# HIGH RESOLUTION SPECTROSCOPY AND *AB INITIO* CALCULATIONS ON HfCl

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The emission spectrum of HfCl has been investigated in the 3000-18500 $cm^{1}$ region at high resolution using a Fourier transform spectrometer. The bands were excited in a microwave discharge through a flowing mixture of $HfCl_4$ and helium. Two bands near 17140 $cm^{-1}$ and 17490 $cm^{-1}$ were also measured in absorption using laser excitation spectroscopy. In this instance the molecules were created by laser ablation in a molecular beam apparatus. The observed bands have been classified into two electronic transitions, $[7.6]^4\Delta_{3/2}$ - $X^2\Delta_{3/2}$ and $[17.1]^2\Delta_{3/2}$ - $X^2\Delta_{3/2}$ involving a common lower state. A rotational analysis of the 0-0 and 1-1 bands of $[7.6]^4\Delta_{3/2}$ - $X^2\Delta_{3/2}$ and 0-0, 1-1 and 1-0 bands of the $[17.1]^2\Delta_{3/2}$ - $X^2\Delta_{3/2}$ transitions, has been carried out and the equilibrium spectroscopic constants have been determined. The ground state principal molecular constants are, $B_e$=0.1097404(54) $cm^{-1}$, $\alpha_e$=0.0004101(68) $cm^{-1}$ and $r_e$=2.290532(57) Å.

The *ab initio* calculations have been performed on HfCl and spectroscopic properties of the low-lying electronic states have been predicted. The ground state is predicted to be a regular $^2\Delta$ state arising from the valence electron configuration, $1\sigma^2 2\sigma^2 3\sigma^2 1\pi^4 1\delta^1$. On the basis of our *ab initio* calculations, we assign the observed transitions as $[7.6]^4\Delta_{3/2}$-$X^2\Delta_{3/2}$ and $[17.1]^2\Delta_{3/2}$-$X^2\Delta_{3/2}$ .