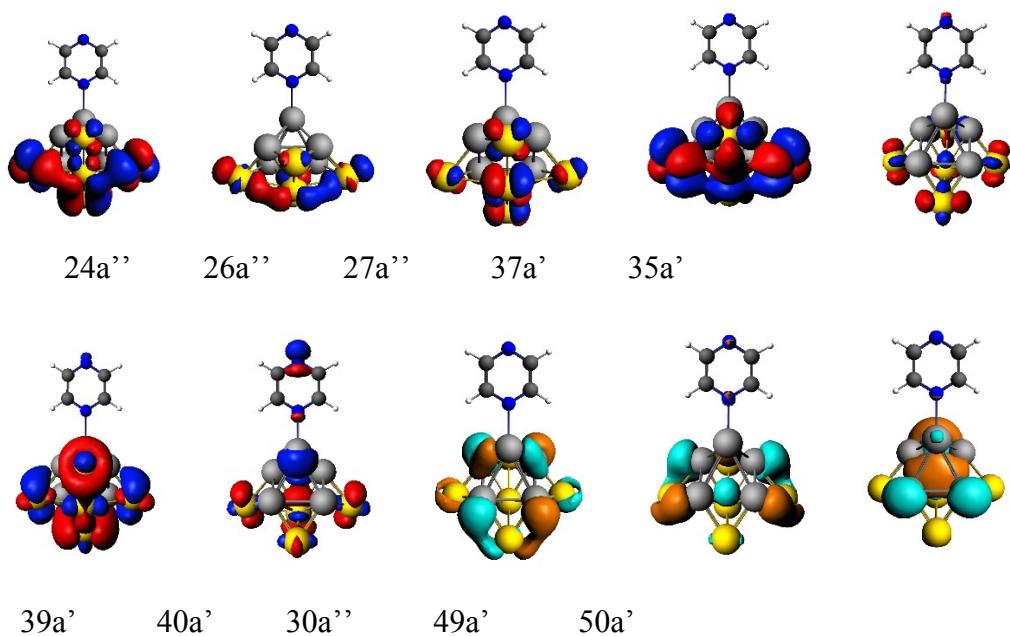
**Part 2.** Molecular orbitals of complexes in different electronic transitions.



**Figure S2.** Molecular orbitals of pyrazine-Al-Au<sub>5</sub>Al<sub>4</sub>-a complex in electronic transition at 277 nm.

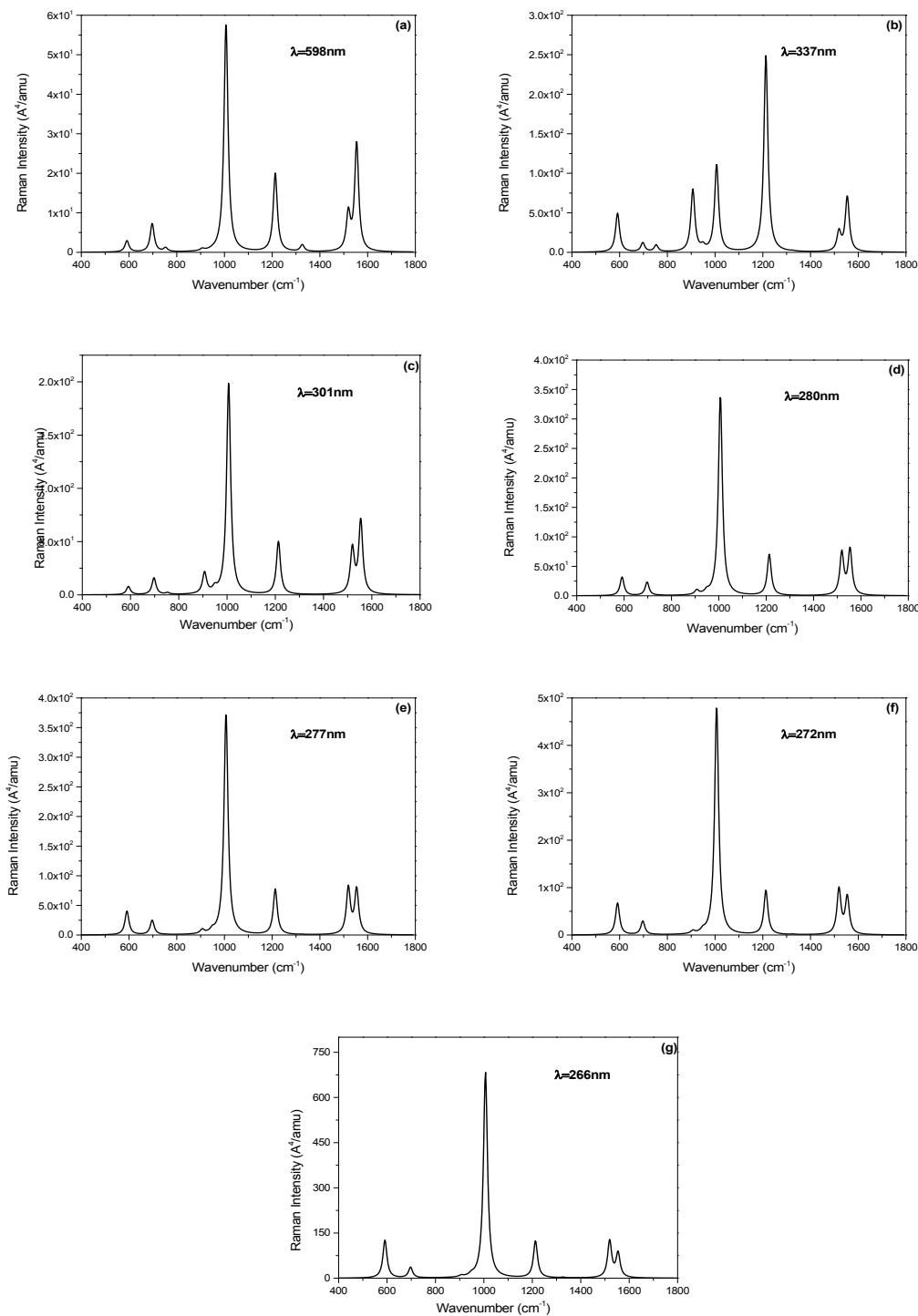


**Figure S3.** Molecular orbitals of pyrazine-Au-Au<sub>4</sub>Al<sub>5</sub>-b complex in electronic transitions at 337 and 266 nm.



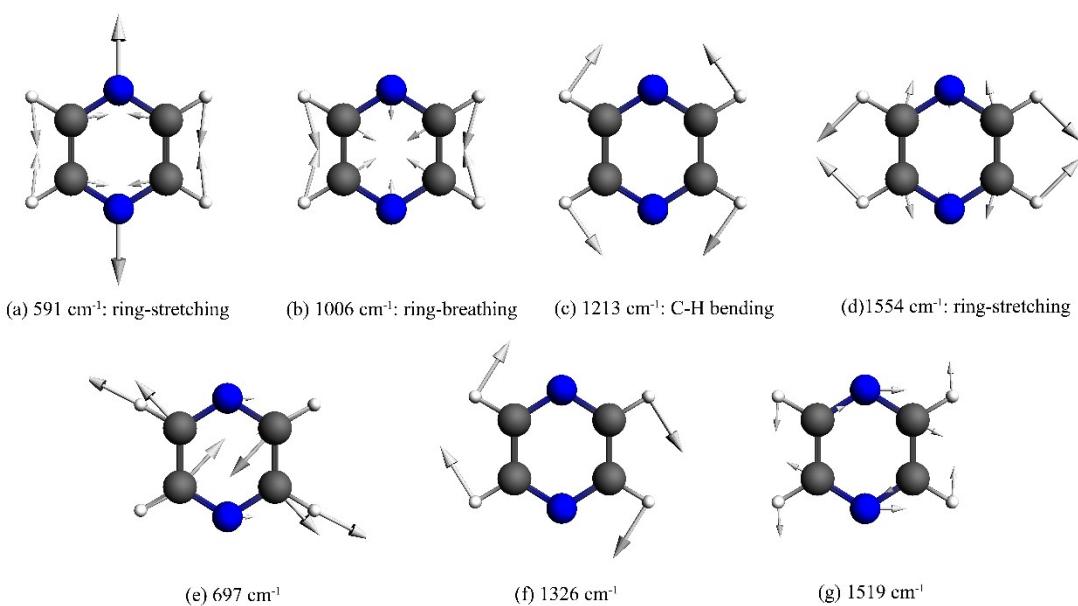
**Figure S4.** Molecular orbitals of pyrazine-Al-Au<sub>5</sub>Al<sub>4</sub>-b complex in electronic transitions at 301 and 272 nm.

**Part 3.** The Raman spectra of pyrazine excited at the different incident lights.



**Figure S5.** The Raman spectra of pyrazine excited at the different incident lights. (a) 598 nm, (b) 337 nm, (c) 301 nm, (d) 280 nm, (e) 277 nm, (f) 272 nm, (g) 266 nm. Spectra were broadened by a Lorentzian having a width of  $20\text{ cm}^{-1}$ .

**Part 4.** Vibrational motions and frequencies of normal modes for pyrazine. .



**Figure S6.** Vibrational motions and frequencies of normal modes for pyrazine.