ROVIBRATIONAL STATES OF $ClHCl^-$ ISOTOPOMERS: A JOINT THEORETICAL AND SPECTROSCOPIC INVESTIGATION

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Explicitly correlated coupled cluster theory at the CCSD(T*)-F12b level[a] and two precise spectroscopic constants[b] were used to construct an analytical potential energy function (PEF) for highly anharmonic $ClHCl^-$. From variational calculations with that PEF, a large number of rovibrational energies of different isotopomers were obtained. Theory helped with assignments of lines observed by IR diode laser spectroscopy and enabled to elucidate rather complex and unusual patterns of rovibrational interactions. In addition, transition dipole moments were predicted and analyzed.

[a] T. B. Adler, G. Knizia, and H.-J. Werner, *J. Chem. Phys.* **127**, 221106 (2007);
G. Knizia, T. B. Adler, and H.-J. Werner, *J. Chem. Phys.* **130**, 054104 (2009).
[b] K. Kawaguchi, *J. Chem. Phys.* **88**, 4186 (1988).