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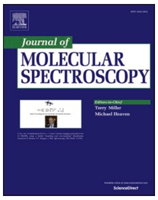

The microwave spectrum of the low energy conformers of 1-ethylsilacyclopentane

Josie R. Glenn [a], J.E. Isert [a], Jacob D. Bethke [b], Gamil A. Guirgis [b], G.S. Grubbs II [a,*]

[a] Department of Chemistry, Missouri University of Science and Technology, 400 W. 11th Street, Rolla, MO 65409, USA
[b] Department of Chemistry and Biochemistry, College of Charleston, 66 George Street, Charleston, SC 29424, USA

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ABSTRACT

The microwave rotational spectrum of 1-ethylsilacyclopentane has been observed using chirped-pulse, Fourier transform microwave spectroscopy and has been reported for the first time. The lowest three energetic conformers were observed and fit to a Watson S semirigid Hamiltonian to within experimental accuracy. The quantum chemical calculations are all within ≈1% of the determined rotational constants, providing confidence that they are accurate representations of the experimental structure. Centrifugal distortion terms D_{JK} and D_K, although seemingly large, have been determined to be physically meaningful as no apparent evidence such as splittings in the spectrum or transition broadening was observed. A second moment analysis was undertaken and compared to similar silacyclopentanes, but it is not clear if this species follows previously determined trends.

1. Introduction

The authors, in recent years, have undertaken investigations into the rotational spectroscopy of a series of silicon-containing molecules for the purposes of understanding the differences in the structure of these molecules from their all-carbon counterparts.[1–7] Studies of these systems have led to interesting physiochemical results like ring puckering motions, planar vs. nonplanar ring structures, or C_2 symmetry in straight-chain alkane species where one may expect C_{2v}. The results often support the understanding that silicon-containing molecular structures are uniquely different from their all-carbon counterparts.

With regards to these studies, we have specifically focused a few projects on the molecular structure and conformations of molecules with functional groups attached to the silicon in the ring molecule silacyclopentane.[1,2] While each of these systems has shown a unique, sometimes unexpected attribute, the basic structure of the ring portion of these molecules has been found to be similar using second moment analysis of the determined rotational constants. In this work, we extend these studies to include the microwave spectra of multiple conformers of 1-ethylsilacyclopentane. This represents the first known report of the molecule's rotational spectra and was achieved utilizing the chirped-pulse, Fourier-transform microwave (CP-FTMW) spectroscopic technique. Analysis, discussion, and conclusions regarding the spectrum and structure are aided by and compared to quantum chemical calculations and second moment analysis.

2. Quantum chemical calculations

All calculations for 1-ethylsilacyclopentane were performed using the Gaussian16 program suite.[8] Because we believed the molecule would have its lowest energy conformation in the equatorial position like many all-carbon ring analogues, we performed an optimization of this structure at the B3LYP-D3BJ/Def2TZVP level. This will be called equatorial 1 in the manuscript. This structure is presented in the *ab*-, *ac*-, and *bc*-principal axis planes in Fig. 1. The ethyl group is pointed toward one of the CH_2 groups coming off the silicon atom.

Just like all-carbon ring analogues, however, we expected there to be other low energy conformations - particularly an axial conformation. Therefore, we performed an optimization of the axial structure at the same level. This conformation has the ethyl group completely pointed up and away from the ring with the hydrogen on the silicon and the concluding methyl group of the ethyl ligand slightly less than 180° apart. This structure is presented in Fig. 2. The surprising result of this calculation was that it was significantly lower in energy than the equatorial 1 conformer result by 64.6 cm^{-1}. This result prompted an energy scan of the C(1)-Si-C(15)-H(17) dihedral angle. This scan is presented in Fig. 3.

This scan provided the confirmation that the axial conformation was

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* Corresponding author.
E-mail address: grubbsg@mst.edu (G.S. Grubbs).

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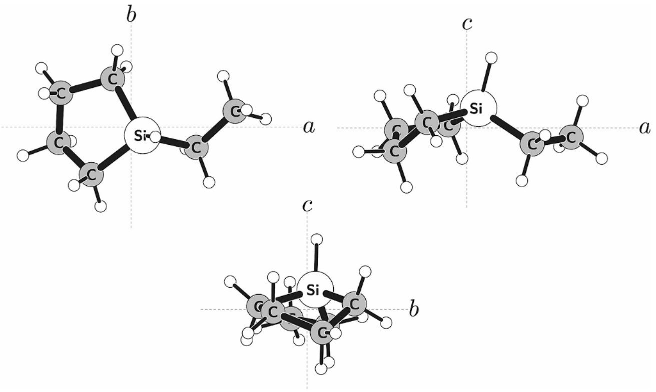

Fig. 1. The equatorial 1 conformation of 1-ethylsilacyclopentane in the *ab*-, *ac*-, and *bc*-planes.

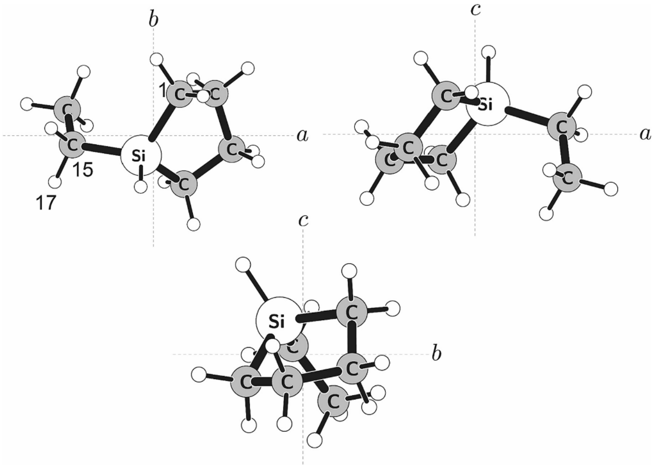

Fig. 2. The axial conformation of 1-ethylsilacyclopentane in the *ab*-, *ac*-, and *bc*-planes. The labelled atoms in the *ab*-plane represent the scanned dihedral atoms referred to in Fig. 3.

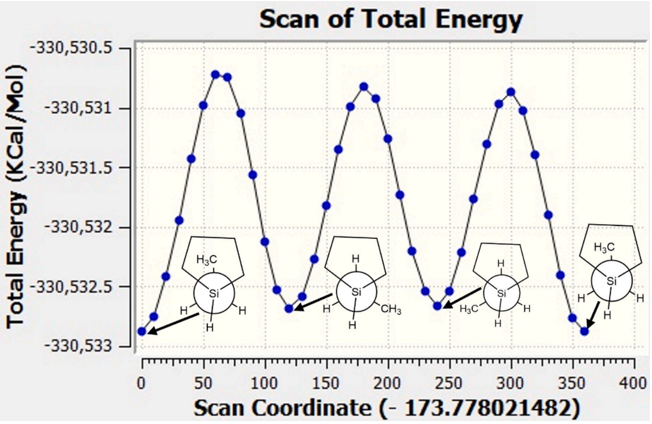

Fig. 3. Potential energy scan of the C(1)-Si-C(15)-H(17) dihedral angle of 1-ethylsilacyclopentane at the B3LYP-D3BJ/Def2TZVP level. The starting dihedral angle is −173.778° with subsequent points taken 10° apart. There are three distinct energy minima with the ethyl group in the axial position being the lowest energy. The lowest energy is the axial conformer (at point 0) and equatorial 1 has the terminal methyl group of the ethyl ligand 120° clockwise and equatorial 2 has the methyl group at 240° clockwise.

the lowest in energy, but also presented a new piece of information. That there was a second equatorial position where the ethyl group pointed toward one CH_2 group on the silicon ring was distinctly different in energy than that of it pointed toward the other CH_2 connected to the silicon atom. The two equatorial conformations were very similar in energy, rotational constants, and dipole moments (see Table 1), though, so it was originally assumed that they were the same structure. However, analysis of the spectrum would show that this wasn't the case and that the conformations were indeed different. This will be discussed more in the *Results and Analysis* section. Therefore, a proper optimization of this structure at the B3LYP-D3BJ/Def2TZVP level was undertaken for what will be called equatorial 2 throughout the manuscript. This structure is presented in Fig. 4. All optimization parameters are presented in Table 1.

3. Experimental methods

3.1. Synthesis

Synthesis of 1-ethylsilacyclopentane was carried out at the College of Charleston. A stepwise scheme for the synthesis is found in Fig. 5. Preliminary basis for this synthetic pathway can be found in the literature. [2,9] The sample of 1-ethylsilacyclopentane was prepared by the coupling of the double Grignard of 1,4-dibromobutane in dry diethyl ether to ethyldichlorosilane in dry diethyl ether and refluxed overnight. The product, 1-ethylsilacyclopentane, was obtained by filtration and washing the solid twice with dry diethyl ether. The diethyl ether was distilled under reduced pressure 100 Torr to 30 mL and then an equal volume of pentane was added to the ethereal solution. Soluble magnesium halides were precipitated and filtered using a sintered glass funnel under dry nitrogen. The diethyl ether and the pentane were separated using trap-to trap distillation and the compound 1-ethylsilacyclopentane was trapped in a bulb at −60 °C and characterized by NMR. ^{1}H NMR (400 MHz, $CHCl_3$): δ (ppm) 3.95 (h, $J = 2.96$ Hz, SiH = 1), 0.99 (multiple t, $J = 8$ Hz, 2 CH_2), 0.65 (m, $J = 1.68$ Hz, 5H). ^{13}C NMR (400 MHz, $CDCl_3$): δ (ppm), 27.52, 8.65, 8.30, 4.48. ^{29}Si NMR (400 MHz, $CHCl_3$): δ (ppm) 4.21.

3.2. Spectroscopy

The microwave experiments were carried out at Missouri University of Science and Technology (Missouri S&T) using a multi-antenna detection, chirped-pulse, Fourier-transform microwave (MAD-CP-FTMW) spectrometer in the standard CP-FTMW orientation. The details of this spectrometer are reported elsewhere.[10–12] 1-ethylsilacyclopentane was liquid at ambient temperature and pressure. A heated nozzle with a sample reservoir, designed to fit on the end of a Parker^{TM} Series 9 solenoid valve, was set to 31 °C to ensure that a reasonable amount of sample was present in the vapor phase above the liquid. [13–15] Argon was used as a backing gas at 20 psig (approximately 2.4 atm absolute pressure). The sample was then introduced into the chamber via a pulsed, free-jet expansion at a rate of 3 Hz with 3 free induction decays (FIDs) per gas pulse. 4 μs chirps over the 5–19 GHz range was utilized. The FIDs were 20 μs in length, and 146,694 FIDs were collected and averaged. The sample provided was completely exhausted during the experiment.

Fourier transformation of the averaged FIDs was performed with Kisiel's FFTS program using a Bartlett windowing function.[16] An example of the resultant spectrum is presented in Fig. 6. Typical linewidths for the spectra were 70–80 kHz (FWHM) with an attributed 10 kHz uncertainty for the line centers. Line center measurements are made through a mathematical routine of the AABS package that automatically reports the transition to 4 decimal places, which is used directly in the spectral fitting process.[17,18].

Table 1
Spectroscopic parameters for the observed conformers of 1-ethylsilacyclopentane compared to structure optimizations for the three lowest energy conformations of 1-ethylsilacyclopentane at the B3LYP-D3BJ/Def2TZVP level.

Parameter	Axial		Equatorial 1		Equatorial 2	
Relative Energy[a] / cm^{-1}	0.00		64.6		75.4	
A / MHz	3202.6064(5)[b]	3189.3	3990.0353(6)	3999.0	4107.234(1)	4108.0
B / MHz	1508.6093(2)	1505.7	1356.2812(2)	1345.9	1338.3345(3)	1330.2
C / MHz	1438.8613(2)	1438.1	1171.2420(2)	1162.0	1157.6299(3)	1149.9
D_J / kHz	0.594(2)	—	0.3194(8)	—	0.270(1)	—
D_{JK} / kHz	−2.048(3)	—	−2.171(5)	—	−1.262(7)	—
D_K / kHz	3.97(1)	—	7.83(3)	—	5.84(9)	—
d_1 / Hz	−7.5(5)	—	−16.3(2)	—	−21.5(3)	—
d_2 / Hz	−4.4(1)	—	−2.07(9)	—	−3.7(1)	—
N[c]	132	—	66	—	55	—
Σ[d]/ kHz	11.2	—	7.8	—	9.7	—
$\|\mu_a\|$[a] / D	0.17		0.03		0.03	
$\|\mu_b\|$[a] / D	0.25		0.06		0.04	
$\|\mu_c\|$[a] / D	0.40		0.55		0.55	

[a] Value taken from quantum chemical calculations.

[b] Numbers in parentheses give standard errors (1 s, 67 % confidence level) in units of the least significant figure.

[c] Number of observed transitions in the fit.

[d] Σ is Microwave RMS and is defined as $\sqrt{\frac{\sum\left[(\text{obs}-\text{calc})^2\right]}{N}}$ where N is defined in footnote b.

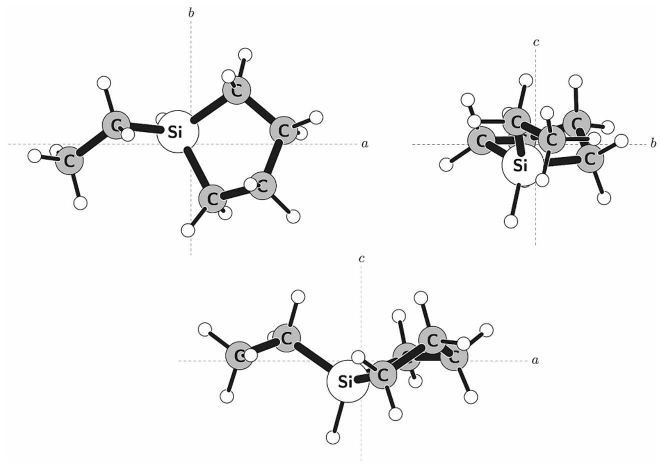

Fig. 4. The equatorial 2 conformation of 1-ethylsilacyclopentane in the *ab*-, *ac*-, and *bc*-planes.

4. Results and analysis

The spectrum of 1-ethylsilacyclopentane was assigned using Kisiel's AABS package used in conjunction with Pickett's SPFIT/SPCAT program suite in the I^r representation. [17–19] Transitions were assigned from 5.7 to 19.1 GHz. A semirigid, Watson S-reduced Hamiltonian was employed for fitting.[20] All rotational constants and quartic centrifugal distortion constants were determined for all three conformers. As expected from quantum chemical calculations, the spectra were predominantly *c*-type for all conformers with observation of a few *a*- and *b*-type transitions in the axial conformation. Isotopologues of the conformers were not identifiable in the spectrum. Determined parameters for each conformer are presented in Table 1 with quality of fit details and assigned transition quantum numbers being reported in the Supporting Information.

Fig. 6 shows the relative scaled intensities of the transitions for all three conformers using the heated (31 °C) temperature as a scaling factor in a Boltzmann distribution. Due to our original expectation that the equatorial conformation was lowest in energy, it was assigned first. As such a search for the equatorial 1 conformer was undertaken using the optimized rotational constants and dipole moment component values from Table 1 as a starting point. Patterns of strong *c*-type, *R*- and *Q*-branch transitions emerged, providing for unambiguous assignment. In all, 66 transitions were assigned to the semirigid Hamiltonian with a microwave RMS of 7.8 kHz.

After assignment of the equatorial 1 conformer, however, and the realization that the axial was lower in predicted energy, the assigned equatorial 1 transitions were subtracted from the spectra using Kisiel's AABS software and a search for axial conformer transitions was undertaken using the optimized rotational constants and dipole moment component values from Table 1 as a starting point. A pattern of strong *c*-type, *R*-branch transitions for the axial conformer were immediately present in the spectrum, allowing for its unambiguous assignment. In addition to these, however, and one of the largest distinctions in the axial and equatorial conformers' spectra is the presence of *a*- and *b*-type transitions in the axial conformation due to the larger dipole components in the *a*- and *b*- principal axes. These additional transition types, along with the lower energy of the conformation, resulted in 132 transitions being assigned with a microwave RMS of 11.2 kHz.

As mentioned previously, equatorial 1 and 2 were not immediately thought to be different conformations due to the similarities in their calculated dipole moments despite there being differences in their calculated energy and rotational constants. After assignment of the axial and equatorial 1 conformations concluded, however, a search for the minor isotopologues of both conformers was undertaken. To do this, the process of subtracting the axial and equatorial 1 conformer transitions out using the AABS subtraction process above was utilized. When this was done, it was noticed that transitions remained that were much more

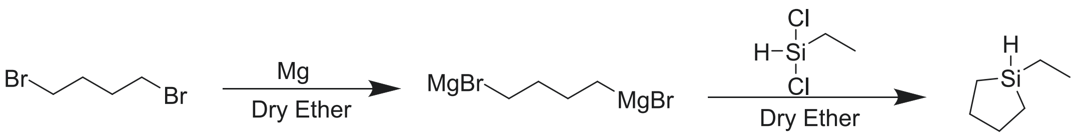

Fig. 5. The stepwise synthetic pathway for 1-ethylsilacyclopentane.

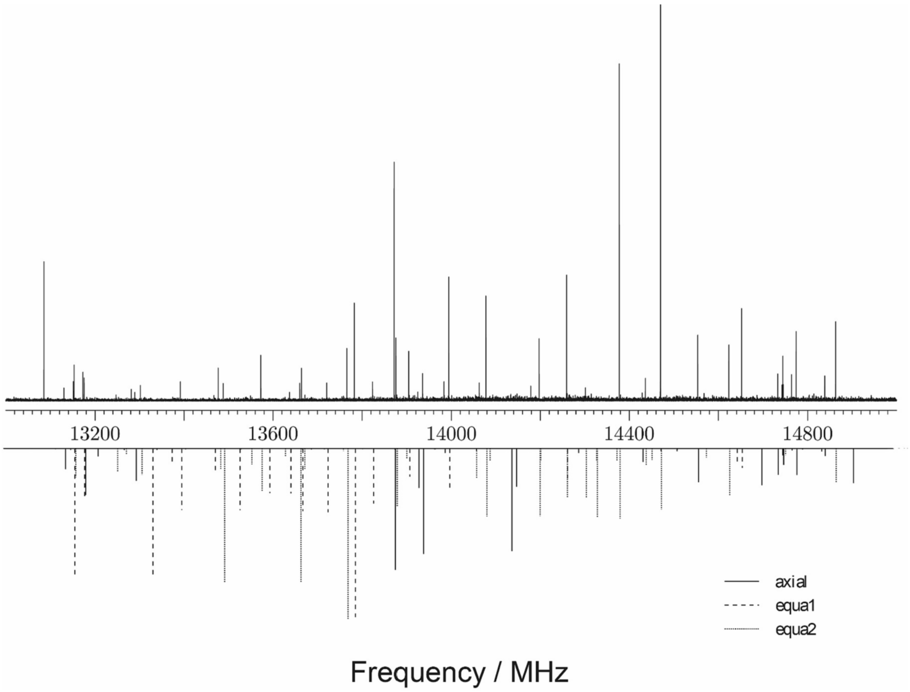

Fig. 6. The 13–15 GHz portion of the collected microwave spectrum of 1-ethylsilacyclopentane. The predicted spectrum with scaled relative intensities at 304 K (31 °C) for axial, equatorial 1 and equatorial 2 is below. The predicted transition positions align well with the observed experimental spectrum.

intense than the ≈4% intensity expected (see Fig. 6) due to the correct relative intensity aspect of the CP-FTMW technique. The patterns again were of strong *c*-type, *R*- and *Q*-branch transitions. In all, 55 transitions were assigned to the semirigid Hamiltonian with a microwave RMS of 9.7 kHz. After assignment of these transitions, the optimized equatorial 2 structure was revisited and it was noticed that the fit spectroscopic rotational constants were $<$ 1 % that of the predicted rotational constants for the conformer, the types of transitions observed matched well to the predicted dipole moment component values, and the observed intensity and number of transitions assigned matched the predicted relative energy scaling at the experimental temperature. Therefore, it was concluded that this unknown conformer assigned belonged to the equatorial 2 conformation.

5. Discussion

Aside from the unexpected observation of the equatorial 2 conformation, it is important to discuss the spectroscopic fits and the structure of the molecule, especially in the context of similar species. The first item that was noteworthy was that the determined D_{JK} and D_K constants were unusually large for a molecule the size of 1-ethylsilacyclopentane. When these constants are unusually large, it is typically an indication of a large amplitude motion in the molecule or some other effect, diminishing the physical meaningfulness of the value. An example of this in previous silicon-ring studies pertains to 1,1-difluorosilacyclopent-3-ene, where D_{JK} was 5.76 kHz and there turned out to be splitting in the spectra despite not being able to clearly identify the source.[5] One test would be to plot centrifugal distortion terms against isotopologue fitted values as we have done in studies of other systems to assess how physically meaningful a centrifugal distortion term may be, but we did not have the isotopologue data to perform this analysis.[7] That meant that the best experimental confirmation would have to be qualitative, so we looked for transition splittings in the spectrum. No such splittings or spectral broadening were observed despite quantum number assignments being reasonably high in *J* and *K*. This led us to conclude that these constants were probably reasonable and had physical meaning, but it is still possible that higher frequency or better resolved measurements of the species may exhibit splittings.

The second item to note is the accuracy of the equilibrium structures in comparison to the experimental structure. Again, this is somewhat difficult to compare directly as only the parent isotopologues were observed for each conformer. However, comparing the equilibrium rotational constants to those of the experimentally determined values in Table 1, the differences are all on the order of 1 % or less, giving confidence that the structures presented in Figs. 1, 2, and 4 are accurate representations of the experimental structure.

Lastly, it is important to characterize these experimental structures in terms of similar silacyclopentane species. However, like 1-ethylsilacyclopentane, many other silacyclopentane derivatives do not necessarily have all the data needed to get accurate, individualized bond lengths and bond angles. To make these comparisons, then, another approach must be used. A very good, generalized comparison approach to molecular structure can be achieved using the second moments approach of Bohn and coworkers.[21] Second moments are a measure of the out-of-plane mass distributions of a molecule in the principal axis system. So, P_{cc} measures the mass distribution out of the *ab*-plane and so on.

Second moments (also called planar moments) have been collected and reported for this molecule and multiple other silacyclopentane species using Kisiel's PLANM program and are presented in Table 2.[22] In the work of 1-chloromethyl-1-fluorosilacyclopentane, it was observed that the silacyclopentane ring exhibits a planar moment value (typically in P_{bb}) of approximately 80 uÅ^2. However, no conformation of 1-ethylsilacyclopentane is consistent with this trend, but the closest values to this lie in P_{bb}. To understand if this is due to the ring or just coincidental, refer to the visual representation of the quantum chemical calculations from this work provided in Figs. 1, 2, and 4. There is a similar twist on the carbons on the ring furthest from the silicon atom as there has been in the previous silacyclopentane derivatives. Furthermore, in all conformers of 1-ethylsilacyclopentane, the ethyl group does stick out of the *ac*-plane, but not much, which would increase the value of P_{bb}. It is difficult to quantify how much this would affect P_{bb} directly, though, without making significant assumptions about the equality of the experimental and equilibrium structures which we are trying to keep separate. Because of this, it is not clear that the previous observation of

Table 2
Comparison of second moments for various silacyclopentanes.

Molecule	P_{aa} / uÅ^2	P_{bb} / uÅ^2	P_{cc} / uÅ^2	References
1-ethylsilacyclopentane (axial)	264.214796(35)[a]	87.020592(35)	70.781818(35)	This Work
1-ethylsilacyclopentane (eq1)	338.725325(47)	92.764500(47)	33.895784(47)	This Work
1-ethylsilacyclopentane (eq2)	345.567663(72)	90.995876(72)	32.050195(72)	This Work
silacyclopentane	109.85405(84)	80.02742(84)	12.30640(84)	[23]
1-chloromethyl-1-fluorosilacyclopentane	365.74541(18)	204.67060(18)	80.10598(18)	[1]
1-fluorosilacyclopentane	185.674479(48)	79.818879(48)	27.703952(48)	[24]
1-chlorosilacyclopentane[b]	286.08	79.50	40.49	[25]
1-bromosilacyclopentane[b]	460.08	79.89	45.22	[26]
1,1-difluorosilacyclopentane	227.27110(12)	83.037692(12)	67.164670(12)	[2]

[a] Numbers in parentheses give standard errors (1 s, 67 % confidence level) in units of the least significant figure.

[b] Reported as an experimental/calculated estimated r_0 value.

80 uÅ^2 holds for 1-ethylsilacyclopentane, despite the structure qualitatively being similar. We are also in the process of analysing 1-ethyl-1-fluorosilacyclopentane in order to see if a new value or trend is being formed.

6. Conclusions

The microwave rotational spectrum of 1-ethylsilacyclopentane has been observed and has been reported for the first time. The lowest three energetic conformers were observed and fit to a Watson S semirigid Hamiltonian to within experimental accuracy. The quantum chemical calculations are all within ≈1% of the determined rotational constants, providing confidence that they are accurate representations of the experimental structure. Centrifugal distortion terms D_{JK} and D_K, although seemingly large, have been determined to be physically meaningful as no apparent evidence such as splittings in the spectrum or transition broadening was observed. A second moment analysis was undertaken and compared to the previous observation of approximately 80 uÅ^2 representing the typical second moment contribution for a silacyclopentane ring, but it is not clear if this species follows that trend or is starting to exhibit a different trend. Studies of 1-ethyl-1-fluorosilacyclopentane are being undertaken in order to understand these differences.

CRediT authorship contribution statement

Josie R. Glenn: Formal analysis, Investigation, Visualization, Writing – original draft, Writing – review & editing. **J.E. Isert:** Investigation, Writing – review & editing. **Jacob D. Bethke:** Investigation, Validation, Writing – review & editing. **Gamil A. Guirgis:** Conceptualization, Investigation, Methodology, Project administration, Supervision, Validation, Writing – original draft, Writing – review & editing. **G. S. Grubbs:** Investigation, Validation, Methodology, Conceptualization, Writing – original draft, Writing – review & editing, Visualization, Data curation, Resources, Project administration, Funding acquisition, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All data has been provided in supplemental information

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jms.2023.111872.

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