Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information for Quantum Chemical Rovibrational Spectroscopic Data for Possible Observation of Thiocarbonic Acid (H_2CS_3) in Interstellar Environments

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Table S1: Optimized Geometry (in Å) of *cis-cis*-thiocarbonic acid

S	0.0000000000	0.0000000000	-1.7388278764
C	0.0000000000	0.0000000000	-0.1137781677
S	0.0000000000	1.4316265193	0.8950580619
S	0.0000000000	-1.4316265193	0.8950580619
H	0.0000000000	2.2817529563	-0.1377619888
H	0.0000000000	-2.2817529563	-0.1377619888

Table S2: Optimized Geometry (in Å) of *trans-trans*-thiocarbonic acid

S	0.0000000000	0.0000000000	-1.6906093597
C	0.0000000000	0.0000000000	-0.0637277599
S	0.0000000000	1.5197880605	0.7928300737
S	0.0000000000	-1.5197880605	0.7928300737
H	0.0000000000	1.0552057055	2.0487855770
H	0.0000000000	-1.0552057055	2.0487855770

Table S3: Optimized Geometry (in Å) of *cis-trans*-thiocarbonic acid

S	0.0000000000	-0.8581422533	-1.4949384022
C	0.0000000000	-0.0605453582	-0.0797147179
S	0.0000000000	1.6847025577	-0.0539084510
S	0.0000000000	-0.7974218721	1.5056924031
H	0.0000000000	1.8487702929	1.2778993964
H	0.0000000000	-2.0541077561	1.0446447499

Table S4: Fermi resonances for *cis-cis*-thiocarbonic acid

$2\omega_7 = \omega_3$
$\omega_{10} + \omega_7 = \omega_4$
$2\omega_8 = 2\omega_9 = \omega_9 + \omega_8 = \omega_{10} + \omega_6 = \omega_{11} + \omega_7 = \omega_5$
$\omega_{10} + \omega_7 = \omega_{12} + \omega_8 = \omega_{12} + \omega_9 = \omega_6$
$2\omega_{10} = 2\omega_{12} = \omega_7$
$\omega_{12} + \omega_{10} = \omega_9$
$2\omega_{12} = \omega_{11}$

Table S5: Fermi resonances for *trans-trans*-thiocarbonic acid

$$2\omega_7 = \omega_9 + \omega_5 = \omega_{11} + \omega_6 = \omega_3$$
$$\omega_9 + \omega_6 = \omega_4$$
$$2\omega_7 = 2\omega_8 = \omega_{10} + \omega_8 = \omega_5$$
$$\omega_{11} + \omega_7 = \omega_6$$
$$2\omega_{12} = \omega_7$$
$$\omega_{12} + \omega_{11} = \omega_8$$
$$2\omega_{12} = \omega_9$$
$$\omega_{12} + \omega_{11} = \omega_{10}$$

Table S6: Fermi resonances for *cis-trans*-thiocarbonic acid

$$2\omega_7 = \omega_3$$
$$2\omega_8 = \omega_9 + \omega_8 = \omega_{11} + \omega_5 = \omega_{11} + \omega_6 = \omega_4$$
$$2\omega_7 = 2\omega_8 = 2\omega_9 = \omega_9 + \omega_8 = \omega_{11} + \omega_7 = \omega_{12} + \omega_8 = \omega_5$$
$$2\omega_9 = \omega_9 + \omega_8 = \omega_{10} + \omega_7 = \omega_{11} + \omega_7 = \omega_{12} + \omega_8 = \omega_{12} + \omega_9 = \omega_6$$
$$2\omega_{12} = \omega_7$$
$$\omega_{12} + \omega_{10} = \omega_8$$

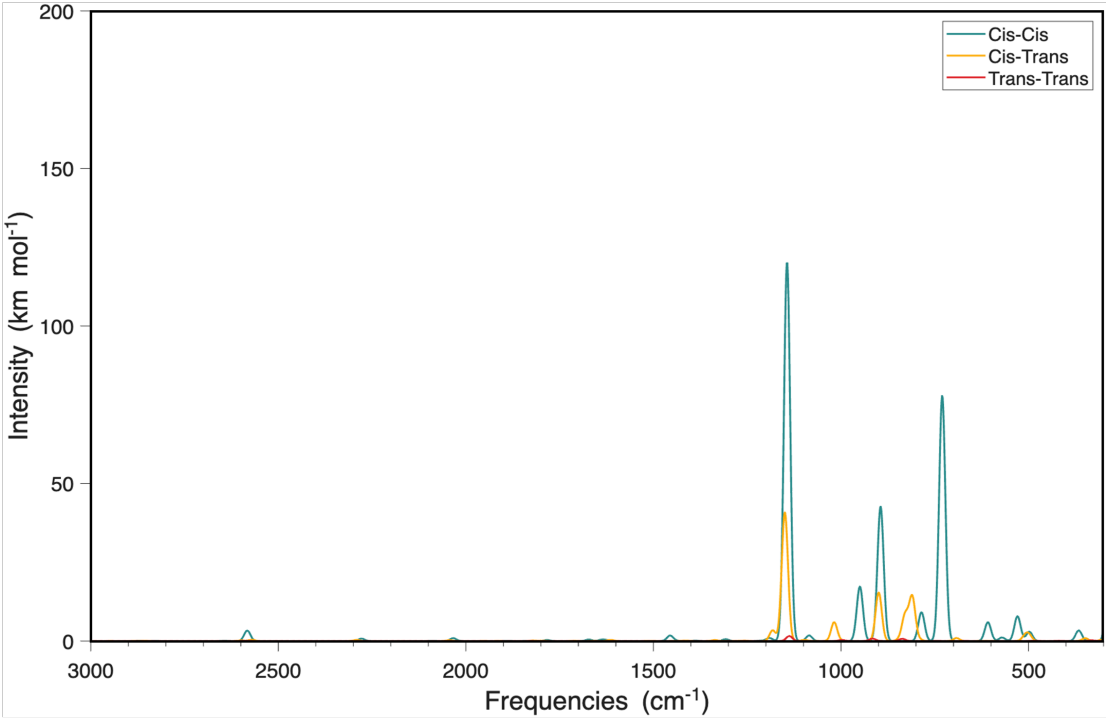

Figure S1: A visual depiction of the IR spectrum for the three conformers of thiocarbonic acid artificially broadened with a FWHM of 3.0 cm^{-1} at 300K computed from the relative energies in the main body of the manuscript.

Table S7: Rotational Constants (in MHz) for all three conformers of thiocarbonic acid

Const.	Units	*cis-cis*	*trans-trans*	*cis-trans*
A_e	MHz	3572.6	3608.5	3551.1
B_e	MHz	3409.1	3368.6	3439.2
C_e	MHz	1744.5	1742.2	1747.1
A_0	MHz	3566.7	3586.1	3534.3
B_0	MHz	3383.4	3354.0	3421.0
C_0	MHz	1735.0	1732.3	1737.0
A_1	MHz	3566.8	3592.1	3534.0
B_1	MHz	3382.2	3348.2	3420.6
C_1	MHz	1734.8	1732.2	1736.8
A_2	MHz	3566.8	3590.4	3538.1
B_2	MHz	3382.3	3350.5	3417.9
C_2	MHz	1734.8	1732.4	1737.1
A_3	MHz	3558.1	3577.9	3526.8
B_3	MHz	3373.6	3347.6	3410.9
C_3	MHz	1730.1	1728.4	1732.3
A_4	MHz	3565.1	3577.6	3527.2
B_4	MHz	3374.4	3345.9	3415.9
C_4	MHz	1731.7	1727.4	1733.2
A_5	MHz	3564.3	3588.1	3529.7
B_5	MHz	3379.0	3344.0	3418.2
C_5	MHz	1732.2	1729.5	1734.2
A_6	MHz	3566.8	3577.6	3527.5
B_6	MHz	3370.9	3346.4	3411.5
C_6	MHz	1730.2	1726.7	1731.2
A_7	MHz	3558.4	3584.7	3528.1
B_7	MHz	3381.2	3345.6	3416.7
C_7	MHz	1732.2	1729.3	1734.0
A_8	MHz	3564.9	3585.1	3532.4
B_8	MHz	3384.0	3352.2	3421.2
C_8	MHz	1736.7	1733.4	1738.4
A_9	MHz	3554.6	3598.7	3529.4
B_9	MHz	3384.6	3348.2	3417.1
C_9	MHz	1733.7	1731.6	1735.9
A_{10}	MHz	3574.3	3579.7	3542.7
B_{10}	MHz	3381.9	3355.2	3419.2
C_{10}	MHz	1734.4	1732.5	1736.5
A_{11}	MHz	3567.6	3588.7	3543.4
B_{11}	MHz	3387.9	3357.7	3427.5
C_{11}	MHz	1734.4	1732.1	1736.4
A_{12}	MHz	3580.9	3547.9	3519.1
B_{12}	MHz	3366.8	3377.4	3418.6
C_{12}	MHz	1736.2	1732.6	1737.0

Table S8: Harmonic fundamental vibrational frequencies (in cm^{-1}) of *cis-cis*-H_2CS_3.

mode	sym.	Description	F12-TcCR	f
ν_1	a_1	SH Stretch	2713.0	1
ν_2	b_2	SH Stretch	2711.2	4
ν_3	a_1	CS Stretch	1175.7	163
ν_4	b_2	IPB	999.9	23
ν_5	a_1	CS Stretch	918.1	58
ν_6	b_2	IPB	766.6	105
ν_7	a_1	CS Stretch	506.6	4
ν_8	b_1	OPB	466.3	5
ν_9	b_2	IPB	296.1	2
ν_{10}	b_1	OPB	408.6	26
ν_{11}	a_1	IPB	254.7	1
ν_{12}	a_2	OPB	211.6	0
ZPT			5536.2	

Table S9: Harmonic fundamental vibrational frequencies (in cm^{-1}) of *trans-trans*-H_2CS_3.

mode	sym.	Description	F12-TcCR	f
ν_1	a_1	SH Stretch	2704.4	8
ν_2	b_2	SH Stretch	2687.8	1
ν_3	a_1	CS Stretch	1161.4	152
ν_4	b_2	IPB	1017.3	31
ν_5	a_1	CS Stretch	930.7	75
ν_6	b_2	IPB	836.1	69
ν_7	a_1	CS Stretch	491.7	10
ν_8	b_1	OPB	478.0	6
ν_{10}	b_1	OPB	284.9	1
ν_{12}	a_2	OPB	150.2	0
ν_9	a_1	IPB	287.5	22
ν_{11}	b_2	IPB	259.8	1
ZPT			5632.1	

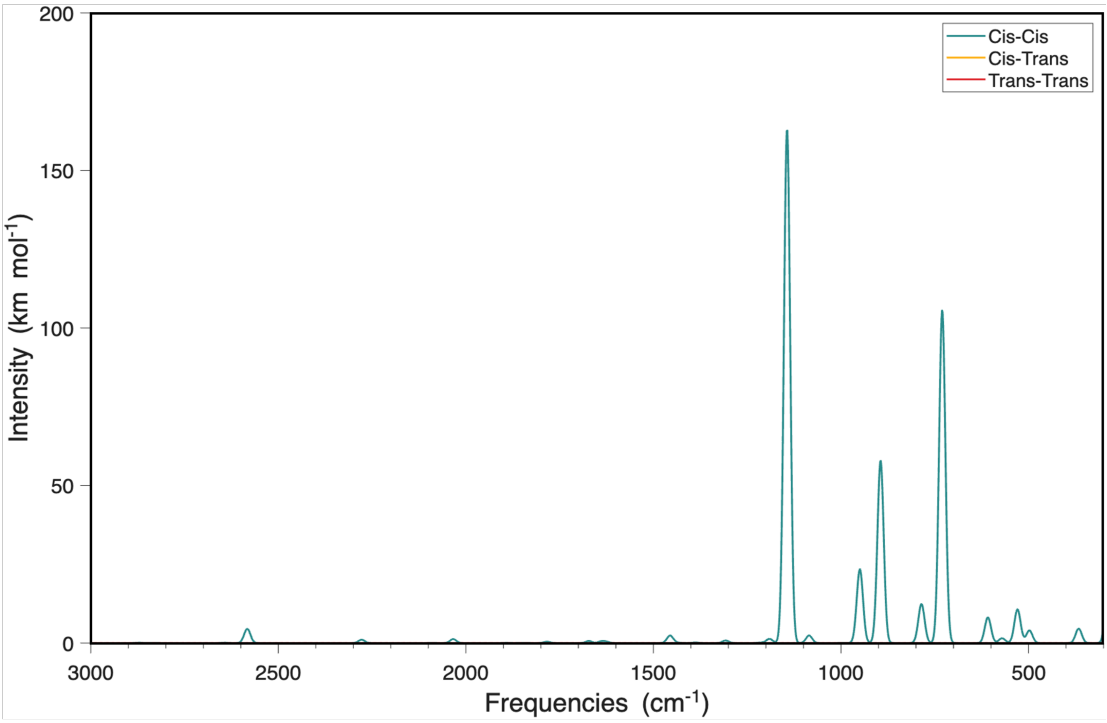

Figure S2: A visual depiction of the IR spectrum for the three conformers of thiocarbonic acid artificially broadened with a FWHM of 3.0 cm^{-1} at 10K computed from the relative energies in the main body of the manuscript.

Table S10: Harmonic fundamental vibrational frequencies (in cm^{-1}) of *cis-trans*-H_2CS_3.

mode	sym.	Description	F12-TcCR	f
ν_1	a′	S(2)H Stretch	2704.7	1
ν_2	a′	S(3)H Stretch	2675.3	2
ν_3	a′	CS Stretch	1174.4	162
ν_4	a′	IPB	1024.6	24
ν_5	a′	CS Stretch	903.5	61
ν_6	a′	IPB	817.5	56
ν_7	a′	CS Stretch	501.7	6
ν_8	a″	OPB	470.5	7
ν_9	a″	OPB	372.3	4
ν_{10}	a′	IPB	281.2	2
ν_{11}	a″	OPB	247.0	23
ν_{12}	a′	IPB	256.8	1
ZPT			5691.4	