

## Higher-order transitions in the IR spectrum of the weak OC...HCL complex dissolved in liquid CO.

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Infrared spectra of HCl-doped CO solutions have been studied at  $T \sim 140-90$  K. First overtone and combination bands of the OC...HCl complex were revealed at the lowest temperature of the liquid solution. Ab initio calculations utilizing the 6-311++G(3df,3pd) basis set with electron correlation at the  $n$ th-order Møller–Plesset (MPn,  $n \leq 4$ ) levels of approximation predict minima for the CO...HCl and OC...HCl linear structures. Based on simplified treatment of anharmonic interactions between CO and HCl constituents, the model estimations of the dipole transition moments have been performed.

### Adres publiczny

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