

CIVP SPECTROSCOPY OF COBINAMIDES IN THE GAS PHASE: CLUES TO THE DESIGN OF VITAMIN B12

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Alkyl and aryl cobinamides are close relatives to adenosylcobalamine, vitamin B12, which is an essential cofactor for a large number of enzymatic transformations. We report gas-phase investigations of the Co-C bond strength by means of energy-resolved collision-induced dissociation experiments, which found unexpected discrepancies to predictions made by dispersion-corrected DFT. Attempted resolution of the discrepancies led us to further cobinamide derivatives, whose ion spectroscopy provide key information on the gas-phase structure of these large molecules (ca. 150 atoms). The structural considerations lead to a hypothesis for the mechanism of control and regulation of vitamin B12 in the enzymatic reactions.