

- Gauche-Anh-B3LYP-D3-6-31+g(d)
- Anti-Anh-B3LYP-D3-6-31+g(d)
- Gauche-Anh-B3LYP-6-31+g(d)
- Anti-Anh-B3LYP-6-31+g(d)
- Experimental

Combination Bands  
+ Overtones

Normalized Intensity

500 1000 1500 2000 2500 3000  
Wavenumbers (cm<sup>-1</sup>)

