

INFRARED ABSORPTION SPECTROSCOPY OF SMALL CARBON CLUSTER · WATER COMPLEXES ISOLATED IN SOLID Ar

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The 1:1 complexes between C_n ($n \leq 13$) carbon clusters and the H_2O molecule formed in Ar matrices at 12K have been investigated experimentally.^{ab} In addition, IR absorption bands found with higher energy than the $C_n \cdot H_2O$ C-C stretching bands have been assigned to 1:2 complexes with the general structure $H_2O \cdot C_n \cdot H_2O$, rather than $C_n \cdot (H_2O)_2$. The proposed structure is supported by geometry optimization and harmonic frequencies calculated at B3LYP/6-31G** level for the $C_n \cdot H_2O$, $H_2O \cdot C_n \cdot H_2O$ and $C_n \cdot (H_2O)_2$ systems. In particular, the ^{13}C -labeled experimental spectra for $^{12/13}C_5 \cdot H_2O$ and $^{12/13}C_6 \cdot H_2O$ complexes will be presented and compared to the calculated ones at the B3LYP/6-31G** level. The C_nO and C_2H_2 final photoproducts observed after UV matrix photolysis will be discussed within the context of possible photo-production of these species in interstellar space.^{cd}

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