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Microwave, r_0 Structural Parameters, Conformational Stability and Vibrational Assignment of (Chloromethyl)fluorosilane

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Scheme S1. Synthesis of (chloromethyl)fluorosilane.

Table S1. Symmetry coordinates for *trans* conformer of (chloromethyl)fluorosilane.

Description		Symmetry Coordinate ^a	
A'	CH ₂ symmetric stretch	S ₁	= r ₁ + r ₂
	SiH ₂ symmetric stretch	S ₂	= r ₃ + r ₄
	CH ₂ deformation	S ₃	= ϕ ₁
	CH ₂ wag	S ₄	= ϕ ₁ + ϕ ₂
	SiH ₂ deformation	S ₅	= ϕ ₂
	SiH ₂ wag	S ₆	= ϕ ₃ + ϕ ₄
	Si-F stretch	S ₇	= R ₁
	C-Cl stretch	S ₈	= R ₂
	C-Si stretch	S ₉	= R ₃
	CSiF in-plane-bend	S ₁₀	= 2θ ₁ - ϕ ₃ - ϕ ₄
	SiCCl in-plane-bend	S ₁₁	= 2θ ₂ - ϕ ₁ - ϕ ₂
A''	CH ₂ antisymmetric stretch	S ₁₂	= r ₁ - r ₂
	SiH ₂ antisymmetric stretch	S ₁₃	= r ₃ - r ₄
	CH ₂ twist	S ₁₄	= σ ₁ - σ ₂
	CH ₂ rock	S ₁₅	= ϕ ₁ - ϕ ₂
	SiH ₂ twist	S ₁₆	= σ ₃ - σ ₄
	SiH ₂ rock	S ₁₇	= ϕ ₃ - ϕ ₄
	torsion	S ₁₈	= σ

^a Not normalized.

Table S2. Temperature and intensity ratios of the conformational bands of (chloromethyl)fluorosilane from the Raman spectra of the liquid krypton solution phase.

T(°C)	1/T ($\times 10^3$ K ⁻¹)	I ₈₁₉ / I ₇₆₃	I ₈₁₉ / I ₁₁₂₄
-133.0	7.144	0.3796	0.5714
-143.0	7.692	0.4080	0.6329
-153.0	8.333	0.4286	0.7059
ΔH^a (cm ⁻¹)		71 $\pm$ 8	123 $\pm$ 31

^a Average value: $\Delta H = 97 \pm 16$ cm⁻¹ (1.16 ± 0.19 kJ mol⁻¹) with the *trans* conformer the more stable form and the statistical uncertainty (σ) obtained by utilizing all of the data as a single set.

Fig. S1 Temperature (-133 to -153°C) dependent Raman spectrum of (chloromethyl)fluorosilane dissolved in liquid krypton solution.

Fig. S2 Internal coordinates for (chloromethyl)fluorosilane.

Fig. S3 Potential function (MP2(full)) governing the internal rotation of the (fluoromethyl)fluorosilane from the trans to the gauche form.

Fig. S4 Potential function (MP2(full)) governing the internal rotation of the (chloromethyl)chlorosilane from the trans to the gauche form.

Fig. S5 Potential function (MP2(full)) governing the internal rotation of the (chloromethyl)bromosilane from the trans to the gauche form.

Fig. S6 Potential function (MP2(full)) governing the internal rotation of the (bromomethyl)fluorosilane from the trans to the gauche form.