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Investigating CO3 Isomers Formed by the Radiation Induced CO2 + O Reaction in Extraterrestrial Ices

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In the ices of comets, on interstellar medium dust grains, and in the Martian polar caps, carbon dioxide plays an important role both directly and indirectly in our understanding of the chemistry that occurs there. The intense solar/ cosmic radiation field that impinges upon molecules of carbon dioxide can lead to dissociation processes giving birth to high energy oxygen atoms. With the large column densities of carbon dioxide in these environments, it is likely for the high energy oxygen atoms to come into contact with carbon dioxide molecules and subsequently initiate non-equilibrium chemistry. An important intermediate of this reaction and one that may play a major role in carbon dioxide chemistry is the carbon trioxide molecule (CO3, C2v). However, the mechanism to its formation and its stability is unknown. We have carried out matrix isolation experiments of the CO3 molecule by irradiating carbon dioxide ices with 5 keV electrons to simulate the electronic effects in carbon dioxide resulting from absorption of radiation. A second isomer of carbon trioxide was found (CO3, D3h) by Fourier Transform Infrared (FTIR) spectroscopy which may be an overlooked intermediate that is essential in interpreting the chemistry of carbon dioxide. Isotopic experiments were also carried out to elucidate the mechanisms of formation and branching ratios to the carbon trioxide intermediate isomers.