

THOCI, CDCCI (Z,L) Wedtenberg A. A. Goldstein J. H. Wilson ...B.

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(D1, Dz)

DCCC

135: 159418v High Resolution FTIR Spectroscopy of DCCCl: Anharmonic Resonances in the v<sub>1</sub> and v<sub>2</sub> Bands. Wang, DongBing: Imajo, Takashi; Tanaka, Keiichi; Tanaka, Takehiko; Burger, Hans (Department of Chemistry, Faculty of Science, Kyushu University 33. Hakozaki, Higashiku, Fukuoka, Japan 812-8581). J. Mol. Spectrosc. 2001, 207(1), 70-76 (Eng), Academic Press. High-resoln. IR spectra of the v1 and v2 bands of DCCCl were obsd. using Bruker IFS 120HR Fourier transform spectrometers at resolns, of 0.0044 and 0.0035 cm<sup>-1</sup>, resp. For the DCC35Cl isotopomer, the  $\nu_1$  as well as the  $\nu_2$  band was found to be heavily perturbed. Detailed analyses revealed that the vi state is in resonance with the l = 0 substate of the  $v_3 + 4v_4$  state and that the  $\nu_2$  state is in resonance with the l=0 substate of the  $\nu_3+4\nu_5$ state. The rotational consts. played a key role in identifying the perturbing states. In contrast, for the DCC37Cl isotopomer, the rotational structures of the  $\nu_1$  and  $\nu_2$  states are almost regular but slightly perturbed by interactions with the  $v_3 + 4v_4$  and  $v_3 + 4v_5$  states, resp. The consts. of resonances as well as the mol. consts. for the  $v_1$ ,  $v_2$ ,  $v_3 + 4v_4$  and  $v_3 +$ 4vs states were detd. (c) 2001 Academic Press.