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Increase of radiative forcing through mid-IR absorption by stable CO2 dimers?

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We have demonstrated that the combination of matrix isolation infrared (MI-IR) spectroscopy and vibration configuration interaction (VCI) calculations [1-3] is a feasible approach [4] to accurately assign and interpret IR spectra of single molecules, such as water [5], fluoroethane [6], carbon dioxide and methane [7].

Relying on our integral experimental-computational methodology for IR spectroscopy, we investigated carbon dioxide dimerization [8], including MI-IR spectroscopy of carbon dioxide monomers CO_2 and dimers $(CO_2)_2$ trapped in neon and air. Based on our VCI calculations accounting for mode-coupling and anharmonicity, we identify additional IR-active bands in the MI-IR spectra due to the $(CO_2)_2$ dimer. In a systematic carbon dioxide mixing ratio study using neon matrices, we observe a significant fraction of the dimer at mixing ratios above 300 ppm, with a steep increase up to 1000 ppm. In neon matrix, the dimer increases the IR absorbance by about 15% at 400 ppm compared to the monomer absorbance alone. This suggests a high fraction of the $(CO_2)_2$ dimer in our matrix experiments.

In atmospheric conditions, such increased absorbance would significantly amplify radiative forcings and, thus, greenhouse warming. In the context of planetary atmospheres, our results improve our understanding of the greenhouse effect for planets of relatively thick CO_2 atmospheres, such as Venus, where a significant fraction of the $(CO_2)_2$ dimer can be expected. There, the necessity of including the mid-IR absorption by stable $(CO_2)_2$ dimers in databases used for modeling radiative forcing, such as HITRAN, arises.

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