Dear Professor Okumura,

We have electronically submitted a revised manuscript (CPLET-10-1679) that addresses the comments of the reviewers. With these modifications, we feel that this contribution is now suitable for publication in Chemical Physics Letters. Specifically, we have addressed the two concerns pointed out by Reviewer 2 and discuss them below.

Response to 1st concern:
With respect to the expectation that one should not obtain good agreement between DFT calculations and small shifts in Raman spectra due to perturbations, we have added text (Page 5, 2nd paragraph, last sentence) and cited recent publications (Refs 5 and 15) that show the DFT procedures employed here and second-order Møller-Plesset perturbation theory (MP2) both do a good job of predicting shifts in similar systems.

Response to 2nd concern:
We agree with Reviewer 2 that comparisons to spectra acquired using isotope labeling is an excellent way to confirm vibrational assignments. To this end, we have added text (Page 8, 1st and 2nd paragraphs) comparing our current assignments to earlier deuterated studies (Ref 25). Our conclusions here agree very well with previous assignments made using earlier deuterated spectra.

Should the revised manuscript require additional peer review, we suggest that you contact Howard Stidham (stidham@chem.umass.edu). Prof. Stidham is the lead author on the earlier study involving five different deuterium substituted pyrimidines.

Sincerely:

Nathan Hammer