

November 16th, 2018

NH₄ + 4H₂O

- Sampling with 6-311G** basis set (step 222, 424, 10)
H: Disappearance of peak? Better agreement with experiment?
- Test IP H: Problem with IP and ammonium:
The one reported by Anna was much higher than the one we got 411 eV.
The diffuse orbital should have = energy, it's not exactly 0.

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TO DO

- Sample NH₃ + 4H₂O with 6-311G** basis set
- sample IPs
 - PE
 - gas Dalton
 - gas Q-Chem