INVESTIGATING THE CO-(D$_2$O)$_2$ AND CO-(D$_2$O)$_3$ COMPLEXES

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In the present contribution we report on the weakly-bound CO-(D$_2$O)$_2$ and CO-(D$_2$O)$_3$ complexes. By using a quantum cascade laser and a supersonic slit-jet apparatus, the infrared spectra of these complexes were investigated in the region of the C-O stretching fundamental of the CO monomer. For the trimer CO-(D$_2$O)$_2$ the observed band is composed of a/b-type transitions thus establishing that the CO monomer lies nearly in the a-b inertial plane. The small value of the inertial defect determined by the rotational constants indicates that the heavy atoms in the trimer are co-planar. No evidence of tunneling splitting was observed, meaning that the large amplitude tunneling that exists in the free D$_2$O dimer is quenched by the presence of the CO monomer. The CO-(D$_2$O)$_3$ band is also composed of a/b-type transitions, so also for this complex the CO monomer lies nearly in the a-b inertial plane. Employing the B2PLYP double-hybrid functional with D3BJ corrections, theoretical calculations were carried out to find minima on the potential energy surfaces for both CO-(D$_2$O)$_2$ and CO-(D$_2$O)$_3$ complexes. Further optimisations were then carried out at different coupled cluster levels of theory, and extrapolating to the complete basis set limit. The rotational parameters, corrected by anharmonic effects, are in very good agreement with those obtained from the observed spectra.