

785
MW $\text{C}_7\text{H}_5\text{O}_2\text{Rh}$ Dicarbonyl(η^5 -2,4-cyclopentadien-1-yl)rhodium G_{20}

Attempts to fit the spectrum using a rigid-rotor model resulted in large deviations between measured and calculated frequencies and an unreasonably large A rotational constant. A better fit, including more transitions, was obtained using a V_{10} -barrier hindered rotor



Hamiltonian, and a much more reasonable A rotational constant was obtained. The barrier height obtained is $V_{10} = 347(13)$ GHz (0.14 kJ mol^{-1}). A DFT calculated structure showed C_2 -symmetry distortions of the cyclopentadienyl moiety. The calculations indicate that there is coupling between the internal rotation and distortions of the cyclopentadienyl ligand, and this could very likely provide the major contribution to deviations between the hindered-rotor calculated frequencies and the measured frequencies.

Kukolich, S.G., Drouin, B.J., Cassak, P., Hubbard, J.L.: *Organometallics* **17** (1998) 4105.