THE ROTATIONAL SPECTRUM OF RUTHENIUM MONOCARBIDE USING PPMODR[a]

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Predicting the properties of simple second row transition metal containing molecules is surprisingly challenging because of the significant relativistic effects as well as the large dynamic electron correlation. Assessing the multitude of computational methodologies being developed for addressing these effects is most readily achieved by comparing of experimentally derived and predicted hyperfine parameters . The interaction between the nuclear electric quadrupole moment and the electric-field gradient at the site of the same nucleus is particularly useful for testing various relativistic effects[b]. As part of our continuing study of RuC[c], here we report on the experimental determination of the electric quadrupole coupling parameter for ^{101}RuC from the analysis of the pure rotational spectrum. The J= 0→1 and J=1→2 transitions for ground state ($X^1\Sigma^+$) ^{101}RuC and ^{102}RuC were recorded using the separated field pump/probe microwave optical double resonance technique.

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[b]Cheng, L; Stopkowicz, S; Stanton, J.F., Gauss, J,; *J. Chem. Phys*, **137**, 224302, 2012.

[c]Steimle, T.C., Virgo, W.L., Brown, J.M.; *J. Chem. Phys*, **118**, 2620, 2003.