LINESHAPE ANALYSIS OF CH_3F-(*ortho*-H_2)$_n$ ABSORPTION SPECTRA IN 3000 cm^{-1} REGION IN SOLID *para*-H_2

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FTIR absorption spectra of CH_3F-(*ortho*-H_2)$_n$ clusters in solid *para*-H_2 were studied in the C-H stretching region ($\sim$3000 cm^{-1}). As shown previously[a], the ν_3 C-F stretching band at 1040 cm^{-1} of the CH_3F-(*ortho*-H_2)$_n$ (n = 0$\sim$12) gives a distinct regular series of absorption lines in solid *para*-H_2, which correspond to each *n*-th component of the cluster. On the other hand, broaden single lines were observed in the 3000 cm^{-1} region, which were assigned to the ν_1 and ν_4 modes with axial rotation[b]. We found that their lineshape varied depending on *ortho*-H_2 concentration in crystals and could be represented as superposition of the cluster components. Least square fitting based on the CH_3F-(*ortho*-H_2)$_n$ cluster model worked very well to resolve the broaden bands and provided us the linewidth and line shift of resolved lines. The large difference of the linewidth and line shift between the vibrational modes shows the distinct nature of each mode in cold quantum solids.

[a] K. Yoshioka and D. T. Anderson *J. Chem. Phys.* **119**, 4731 (2003).
[b] Y. -P. Lee, Y. -J. Wu and J. T. Hougen *J. Chem. Phys.* **129**, 104502 (2008).