respectively. In the ^{13}C NMR spectrum of $Ta_2Cp'_2Cl_4(H)(^{13}CHO)$ at 298K the formyl carbon atom resonance is found as a broad doublet (J_{CH} = 168 Hz) at 168 ppm. The 20 Hz coupling to the hydride could not be resolved under these conditions.

A complicating feature of the ^1H NMR spectrum is its temperature dependence (Fig. 1). As the temperature is raised from 233K to 337K, the formyl and hydride signals broaden, shift toward one another, and then sharpen into doublets with $J_{HH} \simeq 4$ Hz. The resonances due to the Cp' ligands shift somewhat but the molecule remains asymmetric. In the ^{13}C NMR spectrum the resonance for the formyl carbon atom shifts from $\sim$ 168 to $\sim$ 176 ppm and the coupling constant to the formyl proton drops from $\sim$ 175 to 165 Hz over this temperature range. One could ascribe this behavior simply to ordinary temperature dependent chemical shifts if the formyl proton resonance did not collapse to the extent it does. The only explanation we feel comfortable with is that one structural form predominates at low temperatures but at high temperatures there is a significant amount of a second species present with which the first species interconverts rapidly. (Note that the hydride and formyl protons do not exchange during this process.) The structural difference between these two species may be slight. Although we cannot speculate what these two structures might be at this time, we should point out that the inequivalent hydride ligands in $Ta_2Cp'_2Cl_3H_2(R)$ complexes exchange over the same temperature range without destroying the asymmetry of the molecule.[7] The temperature dependent process in $Ta_2Cp'_2Cl_3H_2(R)$ could involve a related structural change. Also note that in the structurally related molecules, $Ta_2Cp'_2Cl_4(H)(O)(Me_3PCH)$ and $Ta_2Cp'_2Cl_4(H)(CHNR)$ (see later), coupling between what were the two initial hydride ligands can be resolved, and it is of the same magnitude as that found in $Ta_2Cp'_2Cl_4(H)(CHO)$ at 70°.