Vibrational signatures of zwitterionic and charge-solvated structures for alkaline earth-tryptophan dimer complexes in the gas phase

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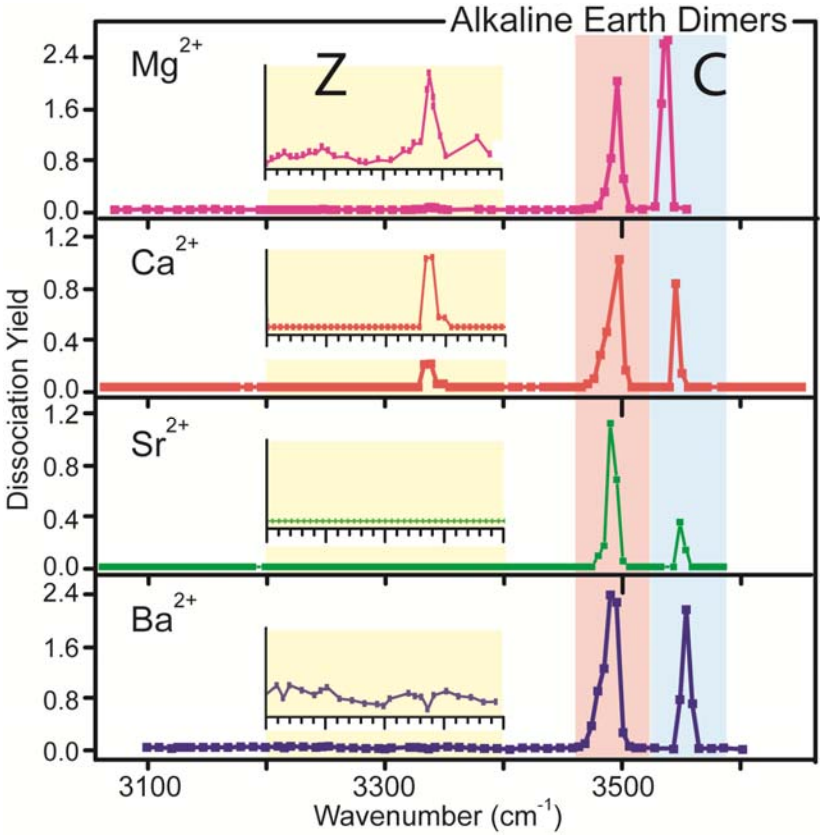
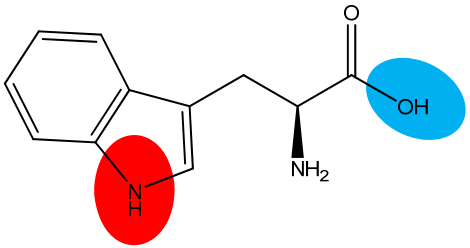
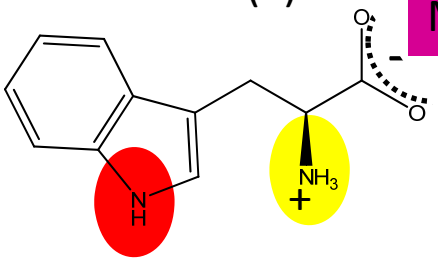


Charge solvation (**C**)



Zwitterion (**Z**)



M^{2+}

A polar solvent such as water generally favors the zwitterionic (**Z**) form of an amino acid, where a proton transfer takes place from the acid to the amino group (H_2N-CHR-COOH $\rightarrow$ H_3N^+-CHR-CO_2^-). In the gas phase, a similar proton transfer can be induced by the interaction of the molecule with a metal cation (M^{2+}) (see top). Structural differentiation between charge solvation (**C**) and zwitterion (**Z**) can then be carried out by infrared photodissociation spectroscopy, based on intense diagnostic vibrations.

The vibrational spectra of a series of alkaline earth-tryptophan complexes has been recorded using a benchtop optical parametric oscillator (OPO) laser (see left).

This shows that smaller alkali earth cation (magnesium and calcium) display a diagnostic band for **Z** (yellow region), whereas the larger cations (strontium and barium) do not. All structures display a diagnostic band for **C** (blue region), indicative of **C**-only for the larger cations, and a **C/Z** mixture for the smaller cations.

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