

IRMPD Spectroscopy Shows That AGG Forms an Oxazolone b_2^+ Ion

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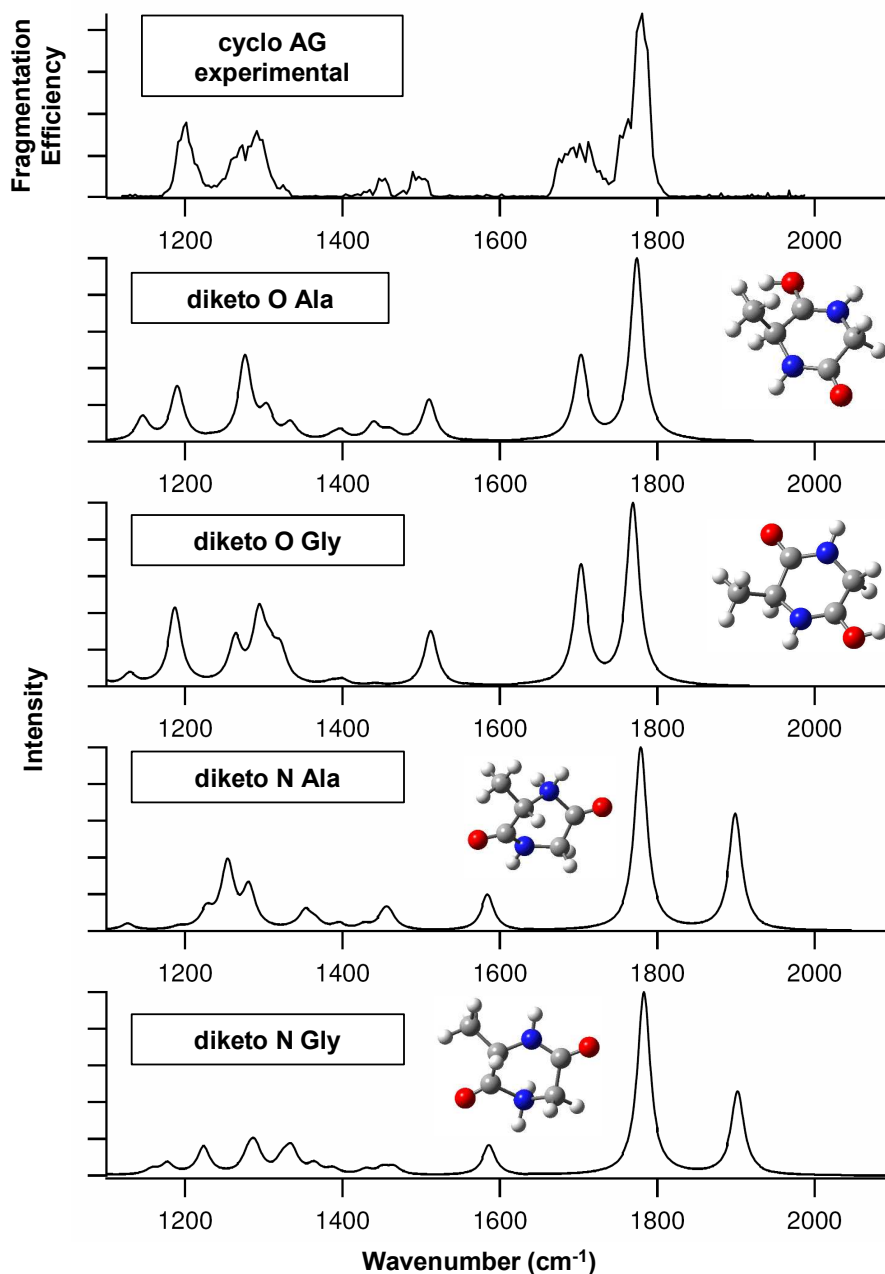


Figure S1: IRMPD spectrum of cAG plotted as fragmentation efficiency for formation of the most abundant fragment ion and calculated spectra of all stable diketopiperazine isomers.

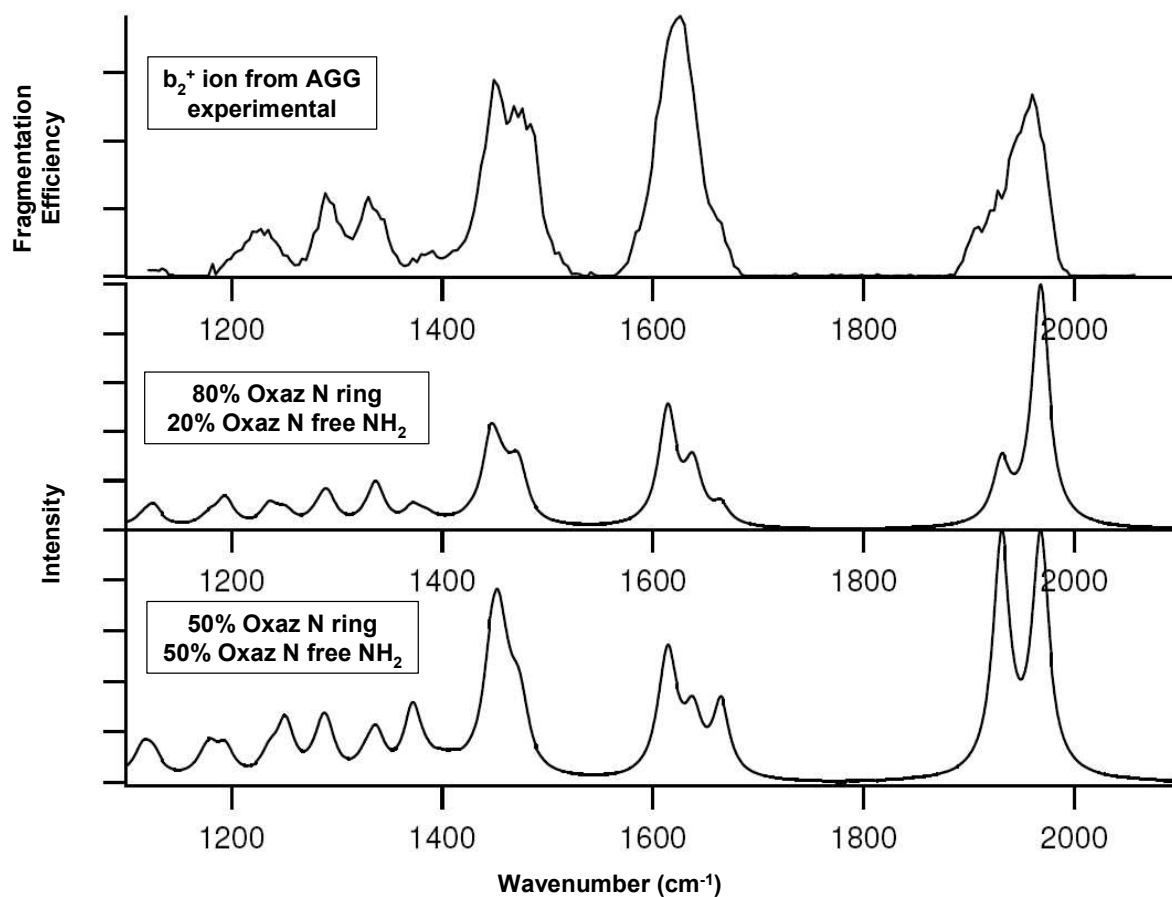


Figure S2: IRMPD spectrum of AGG b_2^+ ion plotted as fragmentation efficiency for formation of the most abundant fragment ion and calculated spectra. The middle panel is a combination of 80% oxazolone protonated on the ring nitrogen and 20% oxazolone protonated on the free NH_2 . The bottom panel is a combination of 50% oxazolone protonated on the ring nitrogen and 50% oxazolone protonated on the free NH_2 .

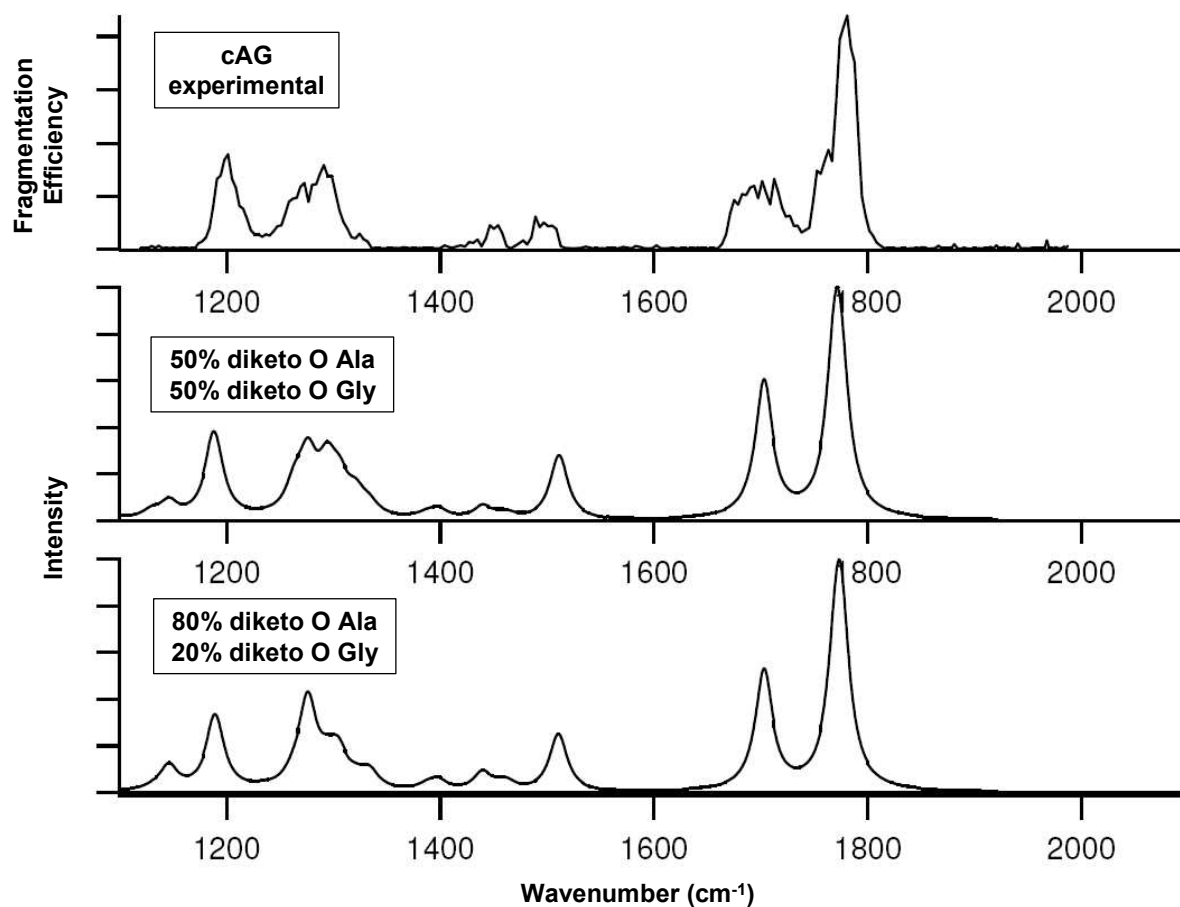


Figure S3: IRMPD spectrum of protonated cAG ion plotted as fragmentation efficiency for formation of the most abundant fragment ion and calculated spectra. The middle panel is a combination of 50% diketopiperazine protonated at the alanine amide oxygen and 50% diketopiperazine protonated at the glycine amide oxygen. The bottom panel is a combination of 80% diketopiperazine protonated at the alanine amide oxygen and 20% diketopiperazine protonated at the glycine amide oxygen.

Further band assignments:

For protonated cAG in Figure 1; the bands at 1446 cm^{-1} is rocking modes of the methyl group; 1284 cm^{-1} is produced by wagging motions of CH_2 .

For b_2^+ ion from protonated AGG in Figure 2; the bands at 1471 cm^{-1} and 1445 cm^{-1} are from scissoring mode of the methyl group (Oxaz N ring) and NH_3 umbrella mode of oxazolone isomer protonated at free NH_2 (Oxaz N free NH_2). The band at 1294 cm^{-1} is from wagging of CH_2 in the ring, and the band at 1239 cm^{-1} is related to twisting of CH_3 .

Full References

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