

STRONG ORTHO/PARA EFFECTS IN THE VIBRATIONAL SPECTRA OF $\text{Cl}^- \text{H}_2$ and $\text{CN}^- \text{H}_2$

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The vibrational predissociation spectra of $\text{Cl}^- \text{H}_2$ and $\text{CN}^- \text{H}_2$ are measured in regions between 450 and 3000 cm^{-1} in an ion trap at different temperatures using the FELIX infrared free electron lasers. Strong differences between the vibrational spectra of the two *para* and *ortho* nuclear spin isomers $\text{X}-(\textit{para}\text{-H}_2)$ or $\text{X}-(\textit{ortho}\text{-H}_2)$, with $\text{X} = \text{Cl}^-$ or CN^- , are detected [1,2]. Above a certain temperature, the removal of the *para* nuclear spin isomer by ligand exchange to the *ortho* isomer is suppressed efficiently. Not only do the transition frequencies agree well with calculated spectra using an accurate quantum approach [3], also the line profile matches with the calculated bands. When comparing the absolute frequency positions of the measured and calculated vibrational bands one finds a redshift of about 5cm^{-1} for the strongest band.

[1] F. Dahlmann, P. Jusko, M. Lara-Moreno et al., *Mol. Phys.*, submitted

[2] F. Dahlmann, C. Lochmann, A. N. Marimuthu et al., *J. Chem. Phys. Comm.* 155, 241101 (2021)

[3] M. Lara-Moreno, P. Halvick, and T. Stoecklin, *Phys. Chem. Chem. Phys.* 22, 25552–25559 (2020)