

ROTATIONAL SPECTROSCOPY AND STRUCTURE OF 1,1-DICHLORO-1-SILACYCLOHEX-2-ENE

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Through a long-standing collaboration with the Guirgis group (College of Charleston, SC), we have been trying to understand the physicochemical differences between silicon-containing species and carbon-containing species. Now, we present the rotational spectrum of 1,1-dichloro-1-silacyclohex-2-ene in the 5.50–18.75 GHz region of the electromagnetic spectrum and discuss the quadrupole coupling within this molecule and present a partial substitution (r_s) structure; the latter arises from the observation of various isotopologues in the free-jet expansion, in their natural abundances. The hyperfine structure is complicated and arises from the two non-equivalent chlorine nuclei ($I = 3/2$), although the quadrupole coupling constants for both atoms are very similar. This leads to challenging analysis as a large portion of the hyperfine splitting is unresolved — even with the resolution we achieve with our chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer. We compare our experimental results to those predicted by high-quality *ab initio* calculations, as well as the related systems 1,1-difluoro-1-silacyclohex-2-ene and 1-silacyclohex-2-ene¹.

¹ N. T. Moon, A. J. Duerden, T. M. C. McFadden, N. A. Seifert, G. A. Guirgis and G. S. Grubbs II, *J. Phys. Chem. A*, **128**, 10–19 (2024).