Supplementary tables for the manuscript:

Isothiocyanato-Containing Carbon Chains: The Laboratory Detection of HCCCCNCS and NCCCNCS via Rotational Spectroscopy

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Appendix I: Equilibrium structures of HC_4NCS and NC_3NCS (Tables S1-S4)

Appendix II: Relative energies of HC_4NCS and NC_3NCS (Table S5)

Appendix I: Equilibrium structures of HC_4NCS and NC_3NCS

Table S1: Cartesian coordinates for HC_4NCS at MP2/cc-pVQZ level of theory

H	-5.63204600	0.00000000	0.00000000
C	-4.56918500	0.00000000	0.00000000
C	-3.34566700	0.00000000	0.00000000
C	-1.98782500	0.00000000	0.00000000
C	-0.75849500	0.00000000	0.00000000
N	0.52668700	0.00000000	0.00000000
C	1.72840700	0.00000000	0.00000000
S	3.29956900	0.00000000	0.00000000

Table S2: Cartesian coordinates for HC_4NCS at CCSD(T)/cc-pVTZ level of theory

H	-5.58617366	0.00000000	0.00000000
C	-4.52220557	0.00000000	0.00000000
C	-3.30572491	0.00000000	0.00000000
C	-1.93419126	0.00000000	0.00000000
C	-0.71447611	0.00000000	0.00000000
N	0.58190098	0.00000000	0.00000000
C	1.77647393	0.00000000	0.00000000
S	3.35710065	0.00000000	0.00000000

Table S3: Cartesian coordinates for NC_3NCS at MP2/cc-pVQZ level of theory

N	-4.48909500	0.00000000	0.00000000
C	-3.31189800	0.00000000	0.00000000
C	-1.95214100	0.00000000	0.00000000
C	-0.72804800	0.00000000	0.00000000
N	0.55159100	0.00000000	0.00000000
C	1.75265100	0.00000000	0.00000000

S	3.31244600	0.00000000	0.00000000

Table S4: Cartesian coordinates for NC_3NCS at CCSD(T)/cc-pVTZ level of theory

N	-4.49198360	0.00000002	0.00000009
C	-3.32325611	-0.00000001	-0.00000001
C	-1.94834132	-0.00000001	-0.00000006
C	-0.73030498	-0.00000001	-0.00000005
N	0.56102391	-0.00000000	-0.00000003
C	1.75881715	0.00000001	-0.00000002
S	3.33261696	0.00000001	0.00000008

Table S5: Relative energies of HC_4NCS and NC_3NCS (in kJ mol^{-1}) as a function of the CNC angle, calculated at the MP2/cc-pVQZ levels of theory.

	180	179	178	177	176	175
HC_4NCS	0	0.002	0.009	0.022	0.039	0.062
NC_3NCS	0	0.001	0.003	0.006	0.012	0.018