Rotational Spectra and Structural Determination of HCCNCS

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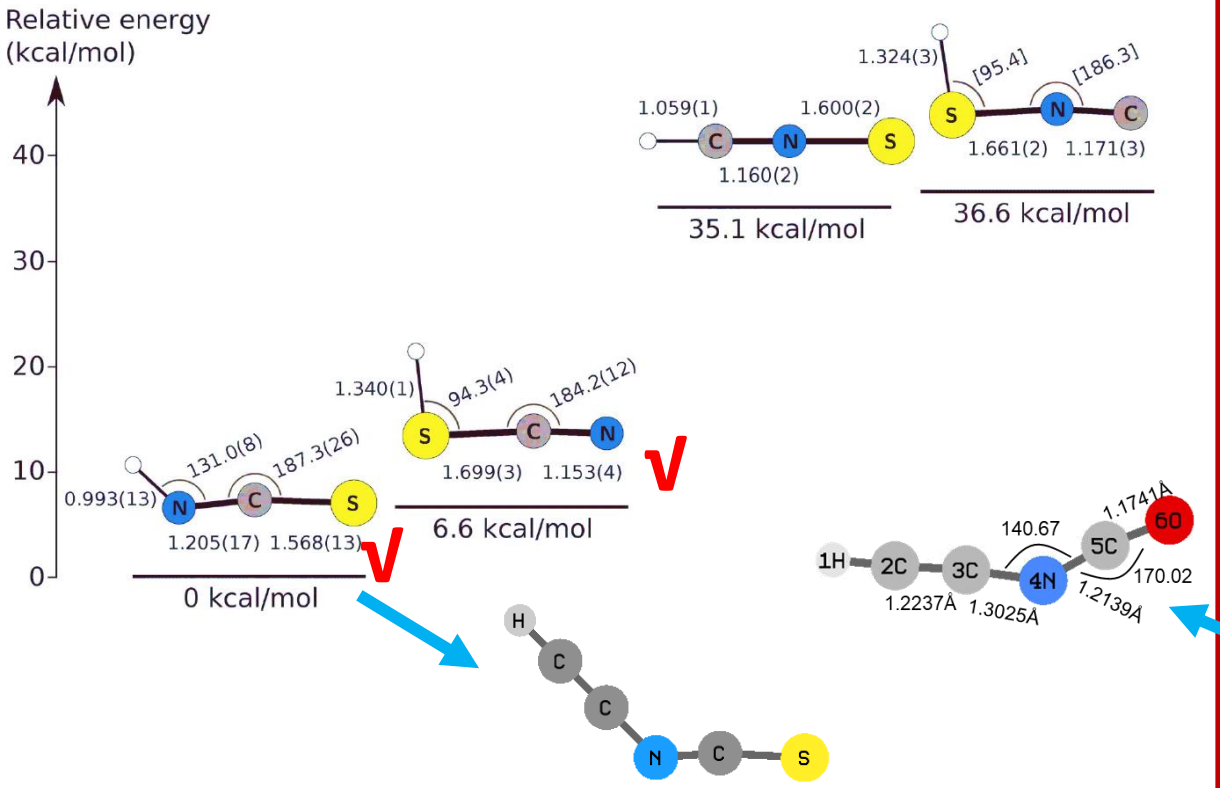
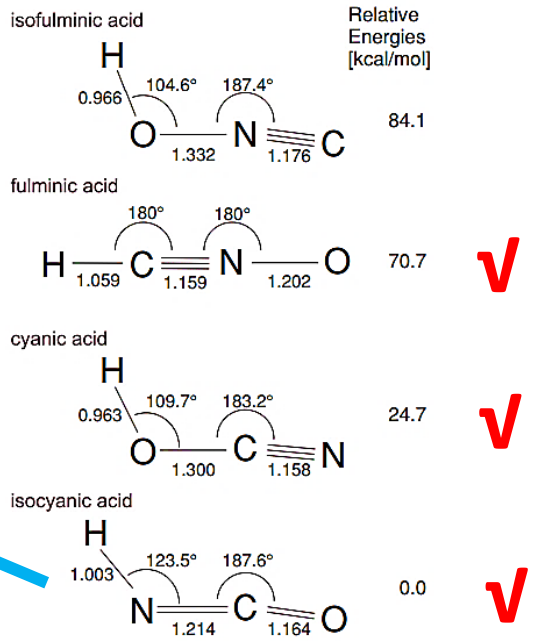
[H, N, C, S] Family



*Energies are calculated at the ae-CCSD(T)/cc-pwCVQZ and corrected for zero-point vibrational contributions calculated at the fc-CCSD(T)/cc-PV(Q+d)Z level.

Similarly, [H, N C, O] family



*Energies are calculated at the CCSD(T)/cc-pCV5Z

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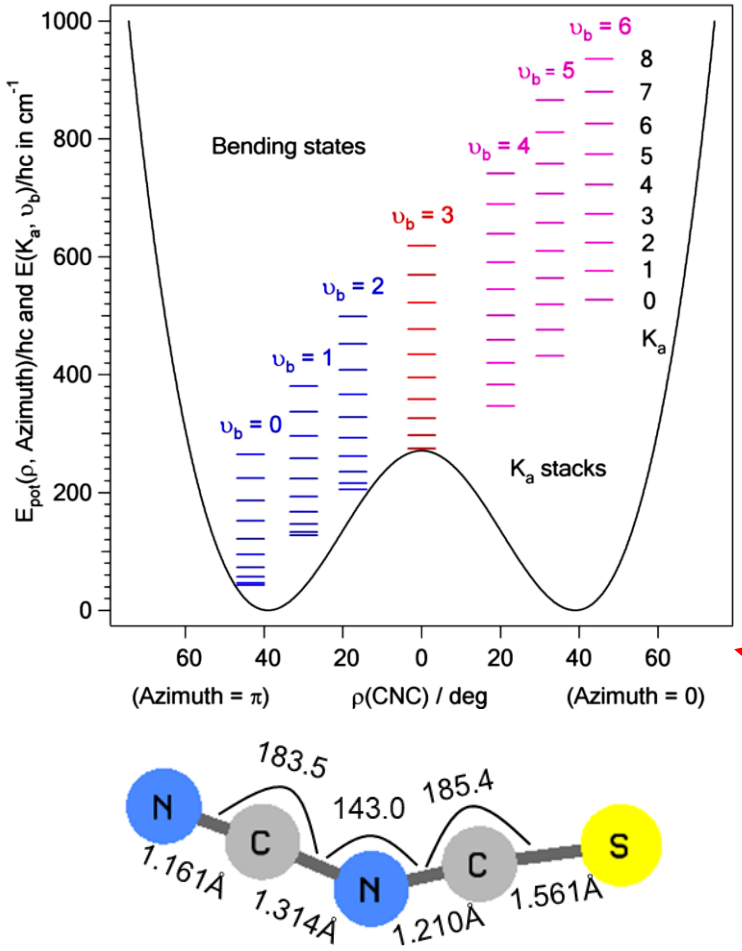
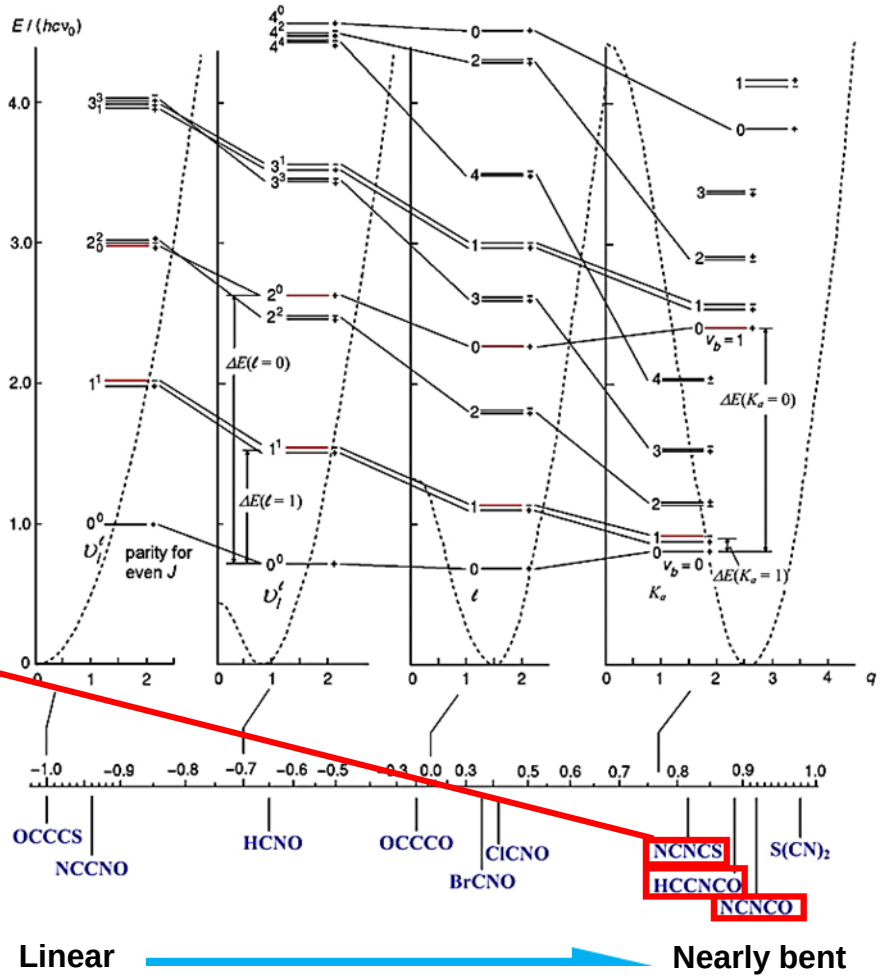
Quantum Monodromy





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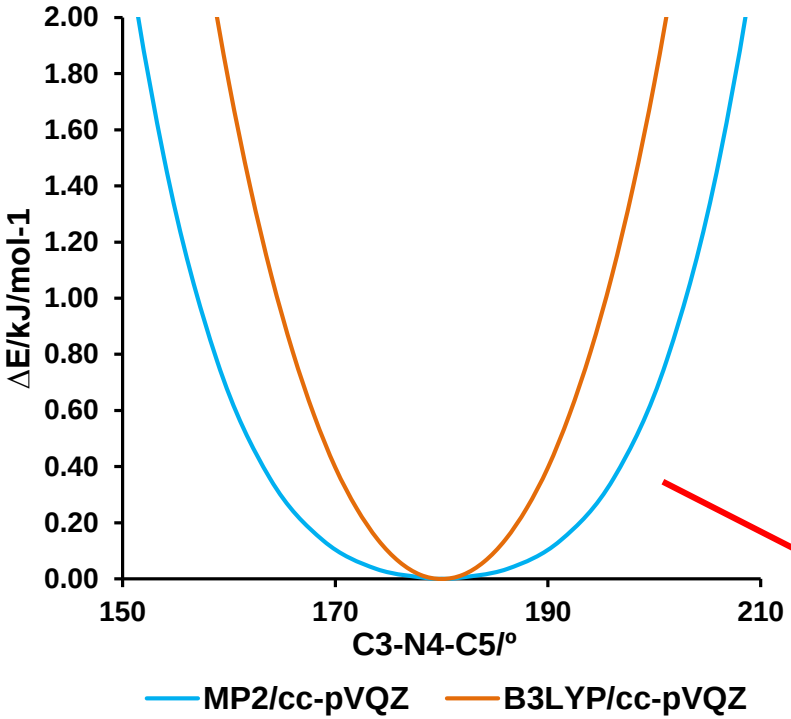
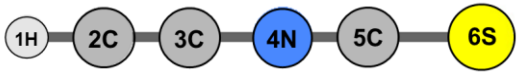
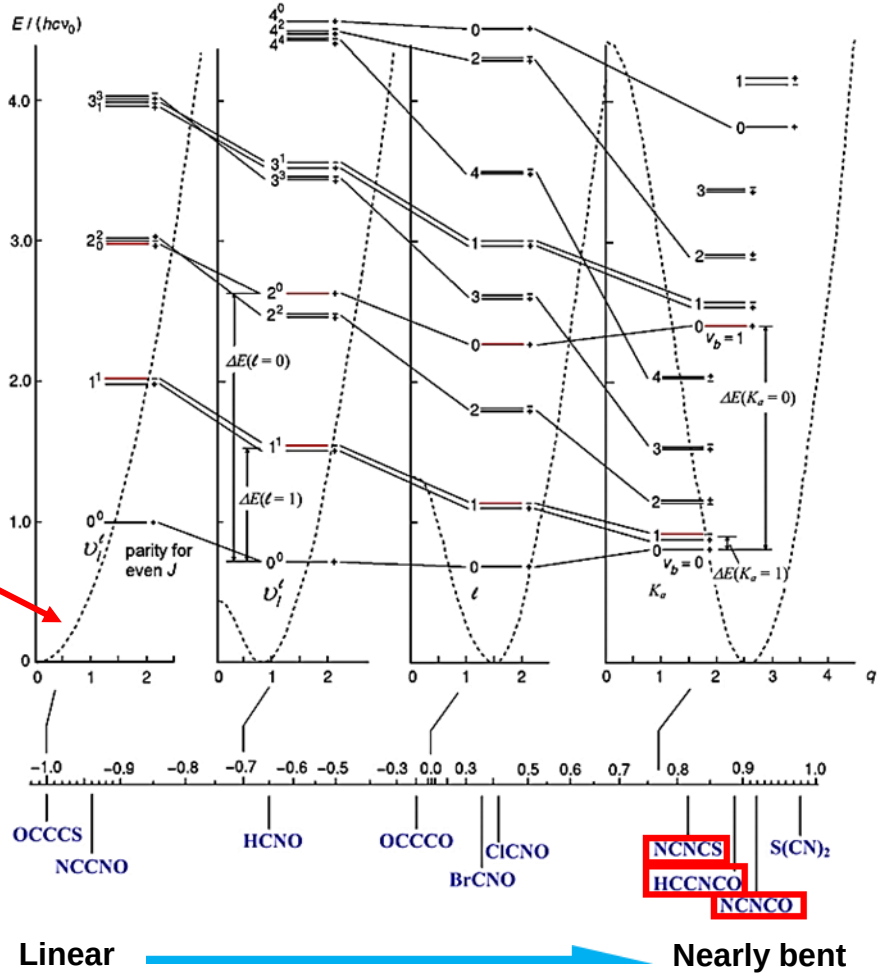
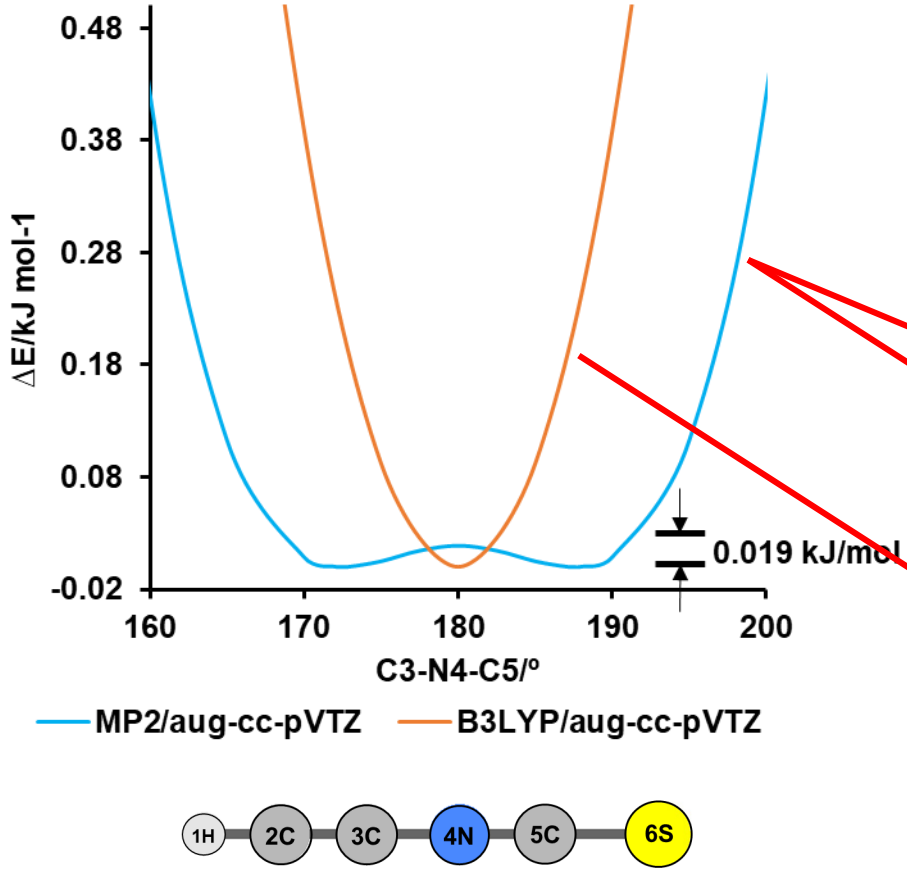
Potential Energy Curve

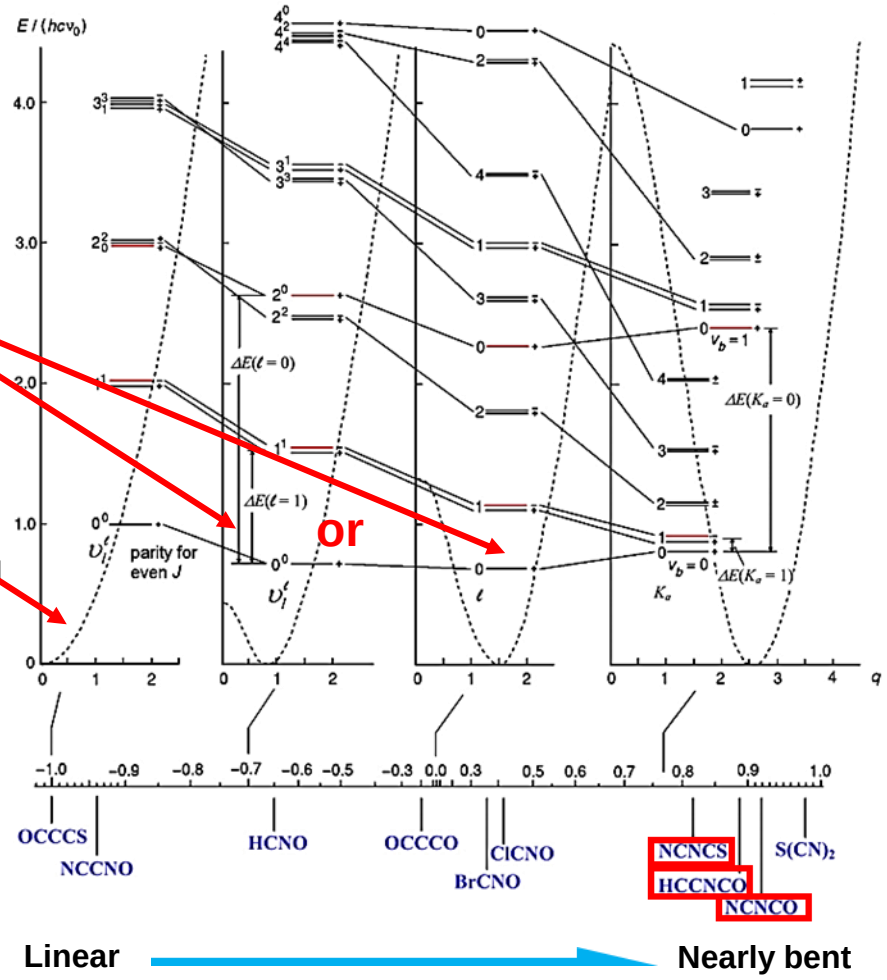




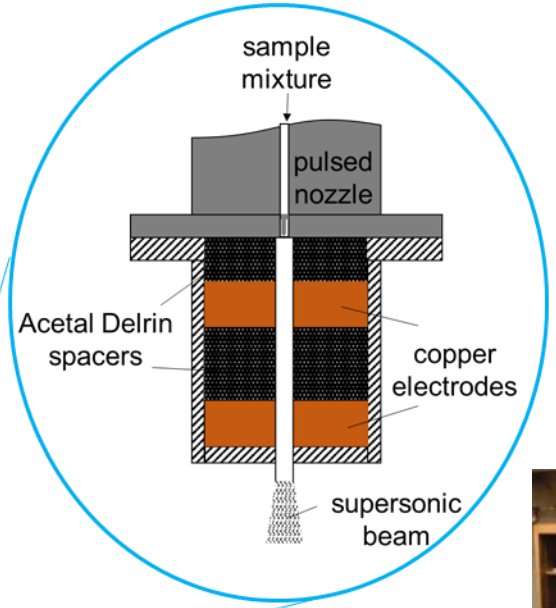


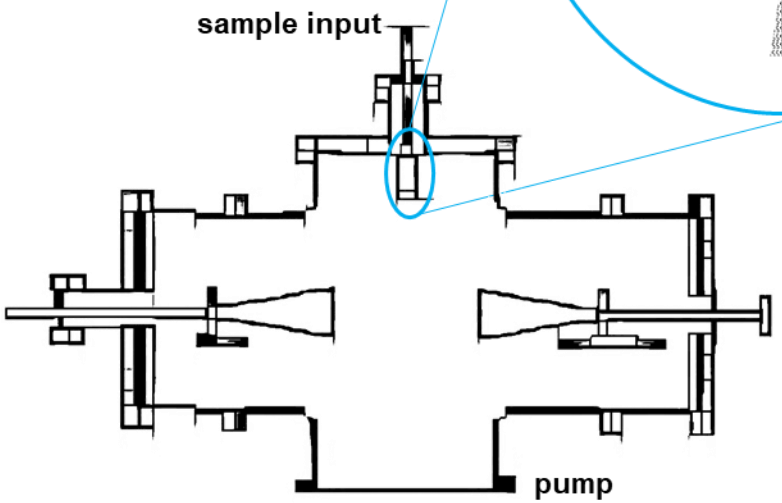
Potential Energy Curve





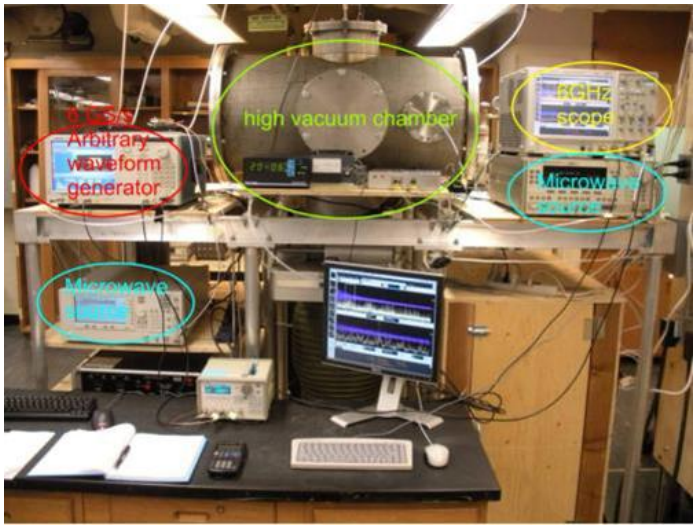
cp FTMW Spectrometer





Experimental conditions:

1. 1% **acetylene** diluted with **Ne** + Bubbler (**CH_3NCS, 37℃**)
2. Acetal Delrin spacers: 5 mm and 8 mm thick; **copper electrodes**: 5 mm thick; channel diameter: 2.5mm
3. High voltage: **700 V**.
4. Expansion duration: 750 µs
   Chirp duration: 4 µs
5. Bandwidth: **1000 MHz**
6. **25 FIDs * 16 µs/FID**



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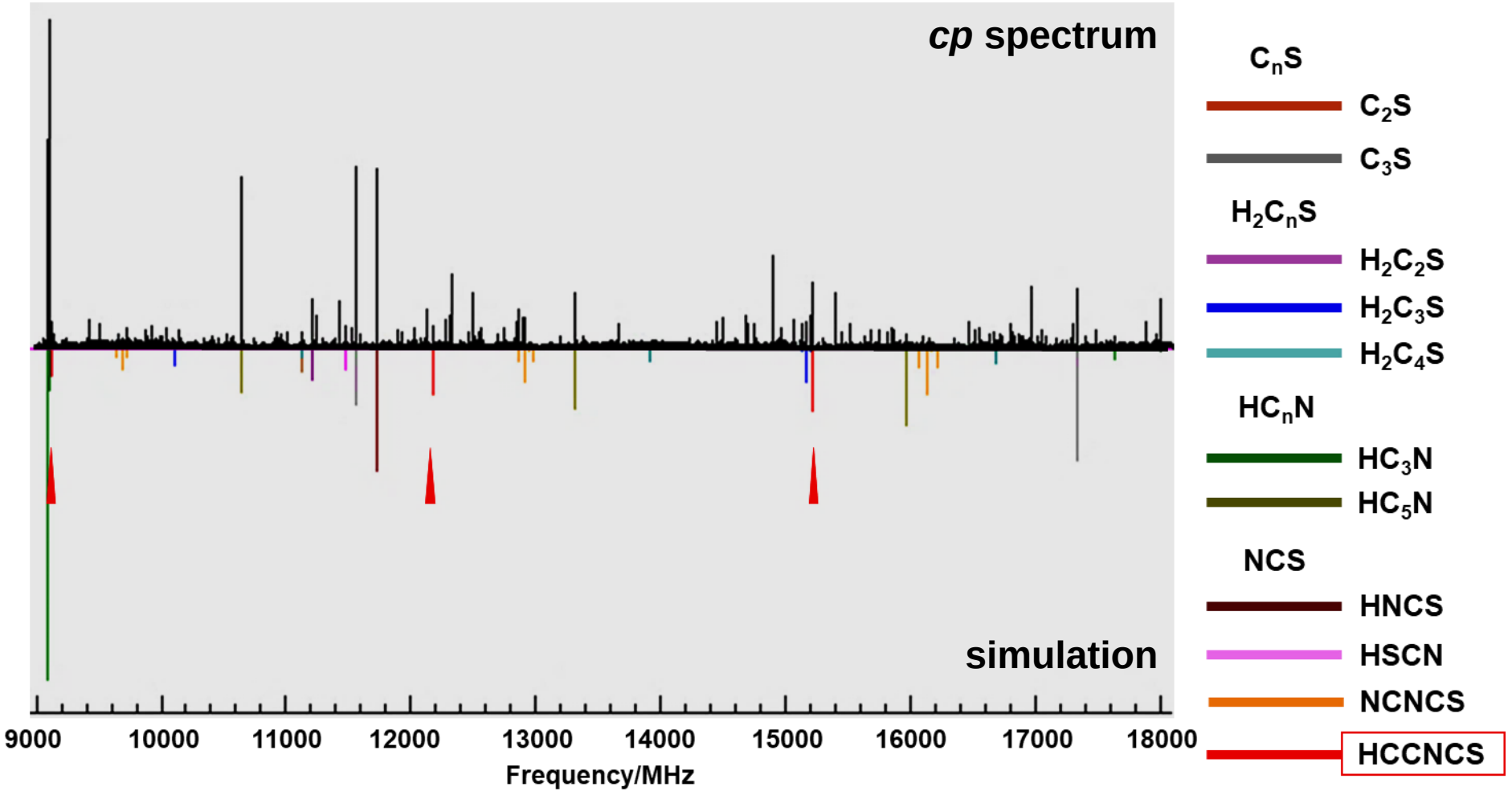
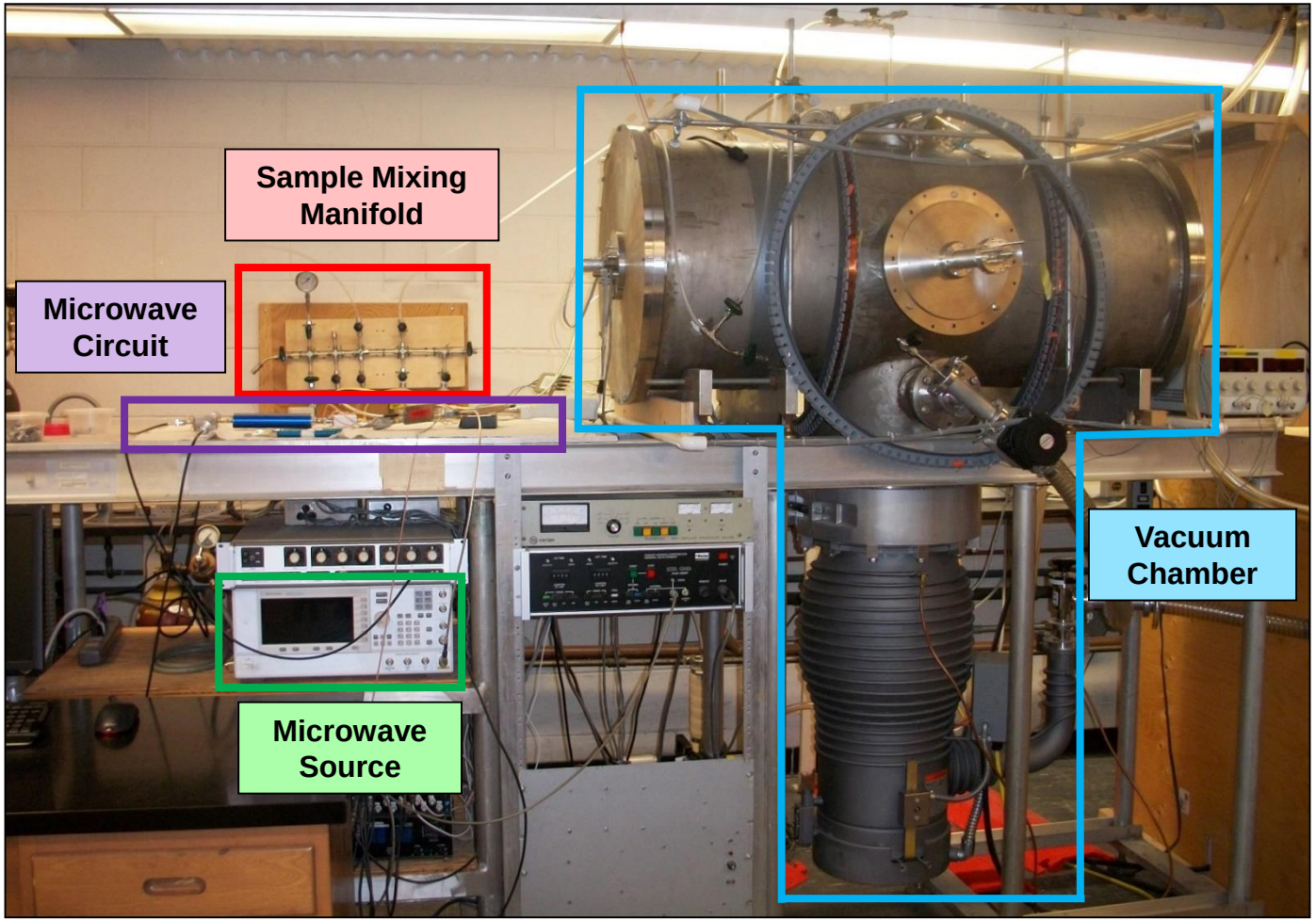
Broadband Microwave Spectra



Balle Flygare FTMW Spectrometer



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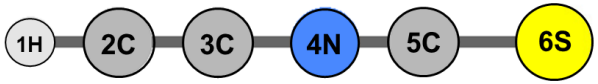
Hyperfine Structure: ^{14}N

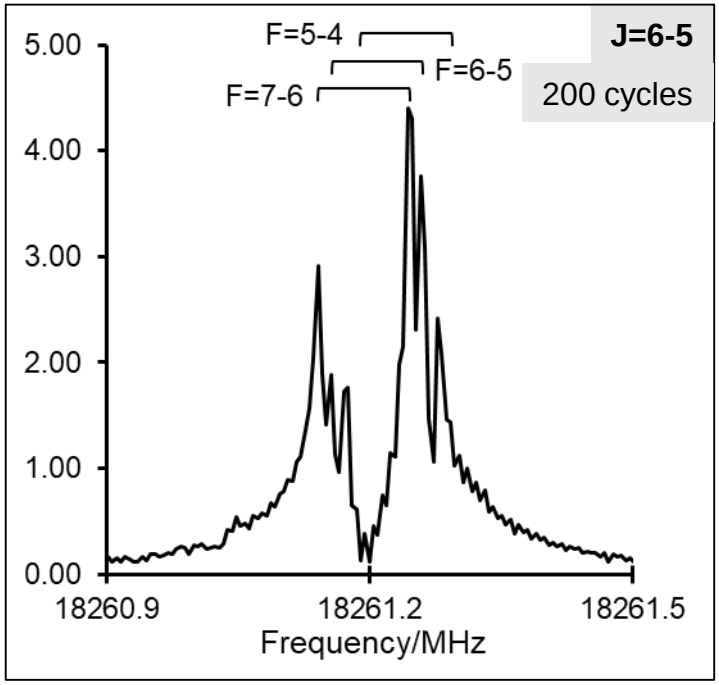


Parent- **29** lines

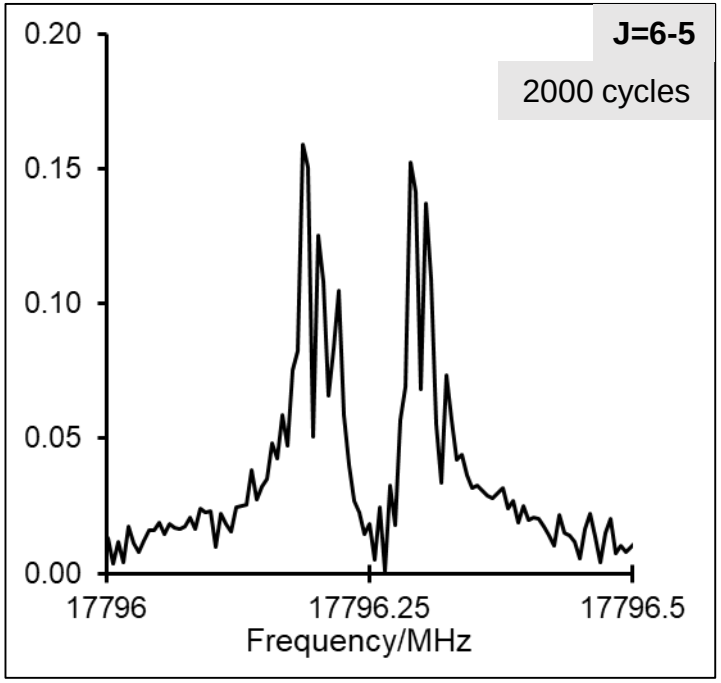
Isotopic lines

5 **7** **8** **16**

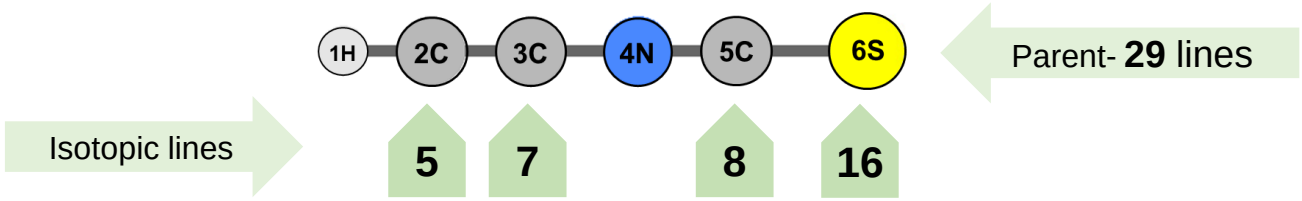
HCCNCS-parent



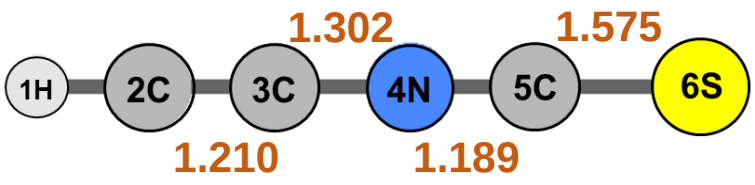
HCCNCS-^{34}S



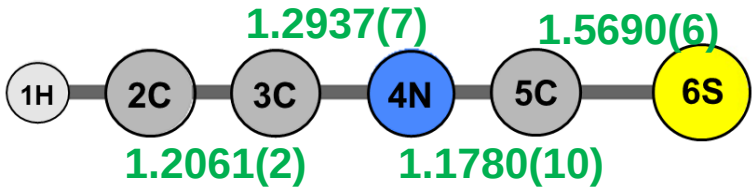
Structural parameters



HCCNCS-r_e



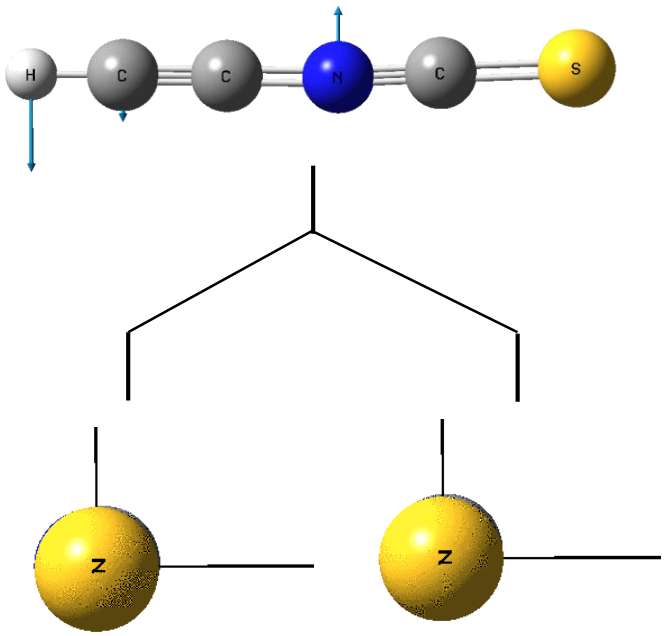
HCCNCS-r_0

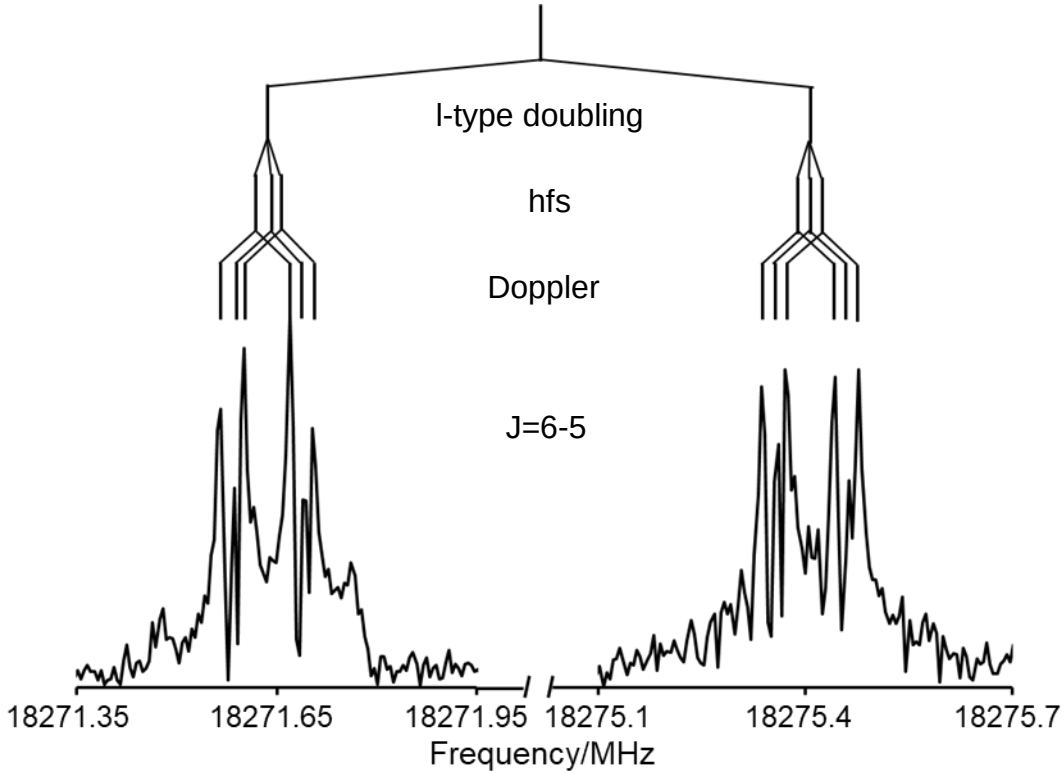


Equilibrium structures are calculated at CCSD(T)/ cc-pVQZ, for H, C, N and cc-pV(Q+d)Z for S.

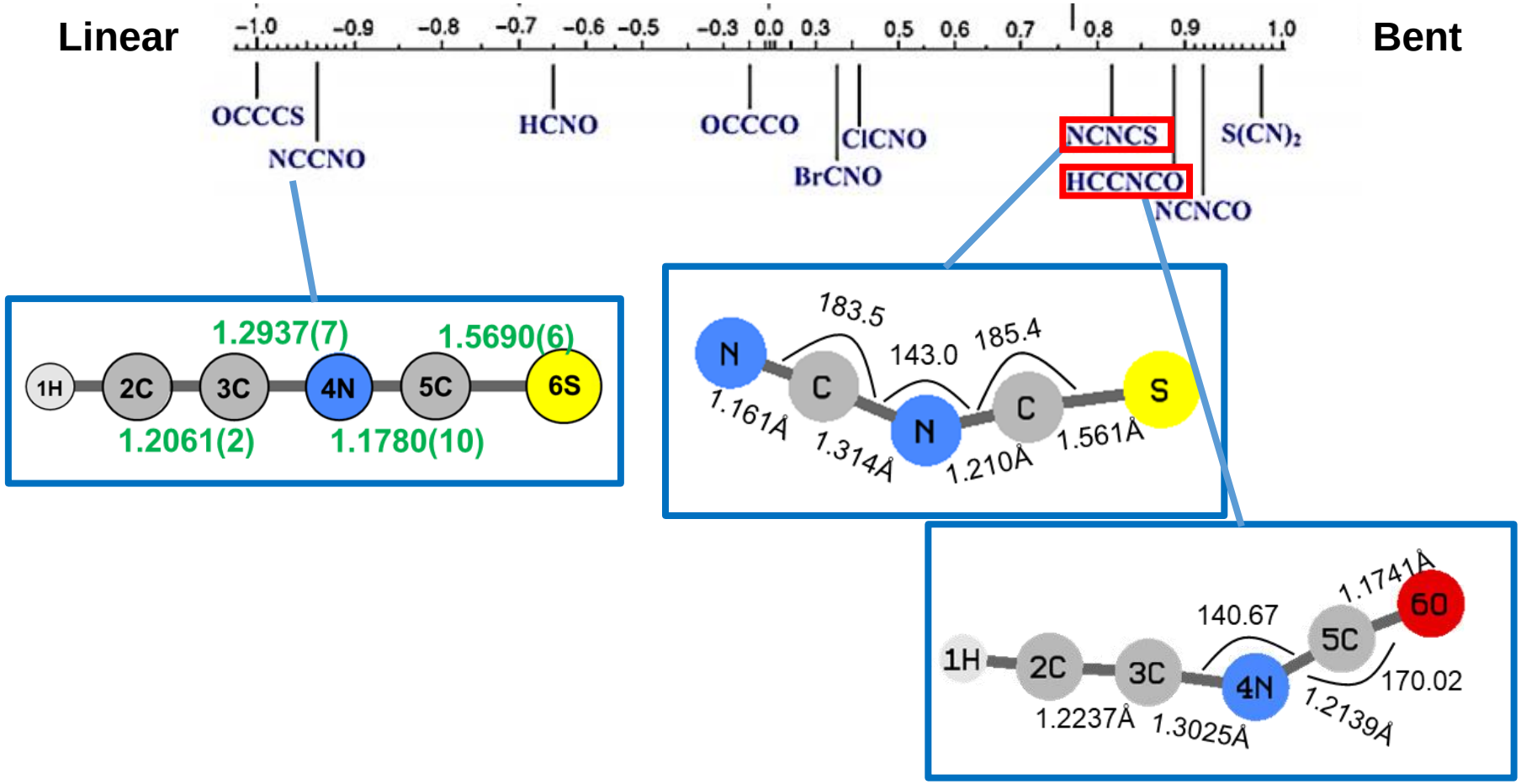
Vibrational State

C-N-C bending mode: $^1\Pi$ state (70.4cm^{-1} above ground state at B3LYP/cc-pVQZ)

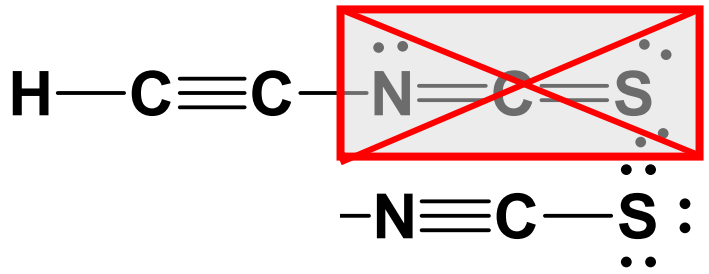


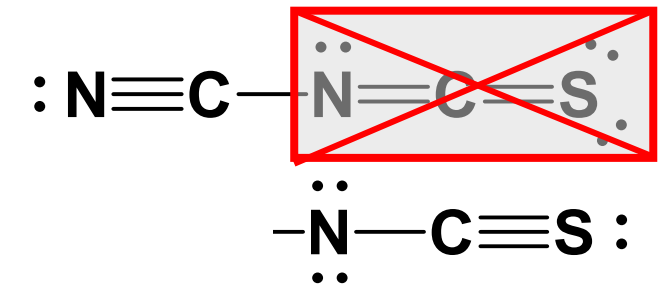


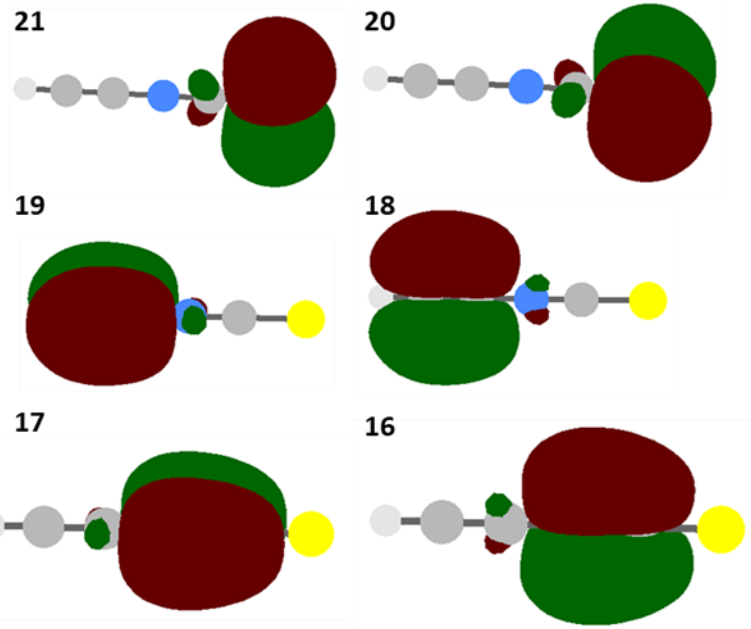
Why is HCCNCS linear?

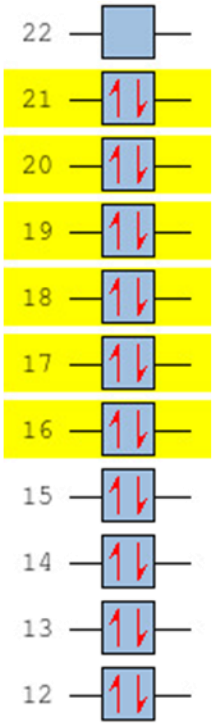


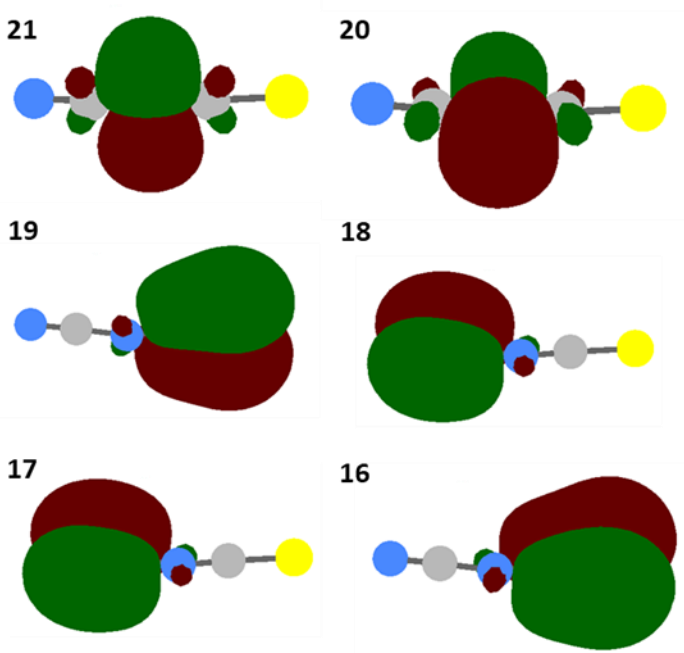
NBO analysis











NBO calculations are calculated at B3LYP/cc-pVQZ.

Acknowledgements