The Conformers of Allyl-Isothiocyanate: A Combined Microwave Spectroscopy and Computational Study

Joseph Stitsky, Weslley G. D. P. Silva, Wenhao Sun and Jennifer van Wijngaarden*

Department of Chemistry, University of Manitoba, Winnipeg, Manitoba, R3T 2N2, Canada

*Corresponding Author
Email: vanwijng@cc.umanitoba.ca
Phone: (204)-474-8379
Fax: (204)-474-7608

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Appendix I: Comparison of Basis Sets Used to Estimate Spectroscopic Constants of Allyl-NCS at the B3LYP-D3BJ Level.

Table S1. Spectroscopic Parameters for Conformer I of Allyl-NCS Calculated at the B3LYP-D3BJ Method Using Different Basis Sets and Comparison with Experimental Values.

Parameter	cc-pVDZ	cc-pVTZ	cc-pVQZ	cc-pV(D+d)Z	cc-pV(T+d)Z	cc-pV(Q+d)Z	aug-cc-pVDZ	aug-cc-pVTZ	aug-cc-pVQZ	aug-cc-pV(D+d)Z	aug-cc-pV(T+d)Z	aug-cc-pV(Q+d)Z
Rotational Constants/MHz												
A	6779.866	7011.024	7018.38	6766.741	7018.203	7019.250	6836.536	7020.493	7016.842	6831.920	7018.336	6997.393
%A*	2.7863	0.5282	0.6337	2.9745	0.6311	0.6462	1.9737	0.6640	0.6116	2.0399	0.6330	0.3328
B	1504.184	1487.146	1488.33	1512.119	1487.449	1489.872	1488.543	1484.007	1488.340	1494.304	1487.211	1493.485
%B	0.2658	0.8699	0.7910	0.7947	0.8497	0.6882	0.7768	1.0792	0.7904	0.3928	0.8656	0.4474
C	1248.566	1241.968	1245.07	1254.042	1244.369	1246.199	1243.583	1242.038	1245.062	1248.726	1244.270	1248.634
%C	0.0054	0.5231	0.2746	0.4440	0.3308	0.1842	0.3938	0.5175	0.2753	0.0182	0.3387	0.0108
Centrifugal Distortion Constants/kHz												
D_J	0.9771	2.803	1.12	0.979	1.109	1.134	1.066	1.084	1.130	1.093	1.115	1.100
D_{JK}	-2.2207	-0.045	-4.43	-1.956	-4.586	-4.339	-4.079	-4.600	-4.251	-4.315	-4.443	-4.222
D_K	34.6944	-0.532	49.06	33.841	48.963	49.575	42.631	48.279	49.387	43.515	49.085	47.195
d_1	-0.3166	0.283	-0.35	-0.321	-0.342	-0.354	-0.330	-0.332	-0.353	-0.338	-0.346	-0.342
d_2	-0.0452	-0.228	-0.04	-0.047	-0.044	-0.046	-0.042	-0.042	-0.046	-0.043	-0.045	-0.044
^{14}N Quadrupole Coupling Constants/kHz												
3/2 χ_{aa}	3.2791	2.803	2.80	3.294	2.805	2.831	2.964	2.773	2.818	2.971	2.789	2.830
1/4 (χ_{bb}-χ_{cc})		-0.045	-0.04		-0.032	-0.035		-0.031	-0.036	0.014	-0.032	-0.036

*The % deviation in the rotational constants were calculated as $\%A = (A_{calc}-A_{exp}/A_{exp})\cdot 100$.

Appendix II: Observed Transitions of Allyl-NCS Conformers I and III.

Table S2. Observed Rotational Transitions for the Parent Species of Conformer I

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
4	0	4	5	3	0	3	4	10910.27500	-0.0008
4	0	4	4	3	0	3	3	10910.28790	0.0012
4	0	4	3	3	0	3	2	10910.32720	-0.0015
3	0	3	4	2	0	2	3	8212.09190	-0.0005
3	0	3	3	2	0	2	2	8212.11150	-0.0003
3	0	3	2	2	0	2	1	8212.20430	-0.0006
3	1	3	4	2	1	2	3	7863.21780	-0.0003
3	1	3	3	2	1	2	2	7863.37740	-0.0011
4	1	3	5	3	1	2	4	11480.31470	-0.0015
4	1	3	3	3	1	2	2	11480.34220	0.0005
4	1	3	4	3	1	2	3	11480.38670	-0.0012
5	2	3	6	4	2	2	5	13890.88660	0.0003
5	2	3	5	4	2	2	4	13891.01780	-0.0004
5	0	5	6	4	0	4	5	13576.20850	-0.0007
5	0	5	5	4	0	4	4	13576.21520	0.0000
5	0	5	4	4	0	4	3	13576.23830	-0.0023
4	1	4	5	3	1	3	4	10474.76030	-0.0005
4	1	4	3	3	1	3	2	10474.78430	0.0017
4	1	4	4	3	1	3	3	10474.83110	-0.0006
5	1	5	6	4	1	4	5	13078.61280	-0.0019
5	1	5	4	4	1	4	3	13078.63350	-0.0002
5	1	5	5	4	1	4	4	13078.65410	0.0010
3	2	1	2	2	2	0	1	8279.45160	-0.0019
3	2	1	4	2	2	0	3	8279.78150	0.0043
3	2	1	3	2	2	0	2	8280.36020	-0.0008
3	2	1	3	2	2	0	2	8280.36020	-0.0008
3	2	1	2	2	2	0	1	8279.45150	-0.0019
3	2	1	4	2	2	0	3	8279.77860	0.0014
4	3	1	3	3	3	0	2	11011.91740	-0.0008
4	3	1	5	3	3	0	4	11012.12840	0.0016
4	3	1	4	3	3	0	3	11012.66580	0.0001
4	2	2	3	3	2	1	2	11072.09800	-0.0006
4	2	2	5	3	2	1	4	11072.16250	0.0000
4	2	2	4	3	2	1	3	11072.41100	-0.0006
4	3	2	3	3	3	1	2	11010.85010	0.0024

4	3	2	5	3	3	1	4	11011.05950	0.0033
4	3	2	4	3	3	1	3	11011.59580	0.0009
5	2	3	4	4	2	2	3	13890.86960	-0.0032
5	2	3	6	4	2	2	5	13890.88670	0.0005
5	2	3	5	4	2	2	4	13891.01780	-0.0004
4	2	3	3	3	2	2	2	10987.89800	-0.0010
4	2	3	5	3	2	2	4	10987.96260	0.0001
4	2	3	4	3	2	2	3	10988.20830	-0.0006
5	2	4	4	4	2	3	3	13724.20330	-0.0021
5	2	4	6	4	2	3	5	13724.22070	0.0022
5	2	4	5	4	2	3	4	13724.34610	-0.0009
5	3	3	4	4	3	2	3	13770.41500	0.0004
5	3	3	6	4	3	2	5	13770.48410	0.0011
5	3	3	5	4	3	2	4	13770.76210	0.0001
5	3	2	4	4	3	1	3	13774.15430	-0.0007
5	3	2	6	4	3	1	5	13774.22400	0.0005
5	3	2	5	4	3	1	4	13774.50240	-0.0004
5	1	4	6	4	1	3	5	14333.04120	-0.0006
5	1	4	4	4	1	3	3	14333.06040	-0.0026
5	1	4	5	4	1	3	4	14333.08170	0.0011
6	0	6	6	5	0	5	5	16204.63960	-0.0022
6	0	6	5	5	0	5	4	16204.66250	0.0026
6	2	4	5	5	2	3	4	16739.73900	0.0001
6	2	4	6	5	2	3	5	16739.81840	-0.0003
6	2	5	5	5	2	4	4	16453.30370	0.0006
6	2	5	6	5	2	4	5	16453.37770	-0.0009
6	3	4	6	5	3	3	5	16533.49690	0.0010
6	1	6	6	5	1	5	5	15673.52280	0.0015
3	2	2	4	2	2	1	3	8245.92750	0.0012
3	2	2	2	2	2	1	1	8245.60250	-0.0006
3	1	2	3	2	1	1	2	8618.22320	-0.0007
7	1	7	6	6	1	6	6	18257.85500	0.0000
7	1	7	6	6	1	6	5	18258.51500	0.0011
7	0	7	6	6	0	6	5	18793.43290	0.0027
7	2	5	6	6	2	4	5	19619.35910	-0.0010
7	2	5	6	6	2	4	6	19618.81710	0.0001
7	1	6	6	6	1	5	6	19996.54470	0.0011
7	2	6	6	6	2	5	5	19173.83870	-0.0020
7	3	4	6	6	3	3	5	19321.68400	-0.0012
7	3	5	6	6	3	4	5	19299.41930	-0.0010
7	0	7	6	6	0	6	6	18792.70560	-0.0001

6	1	5	5	5	1	4	5	17172.49990	-0.0003
6	1	5	6	5	1	4	6	17173.79250	0.0003
6	1	5	6	5	1	4	5	17173.21160	0.0025
5	1	5	6	4	0	4	5	17525.04920	-0.0005
5	1	5	4	4	0	4	3	17525.09720	0.0005
5	1	5	5	4	0	4	4	17524.98040	0.0008
3	1	3	4	2	0	2	3	13094.04330	0.0008
3	1	3	3	2	0	2	2	13093.89340	0.0000
3	1	3	2	2	0	2	1	13094.21560	0.0016
4	1	4	4	3	0	3	3	15356.61200	-0.0012
4	1	4	5	3	0	3	4	15356.71370	0.0028
4	1	4	3	3	0	3	2	15356.79000	-0.0016
1	1	1	1	0	0	0	1	8222.39680	-0.0011
1	1	1	2	0	0	0	1	8222.68850	0.0005
6	1	6	6	5	0	5	5	19622.28490	-0.0007
7	1	7	6	6	0	6	5	21676.22170	-0.0014
2	1	2	2	1	0	1	1	10719.38980	0.0001
2	1	2	3	1	0	1	2	10719.66320	0.0015
5	1	5	5	4	0	4	4	17524.97980	0.0002
6	0	6	5	5	1	5	4	12255.8077	0.0038
6	0	6	6	5	1	5	5	12255.8766	-0.0008

Table S3. Observed Rotational Transitions for the ^{34}S Substituted Species of Conformer I

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
3	1	3	4	2	1	2	3	7660.9906	0.0003
3	1	3	2	2	1	2	1	7660.9906	0.0008
3	1	3	3	2	1	2	2	7661.1511	-0.0005
3	1	2	4	2	1	1	3	8377.7588	-0.0012
3	1	2	3	2	1	1	2	8377.9223	-0.0004
4	0	4	5	3	0	3	4	10623.0588	-0.0011
4	0	4	4	3	0	3	3	10623.0740	0.0030
4	0	4	3	3	0	3	2	10623.1128	-0.0002
5	1	5	6	4	1	4	5	12744.2037	-0.0006
5	1	5	4	4	1	4	3	12744.2247	0.0012
5	1	5	5	4	1	4	4	12744.2415	-0.0013
4	1	4	5	3	1	3	4	10206.0729	-0.0007
4	1	4	4	3	1	3	3	10206.1449	0.0000
5	1	4	6	4	1	3	5	13935.7083	0.0011

5	1	4	4	4	1	3	3	13935.7267	-0.0017
5	1	4	5	4	1	3	4	13935.7478	0.0016
5	0	5	6	4	0	4	5	13223.2572	-0.0006
5	0	5	5	4	0	4	4	13223.2650	0.0009
5	0	5	4	4	0	4	3	13223.2894	0.0000
3	1	3	4	2	0	2	3	12931.1952	0.0013
3	1	3	3	2	0	2	2	12931.0437	-0.0004
3	1	3	2	2	0	2	1	12931.3667	0.0005
1	1	1	1	0	0	0	1	8175.9996	-0.0019
1	1	1	2	0	0	0	1	8176.2936	0.0005
3	0	3	4	2	0	2	3	7993.7278	0.0000
3	0	3	3	2	0	2	2	7993.7479	0.0004
3	0	3	2	2	0	2	1	7993.8403	-0.0005
6	0	6	5	5	0	5	4	15789.3482	0.0023
6	1	6	6	5	1	5	5	15274.2172	0.0012
4	2	3	3	3	2	2	2	10692.8311	-0.0016
4	2	3	4	3	2	2	3	10693.1430	-0.0012
4	2	3	5	3	2	2	4	10692.8974	0.0009
4	1	3	5	3	1	2	4	11160.9942	0.0002
4	1	3	3	3	1	2	2	11161.0211	0.0016
4	1	3	4	3	1	2	3	11161.0659	-0.0002
5	2	4	4	4	2	3	3	13356.4585	-0.0032
5	2	4	6	4	2	3	5	13356.4752	0.0002
5	2	4	5	4	2	3	4	13356.6019	-0.0022
5	2	3	4	4	2	2	3	13506.4317	-0.0011
5	2	3	6	4	2	2	5	13506.4496	0.0032
5	2	3	5	4	2	2	4	13506.5801	0.0012
5	3	2	4	4	3	1	3	13401.2321	0.0007
5	3	2	6	4	3	1	5	13401.3010	0.0009
5	3	2	5	4	3	1	4	13401.5804	-0.0004
6	2	5	5	5	2	4	4	16013.5999	-0.0026
6	2	5	6	5	2	4	5	16013.6748	-0.0038
6	3	4	5	5	3	3	4	16085.7015	0.0022
6	3	4	6	5	3	3	5	16085.8895	-0.0001
6	3	3	6	5	3	2	5	16094.3443	0.0007

Table S4. Observed Rotational Transitions for the ^{13}C1 Substituted Species of Conformer I

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
6	0	6	6	5	0	5	5	16008.3709	-0.0009
6	0	6	5	5	0	5	4	16008.3893	-0.0006
5	0	5	6	4	0	4	5	13415.7750	-0.0001
5	0	5	5	4	0	4	4	13415.7828	0.0018
5	0	5	4	4	0	4	3	13415.8059	-0.0005
5	1	4	6	4	1	3	5	14183.5567	0.0015
5	1	4	4	4	1	3	3	14183.5736	-0.0026
5	1	4	5	4	1	3	4	14183.5937	0.0000
5	1	5	6	4	1	4	5	12919.6065	0.0003
5	1	5	4	4	1	4	3	12919.6246	-0.0005
5	1	5	5	4	1	4	4	12919.6443	0.0001
4	0	4	5	3	0	3	4	10784.2236	-0.0016
4	0	4	4	3	0	3	3	10784.2386	0.0027
4	0	4	3	3	0	3	2	10784.2775	-0.0003
4	1	3	5	3	1	2	4	11361.4531	-0.0002
4	1	3	3	3	1	2	2	11361.4790	0.0002
4	1	3	4	3	1	2	3	11361.5253	0.0006
3	0	3	4	2	0	2	3	8118.9782	-0.0001
3	1	2	4	2	1	1	3	8529.3149	-0.0002
4	2	3	4	3	2	2	3	10865.9681	-0.0012
6	2	5	6	5	2	4	5	16268.6138	-0.0009
6	2	5	5	5	2	4	4	16268.5408	0.0012
6	2	4	5	5	2	3	4	16568.3399	-0.0004
6	2	4	6	5	2	3	5	16568.4202	0.0001
4	2	3	3	3	2	2	2	10865.6594	-0.0018
4	2	3	5	3	2	2	4	10865.7261	0.0018
3	1	3	2	2	1	2	1	7768.5629	-0.0003
5	2	4	4	4	2	3	3	13570.8754	-0.0037
5	2	4	6	4	2	3	5	13570.8926	0.0004
5	2	4	5	4	2	3	4	13571.0200	0.0000
4	1	4	5	3	1	3	4	10348.1001	0.0000
4	1	4	4	3	1	3	3	10348.1706	0.0000
5	2	3	6	4	2	2	5	13745.5868	0.0003
5	2	3	5	4	2	2	4	13745.7177	-0.0002
6	1	5	5	5	1	4	4	16992.3920	-0.0006
6	1	5	6	5	1	4	5	16992.4018	0.0023

5	3	3	6	4	3	2	5	13619.3850	0.0000
4	3	2	5	3	3	1	4	10889.9525	0.0002
4	3	2	3	3	3	1	2	10889.7456	0.0007
4	3	2	4	3	3	1	3	10890.4907	0.0025
6	1	6	6	5	1	5	5	15481.7952	0.0014
5	3	2	6	4	3	1	5	13623.4755	0.0018
5	3	2	5	4	3	1	4	13623.7483	-0.0031

Table S5. Observed Rotational Transitions for the ^{13}C2 Substituted Species of Conformer I

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
4	0	4	5	3	0	3	4	10752.0403	-0.0009
4	0	4	4	3	0	3	3	10752.0538	0.0014
4	0	4	3	3	0	3	2	10752.0943	0.0002
3	0	3	4	2	0	2	3	8091.7125	-0.0007
3	0	3	3	2	0	2	2	8091.7365	0.0038
5	0	5	6	4	0	4	5	13381.9134	0.0001
5	0	5	5	4	0	4	4	13381.9213	0.0019
5	0	5	4	4	0	4	3	13381.9442	-0.0003
4	1	3	5	3	1	2	4	11303.8094	-0.0006
4	1	3	3	3	1	2	2	11303.8371	0.0015
4	1	3	4	3	1	2	3	11303.8816	0.0000
4	1	4	5	3	1	3	4	10326.9672	-0.0005
4	1	4	3	3	1	3	2	10326.9912	0.0016
4	1	4	4	3	1	3	3	10327.0390	0.0004
6	0	6	6	5	0	5	5	15976.2190	0.0001
6	0	6	5	5	0	5	4	15976.2370	0.0003
3	1	3	4	2	1	2	3	7751.9641	0.0010
3	1	3	2	2	1	2	1	7751.9641	0.0016
3	1	3	3	2	1	2	2	7752.1197	-0.0034
3	1	2	3	2	1	1	2	8485.3756	-0.0007
4	2	3	5	3	2	2	4	10825.2058	-0.0038
4	2	2	3	3	2	1	2	10904.4288	-0.0024
4	2	2	5	3	2	1	4	10904.4974	0.0024
4	2	2	4	3	2	1	3	10904.7439	0.0002
5	1	5	6	4	1	4	5	12894.7073	-0.0002
5	1	5	4	4	1	4	3	12894.7250	-0.0015
5	1	5	5	4	1	4	4	12894.7443	-0.0014
5	2	4	4	4	2	3	3	13521.3893	-0.0027

5	2	4	6	4	2	3	5	13521.4062	0.0011
5	2	4	5	4	2	3	4	13521.5336	0.0001
6	2	5	5	5	2	4	4	16210.8450	0.0005
6	2	4	5	5	2	3	4	16481.0063	-0.0001
6	2	4	6	5	2	3	5	16481.0875	0.0014
5	1	4	6	4	1	3	5	14113.4598	0.0003
5	1	4	4	4	1	3	3	14113.4773	-0.0033
5	1	4	5	4	1	3	4	14113.4979	-0.0003
5	2	3	4	4	2	2	3	13678.4245	-0.0022
5	2	3	6	4	2	2	5	13678.4414	0.0012
5	2	3	5	4	2	2	4	13678.5731	0.0013
4	2	3	3	3	2	2	2	10825.1480	0.0016
4	2	3	5	3	2	2	4	10825.2121	0.0024
4	2	3	4	3	2	2	3	10825.4562	0.0004

Table S6. Observed Rotational Transitions for the ^{13}C3 Substituted Species of Conformer I

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
4	0	4	5	3	0	3	4	10818.9641	-0.0008
4	0	4	4	3	0	3	3	10818.9768	0.0009
4	0	4	3	3	0	3	2	10819.0181	-0.0004
5	0	5	6	4	0	4	5	13461.1693	-0.0005
5	0	5	5	4	0	4	4	13461.1766	0.0006
5	0	5	4	4	0	4	3	13461.2025	0.0007
3	0	3	4	2	0	2	3	8144.0593	0.0001
3	0	3	3	2	0	2	2	8144.0810	0.0021
3	0	3	2	2	0	2	1	8144.1729	-0.0001
4	1	3	5	3	1	2	4	11389.7734	-0.0010
4	1	3	3	3	1	2	2	11389.8037	0.0036
4	1	3	4	3	1	2	3	11389.8443	-0.0027
5	1	5	6	4	1	4	5	12965.9127	-0.0001
5	1	5	4	4	1	4	3	12965.9345	0.0022
5	1	5	5	4	1	4	4	12965.9511	-0.0005
4	1	4	4	3	1	3	3	10384.8377	-0.0002
5	2	3	5	4	2	2	4	13780.7640	0.0006
5	2	3	6	4	2	2	5	13780.6311	0.0015
5	2	3	4	4	2	2	3	13780.6135	-0.0024
6	0	6	6	5	0	5	5	16065.4359	-0.0010
3	1	3	2	2	1	2	1	7795.8266	0.0001

3	1	3	3	2	1	2	2	7795.9869	-0.0025
3	1	3	4	2	1	2	3	7795.8266	-0.0003
4	1	4	5	3	1	3	4	10384.7660	-0.0001
5	1	4	6	4	1	3	5	14219.5836	0.0016
5	1	4	4	4	1	3	3	14219.6028	-0.0006
5	1	4	5	4	1	3	4	14219.6212	0.0000
5	2	4	6	4	2	3	5	13611.4040	0.0005
5	2	4	5	4	2	3	4	13611.5332	-0.0005
3	1	2	4	2	1	1	3	8550.2776	-0.0013
3	1	2	2	2	1	1	1	8550.2888	0.0026
3	1	2	3	2	1	1	2	8550.4397	-0.0032
4	3	2	4	3	3	1	3	10921.8012	0.0018
5	3	3	4	4	3	2	3	13658.2598	0.0010
5	3	3	6	4	3	2	5	13658.3254	-0.0025
4	2	3	5	3	2	2	4	10897.8386	0.0006

Table S7. Observed Rotational Transitions for the ^{13}C4 Substituted Species of Conformer I

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
6	0	6	6	5	0	5	5	16172.1834	-0.0019
6	0	6	5	5	0	5	4	16172.2067	0.0033
5	1	5	6	4	1	4	5	13052.4172	0.0001
5	1	5	4	4	1	4	3	13052.4362	0.0001
5	1	5	5	4	1	4	4	13052.4541	-0.0010
4	0	4	5	3	0	3	4	10888.4363	-0.0015
4	0	4	4	3	0	3	3	10888.4509	0.0021
4	0	4	3	3	0	3	2	10888.4890	-0.0016
4	1	4	5	3	1	3	4	10453.7805	-0.0001
4	1	4	3	3	1	3	2	10453.8052	0.0028
4	1	4	4	3	1	3	3	10453.8515	0.0001
3	0	3	4	2	0	2	3	8195.6588	-0.0004
3	0	3	3	2	0	2	2	8195.6809	0.0022
3	0	3	2	2	0	2	1	8195.7714	-0.0002
3	1	2	4	2	1	1	3	8600.8396	-0.0004
3	1	2	2	2	1	1	1	8600.8479	0.0006
3	1	2	3	2	1	1	2	8601.0019	0.0002
3	1	3	2	2	1	2	1	7847.4693	0.0000
3	1	3	4	2	1	2	3	7847.4693	-0.0004
3	1	3	3	2	1	2	2	7847.6285	-0.0013

5	0	5	6	4	0	4	5	13549.0261	-0.0006
5	0	5	5	4	0	4	4	13549.0338	0.0010
5	0	5	4	4	0	4	3	13549.0570	-0.0011
6	1	6	5	5	1	5	4	15642.1125	-0.0019
6	1	6	6	5	1	5	5	15642.1236	0.0009
4	2	3	3	3	2	2	2	10965.9194	-0.0027
4	2	3	5	3	2	2	4	10965.9864	0.0010
4	2	3	4	3	2	2	3	10966.2309	-0.0003
4	3	1	5	3	3	0	4	10990.1101	-0.0012
4	3	1	4	3	3	0	3	10990.6462	-0.0028
4	2	2	5	3	2	1	4	11050.0302	0.0012
4	2	2	4	3	2	1	3	11050.2771	-0.0006
4	1	3	5	3	1	2	4	11457.3728	-0.0003
4	1	3	3	3	1	2	2	11457.3992	0.0006
4	1	3	4	3	1	2	3	11457.4448	0.0000
5	2	4	6	4	2	3	5	13696.7684	0.0010
5	2	4	5	4	2	3	4	13696.8962	0.0005
5	3	3	6	4	3	2	5	13742.9570	0.0032
5	3	3	5	4	3	2	4	13743.2323	0.0000
5	3	2	4	4	3	1	3	13746.6179	-0.0015
5	3	2	6	4	3	1	5	13746.6891	0.0013
5	3	2	5	4	3	1	4	13746.9668	0.0003
5	2	3	4	4	2	2	3	13863.1087	-0.0031
5	2	3	6	4	2	2	5	13863.1263	0.0010
5	2	3	5	4	2	2	4	13863.2584	0.0014
5	1	4	6	4	1	3	5	14304.3963	0.0005
5	1	4	4	4	1	3	3	14304.4160	-0.0009
5	1	4	5	4	1	3	4	14304.4344	0.0000
6	2	5	5	5	2	4	4	16420.3919	0.0006
6	2	5	6	5	2	4	5	16420.4649	-0.0018
6	3	3	6	5	3	2	5	16510.3701	-0.0016
6	2	4	5	5	2	3	4	16706.2945	0.0008
6	2	4	6	5	2	3	5	16706.3731	-0.0003
6	1	5	5	5	1	4	4	17138.8748	-0.0015
6	1	5	6	5	1	4	5	17138.8843	0.0010
3	2	1	2	2	2	0	1	8262.8986	-0.0007
3	2	1	3	2	2	0	2	8263.8069	0.0021
6	3	4	5	5	3	3	4	16500.2566	0.0012
6	3	4	6	5	3	3	5	16500.4447	0.0003

Table S8. Observed Rotational Transitions for the ^{15}N Substituted Species of Conformer I

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
4	0	4	3	0	3	10895.7083	0.0000
3	0	3	2	0	2	8202.1958	-0.0001
5	0	5	4	0	4	13555.9263	0.0002
4	1	3	3	1	2	11473.0403	-0.0001
3	1	2	2	1	1	8612.9154	-0.0005
3	1	3	2	1	2	7850.6428	-0.0004
4	1	4	3	1	3	10457.6326	0.0002
4	2	3	3	2	2	10976.1714	0.0000
4	2	2	3	2	1	11063.3248	0.0005
5	1	5	4	1	4	13056.6980	-0.0001
5	2	4	4	2	3	13709.0622	-0.0003
5	3	3	4	3	2	13756.9600	0.0008
5	3	2	4	3	1	13760.9294	-0.0006
5	2	3	4	2	2	13881.4874	0.0004
5	1	4	4	1	3	14323.2929	0.0002
6	1	6	5	1	5	15646.5273	0.0000
6	0	6	5	0	5	16177.5612	0.0000
6	2	5	5	2	4	16434.5491	0.0005
6	3	4	5	3	3	16517.3129	-0.0012
6	3	3	5	3	2	16527.8703	0.0008
6	2	4	5	2	3	16730.6204	-0.0004
6	1	5	5	1	4	17160.4806	0.0000

Table S9. Observed Rotational Transitions for the Parent Species of Conformer III

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
6	0	6	6	5	0	5	5	14190.2211	-0.0030
6	0	6	5	5	0	5	4	14190.2466	0.0034
3	0	3	4	2	0	2	3	7121.7636	0.0000
3	0	3	3	2	0	2	2	7121.7847	0.0010
3	0	3	2	2	0	2	1	7121.8802	0.0008
5	0	5	6	4	0	4	5	11843.1719	-0.0010
5	0	5	5	4	0	4	4	11843.1789	0.0000
5	0	5	4	4	0	4	3	11843.2017	-0.0037
4	0	4	5	3	0	3	4	9486.4122	-0.0012

4	0	4	4	3	0	3	3	9486.4253	0.0007
4	0	4	3	3	0	3	2	9486.4671	-0.0007
4	1	4	5	3	1	3	4	9235.8514	0.0009
4	1	4	3	3	1	3	2	9235.8682	-0.0005
4	1	4	4	3	1	3	3	9235.9233	0.0011
5	1	4	6	4	1	3	5	12207.0716	0.0000
5	1	4	4	4	1	3	3	12207.0942	-0.0016
5	1	4	5	4	1	3	4	12207.1118	-0.0003
5	1	5	6	4	1	4	5	11541.0187	0.0006
5	1	5	4	4	1	4	3	11541.0368	0.0016
6	1	6	5	5	1	5	4	13843.7545	-0.0010
6	1	6	6	5	1	5	5	13843.7656	0.0005
3	1	2	3	2	1	1	2	7328.8676	-0.0001
3	1	2	4	2	1	1	3	7328.6990	-0.0005
3	1	2	2	2	1	1	1	7328.7199	0.0040
6	1	5	5	5	1	4	4	14642.2043	-0.0006
6	1	5	6	5	1	4	5	14642.2117	0.0005
7	1	7	6	6	1	6	5	16143.6485	0.0019
7	0	7	6	6	0	6	5	16525.9345	-0.0005
6	2	5	5	5	2	4	4	14252.0606	0.0004
6	2	5	6	5	2	4	5	14252.1372	-0.0007
6	2	4	5	5	2	3	4	14319.5694	-0.0029
6	2	4	6	5	2	3	5	14319.6555	0.0005
1	1	1	1	0	0	0	1	9165.9359	-0.0004
1	1	1	2	0	0	0	1	9166.2768	-0.0009
2	1	2	1	1	0	1	0	11410.3881	-0.0031
2	1	2	3	1	0	1	2	11409.6823	-0.0006
2	1	2	2	1	0	1	1	11409.3570	-0.0001
4	1	3	5	3	1	2	4	9769.0336	-0.0002
4	1	3	4	3	1	2	3	9769.1110	0.0023
3	2	2	2	2	2	1	1	7130.6342	-0.0002
3	2	2	4	2	2	1	3	7130.9675	0.0008
3	2	2	3	2	2	1	2	7131.5642	-0.0005
3	2	1	2	2	2	0	1	7138.4102	-0.0014
3	2	1	4	2	2	0	3	7138.7447	0.0003
3	2	1	3	2	2	0	2	7139.3460	0.0014
4	2	3	3	3	2	2	2	9506.2487	-0.0010
4	2	3	5	3	2	2	4	9506.3155	0.0005
4	2	3	4	3	2	2	3	9506.5680	-0.0003
4	3	1	4	3	3	0	3	9514.8176	0.0024
6	1	5	6	6	0	6	6	8364.1018	0.0002

4	1	4	4	3	0	3	3	15701.1430	0.0001
4	1	4	5	3	0	3	4	15701.2920	-0.0002
4	1	4	3	3	0	3	2	15701.3904	0.0024
3	1	3	3	2	0	2	2	13587.0034	-0.0009
3	1	3	4	2	0	2	3	13587.2068	0.0013
5	2	4	4	4	2	3	3	11880.1119	-0.0031
5	2	4	6	4	2	3	5	11880.1291	0.0007
5	2	4	5	4	2	3	4	11880.2604	-0.0001
5	1	5	6	4	0	4	5	17755.8965	-0.0002
4	1	3	5	4	0	4	5	7548.2043	0.0038
4	1	3	3	4	0	4	3	7548.2043	-0.0010
7	2	6	6	6	2	5	6	16621.2123	0.0002
7	2	6	6	6	2	5	5	16621.7529	-0.0009
7	1	6	6	6	1	5	6	17072.9325	0.0006
7	1	6	6	6	1	5	5	17073.7219	0.0022
6	1	6	5	5	0	5	4	19756.5041	-0.0012
5	1	5	4	4	0	4	3	17755.9574	0.0022
5	2	3	6	4	2	2	5	11918.8681	-0.0003
5	2	3	5	4	2	2	4	11919.0030	-0.0013

Table S10. Observed Rotational Transitions for the ^{34}S Substituted Species of Conformer III

J'	K_a'	K_c'	F'	J"	K_a"	K_c"	F"	ν_{obs} /MHz	$\nu_{obs-calc}$ /MHz
4	0	4	5	3	0	3	4	9245.0633	-0.0021
4	0	4	4	3	0	3	3	9245.0762	-0.0006
4	0	4	3	3	0	3	2	9245.1210	0.0006
5	0	5	6	4	0	4	5	11542.6874	-0.0021
5	0	5	5	4	0	4	4	11542.6952	-0.0006
5	0	5	4	4	0	4	3	11542.7191	-0.0031
6	0	6	6	5	0	5	5	13831.3751	0.0007
6	0	6	5	5	0	5	4	13831.3949	0.0015
5	1	4	6	4	1	3	5	11889.7654	0.0015
5	1	4	4	4	1	3	3	11889.7878	-0.0005
5	1	4	5	4	1	3	4	11889.8054	0.0003
4	1	4	5	3	1	3	4	9004.6840	0.0024
4	1	4	4	3	1	3	3	9004.7559	0.0016
6	1	5	5	5	1	4	4	14261.9455	-0.0022
6	1	5	6	5	1	4	5	14261.9544	0.0003
4	1	3	5	3	1	2	4	9514.9165	0.0023
4	1	3	4	3	1	2	3	9514.9913	0.0013

6	3	4	5	5	3	3	4	13909.5218	-0.0012
6	3	3	5	5	3	2	4	13910.3939	0.0014
5	2	3	5	4	2	2	4	11612.4313	-0.0008
5	2	3	4	4	2	2	3	11612.2784	-0.0023
5	2	3	6	4	2	2	5	11612.2958	0.0010
7	0	7	6	6	0	6	5	16109.5922	0.0000
7	1	6	6	6	1	5	5	16630.8100	0.0008

Appendix III: Ground State Effective (r_0) Geometry and Atomic Coordinates (Å) Used to Derive the Ground State Effective Geometry of Allyl-NCS Conformer I

FINAL RESULTS OF LEAST SQUARES FIT

R(6, 4) =	1.504338 +- 0.006182	R(C2-C3)
R(9, 6) =	1.429099 +- 0.007674	R(N-C3)
R(4, 1) =	1.338813 +- 0.006579	R(C1-C2)
R(10, 9) =	1.178425 +- 0.010268	R(C4-N)
R(11,10) =	1.583125 +- 0.005978	R(C5-S)
A(9, 6, 4) =	114.515754 +- 0.318809	A(C2-C3-N)
A(6, 4, 1) =	125.770102 +- 0.169074	A(C1-C2-C3)
A(10, 9, 6) =	152.555429 +- 0.293072	A(C3-N-C4)
D(10, 9, 6, 4) =	-33.945843 +- 0.443723	D(C3-N-C4-S)

Chi-squared = 0.0014313833
Deviation of fit = 0.010922

ATOM NO.	A	dA	B	dB	C	dC	MASS
1	-1.80224	0.00226	1.46224	0.00274	-0.06881	0.00035	12.0000000
2	-0.74244	0.00241	1.60161	0.00450	-0.22623	0.00094	1.0078250
3	-2.41334	0.00369	2.35237	0.00244	-0.03996	0.00086	1.0078250
4	-2.34959	0.00157	0.25025	0.00408	0.08580	0.00051	12.0000000
5	-3.41834	0.00173	0.14918	0.00602	0.24005	0.00121	1.0078250
6	-1.60784	0.00246	-1.05838	0.00344	0.06787	0.00052	12.0000000
7	-1.76899	0.00358	-1.58239	0.00327	1.01548	0.00078	1.0078250
8	-2.02784	0.00305	-1.70223	0.00308	-0.70797	0.00084	1.0078250
9	-0.20118	0.00631	-0.93969	0.00315	-0.15476	0.00050	14.0030740
10	0.83177	0.00431	-0.38330	0.00354	-0.04472	0.00068	12.0000000
11	2.26460	0.00075	0.28412	0.00170	0.04385	0.00022	31.9720710

Appendix IV: Kraitchman Coordinates (Å) Used to Derive the Substitution Structure of Allyl-NCS Conformer I. (note that the imaginary value was set to zero).

C(1)	1.79671	0.00084	1.46231	0.00103	0.03384*i	0.04435
C(2)	2.34514	0.00064	0.23704	0.00634	0.11079	0.01356
C(3)	1.60149	0.00094	1.05796	0.00142	0.04443	0.03381
C(4)	0.82082	0.00183	0.38090	0.00394	0.06605	0.02272
N15	0.09715	0.01544	0.93632	0.00160	0.19933	0.00753
S34	2.26180	0.00066	0.29308	0.00512	0.03552	0.04224

Appendix V: Calculated Atomic Coordinates (Å) in the Principal Axis System for the Equilibrium Geometry of Conformer I and the Transition State for the Interconversion of Ia/Ib. (note that the numbering scheme is the same as that used in Appendix 2).

<u>Conformer I</u>

ATOM NO.	A	B	C	MASS
1	1.850687	1.444860	-0.089780	12.0000000
2	0.804624	1.610775	-0.303353	1.0078252
3	2.485509	2.317719	-0.048175	1.0078252
4	2.347628	0.236366	0.114358	12.0000000
5	3.403902	0.108406	0.324437	1.0078252
6	1.584588	-1.059048	0.089144	12.0000000
7	1.689539	-1.563438	1.055122	1.0078252
8	2.030558	-1.727821	-0.650265	1.0078252
9	0.197559	-0.928476	-0.203916	14.0030740
10	-0.839734	-0.376708	-0.061230	12.0000000
11	-2.270109	0.291017	0.057701	31.9720710

<u>Transition State Ia-Ib</u>

ATOM NO.	A	B	C	MASS
1	-1.786792	1.468506	0.000000	12.0000000
2	-0.716218	1.613735	0.000000	1.0078252
3	-2.399420	2.358111	-0.000001	1.0078252
4	-2.340172	0.267459	0.000000	12.0000000
5	-3.419883	0.164215	-0.000001	1.0078252
6	-1.619732	-1.052420	0.000000	12.0000000
7	-1.929536	-1.635335	-0.872161	1.0078252
8	-1.929535	-1.635333	0.872164	1.0078252
9	-0.202016	-0.967811	0.000000	14.0030740
10	0.830163	-0.393085	0.000000	12.0000000
11	2.261448	0.287583	0.000000	31.9720710

Appendix VI: Transition State Geometries for the Interconversion Pathway Between the Enantiomeric Forms of Conformer I.

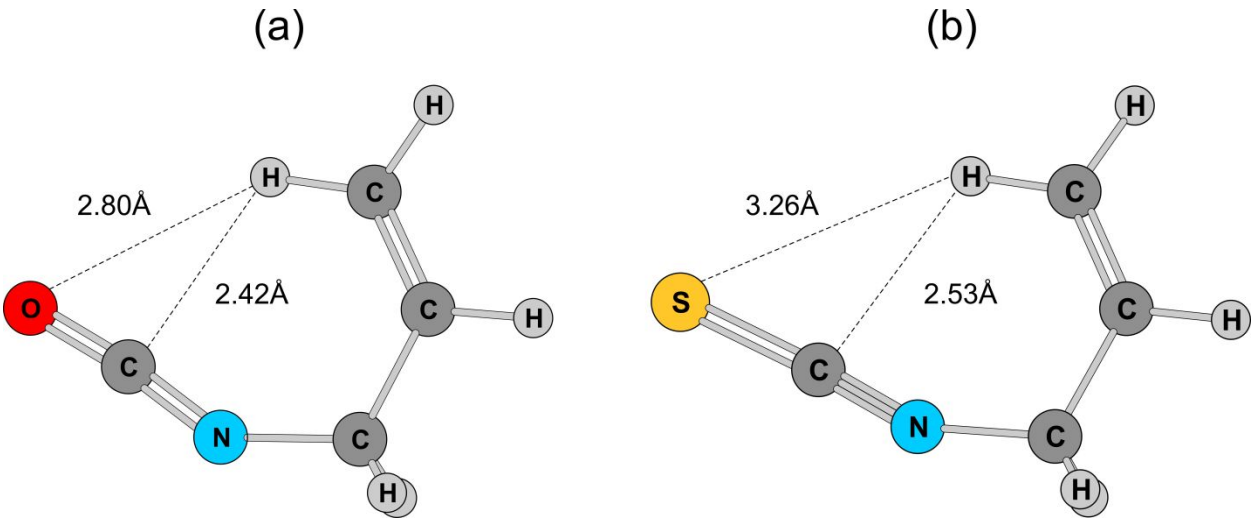

Figure S1. Optimized transition state geometries (B3LYP-D3(BJ)/cc-pVQZ) of (a) allyl-NCO and (b) allyl-NCS for the interconversion pathway between conformers Ia and Ib.

Appendix VII: Diagonalization of Nuclear Quadrupole Coupling Tensors of Conformers I of Allyl-NCS and Allyl-NCO.

<u>Allyl-NCS Confomer I</u>
Inertial tensor:

	a	b	c
a	1.80980 +- 0.00000	-0.54740 +- 0.00000	-0.27220 +- 0.00000
b	-0.54740 +- 0.00000	-0.96678 +- 0.00000	0.33330 +- 0.00000
c	-0.27220 +- 0.00000	0.33330 +- 0.00000	-0.84302 +- 0.00000

Principal tensor components:		SPFIT diagonal components:	
x	1.95304 +- 0.00000		
z	-1.26707 +- 0.00000	3/2 chi.aa	2.71470 +- 0.00000
y	-0.68597 +- 0.00000	1/4(bb-cc)	-0.03094 +- 0.00000

Direction cosines:

	a	b	c
x	0.973465 +-0.000000	-0.195987 +-0.000000	-0.118130 +-0.000000
z	0.093180 +-0.000000	0.810975 +-0.000000	-0.577613 +-0.000000
y	0.209006 +-0.000000	0.551278 +-0.000000	0.807718 +-0.000000

Rotation angles:

	a	b	c
x	13.2285 +- 0.0000	101.3024 +- 0.0000	96.7842 +- 0.0000
z	84.6534 +- 0.0000	35.8087 +- 0.0000	125.2828 +- 0.0000
y	77.9359 +- 0.0000	56.5452 +- 0.0000	36.1264 +- 0.0000

Eta = (chixx-chiyy)/chizz = -2.0827736 +- 0.0000000- ----allylnco

<u>Allyl-NCO Confomer I</u>

Inertial tensor:

	a	b	c
a	1.98167 +- 0.00000	-1.74530 +- 0.00000	0.22250 +- 0.00000
b	-1.74530 +- 0.00000	-0.65683 +- 0.00000	0.32970 +- 0.00000
c	0.22250 +- 0.00000	0.32970 +- 0.00000	-1.32483 +- 0.00000

Principal tensor components:		SPFIT diagonal components:	
x	2.85088 +- 0.00000		
z	-1.83218 +- 0.00000	3/2 chi.aa	2.97250 +- 0.00000
y	-1.01870 +- 0.00000	1/4(bb-cc)	0.16700 +- 0.00000

Direction cosines:

	a	b	c
x	0.895701 +-0.000000	-0.444478 +-0.000000	0.012632 +-0.000000
z	0.357765 +-0.000000	0.703506 +-0.000000	-0.614071 +-0.000000
y	0.264054 +-0.000000	0.554543 +-0.000000	0.789150 +-0.000000

Rotation angles:

	a	b	c
x	26.4014 +- 0.0000	116.3899 +- 0.0000	89.2762 +- 0.0000
z	69.0370 +- 0.0000	45.2910 +- 0.0000	127.8845 +- 0.0000
y	74.6893 +- 0.0000	56.3207 +- 0.0000	37.8939 +- 0.0000

Eta = (chixx-chiyy)/chizz = -2.1120070 +- 0.0000000

allylncs-conformerI-B3LYP-D3(BJ)/cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=vibrot b3lyp/cc-pvqz geom=connectivity empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	484
Electronic Energy (Eh)	-608.491564318
Sum of electronic and zero-point Energies (Eh)	-608.409849
Sum of electronic and thermal Energies (Eh)	-608.403133
Sum of electronic and enthalpy Energies (Eh)	-608.402188
Sum of electronic and thermal Free Energies (Eh)	-608.442
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C         1.757664       1.431514      -0.079048
H         0.711625       1.604746      -0.286851
H         2.396278       2.301060      -0.027331
C         2.250179       0.218228       0.106550
H         3.306577       0.082953       0.311356
C         1.481626      -1.073525       0.065736
H         1.587567      -1.591810       1.024222
H         1.922399      -1.733736      -0.684405
N         0.094221      -0.933103      -0.220921
C        -0.940279      -0.379079      -0.067138
S        -2.367446       0.292855       0.065803
```

__Frequencies__ (27 in total)

```
 1.     40.7144 cm-1
 2.     74.8403 cm-1
 3.    177.6899 cm-1
 4.    294.5812 cm-1
 5.    456.4883 cm-1
```

6. 467.3371 cm-1
7. 561.2638 cm-1
8. 589.9981 cm-1
9. 712.8594 cm-1
10. 906.1206 cm-1
11. 966.4435 cm-1
12. 995.2390 cm-1
13. 1027.3454 cm-1
14. 1054.3452 cm-1
15. 1167.1204 cm-1
16. 1280.4435 cm-1
17. 1327.3648 cm-1
18. 1375.5688 cm-1
19. 1456.1556 cm-1
20. 1484.6881 cm-1
21. 1716.1483 cm-1
22. 2174.5301 cm-1
23. 3003.7992 cm-1
24. 3037.8491 cm-1
25. 3137.0286 cm-1
26. 3152.0885 cm-1
27. 3230.9831 cm-1

```
***
```

allylncs-conformerI-MP2/cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=vibrot mp2/cc-pvqz geom=connectivity output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	484
Electronic Energy (Eh)	-606.428904598
Sum of electronic and zero-point Energies (Eh)	-607.425044
Sum of electronic and thermal Energies (Eh)	-607.418376
Sum of electronic and enthalpy Energies (Eh)	-607.417432
Sum of electronic and thermal Free Energies (Eh)	-607.456905
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.709388       1.431022      -0.089352
H          0.661714       1.559224      -0.317056
H          2.324071       2.315807      -0.035385
C          2.239858       0.230490       0.119975
H          3.294835       0.132375       0.345300
C          1.494087      -1.069701       0.077359
H          1.566879      -1.570134       1.045311
H          1.953288      -1.732925      -0.655083
N          0.118835      -0.923687      -0.254730
C         -0.928492      -0.374366      -0.070938
S         -2.357605       0.278550       0.073610
```

__Frequencies__ (27 in total)

```
```

1. 50.3052 cm-1 (Symmetry: A)
2. 83.1354 cm-1 (Symmetry: A)
3. 180.5874 cm-1 (Symmetry: A)
4. 302.9094 cm-1 (Symmetry: A)

5. 447.7729 cm-1 (Symmetry: A)
6. 462.5387 cm-1 (Symmetry: A)
7. 559.6087 cm-1 (Symmetry: A)
8. 591.8587 cm-1 (Symmetry: A)
9. 722.1108 cm-1 (Symmetry: A)
10. 927.1952 cm-1 (Symmetry: A)
11. 955.1612 cm-1 (Symmetry: A)
12. 1002.3921 cm-1 (Symmetry: A)
13. 1023.0301 cm-1 (Symmetry: A)
14. 1052.0303 cm-1 (Symmetry: A)
15. 1193.6131 cm-1 (Symmetry: A)
16. 1285.0261 cm-1 (Symmetry: A)
17. 1318.1757 cm-1 (Symmetry: A)
18. 1379.6542 cm-1 (Symmetry: A)
19. 1454.3509 cm-1 (Symmetry: A)
20. 1497.1000 cm-1 (Symmetry: A)
21. 1703.8689 cm-1 (Symmetry: A)
22. 2142.9292 cm-1 (Symmetry: A)
23. 3070.1203 cm-1 (Symmetry: A)
24. 3120.6384 cm-1 (Symmetry: A)
25. 3188.5791 cm-1 (Symmetry: A)
26. 3200.3783 cm-1 (Symmetry: A)
27. 3292.4266 cm-1 (Symmetry: A)

```
***
# allylncs-conformerI-B3LYP-D3(BJ)/cc-pVDZ


__Requested operations__

Run with Gaussian 16revisionB.01.

# opt freq=(vibrot,noraman) b3lyp/cc-pvdz empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__


| Datum | Value |
|:---|---:|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C4H5NS |
| Number of Basis Functions | 113 |
| Electronic Energy (Eh) | -608.387009163 |
| Sum of electronic and zero-point Energies (Eh) | -608.305562 |
| Sum of electronic and thermal Energies (Eh) | -608.298814 |
| Sum of electronic and enthalpy Energies (Eh) | -608.29787 |
| Sum of electronic and thermal Free Energies (Eh) | -608.337726 |
| Number of Imaginary Frequencies | 0 |
```

| Mean of alpha and beta Electrons | 26 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C 1.706094 1.455258 -0.083218
H 0.643604 1.600880 -0.290124
H 2.330151 2.349911 -0.032947
C 2.236500 0.247463 0.105127
H 3.308533 0.141604 0.309273
C 1.503748 -1.070303 0.069446
H 1.626072 -1.587921 1.039706
H 1.970819 -1.729680 -0.682414
N 0.107146 -0.979623 -0.222915
C -0.925259 -0.396236 -0.063384
S -2.359731 0.291592 0.065568
```

__Frequencies__ (27 in total)

```
1. 39.1745 cm-1 (Symmetry: A)
2. 80.6964 cm-1 (Symmetry: A)
3. 176.0349 cm-1 (Symmetry: A)
4. 292.9207 cm-1 (Symmetry: A)
5. 438.3766 cm-1 (Symmetry: A)
6. 456.9628 cm-1 (Symmetry: A)
7. 554.8208 cm-1 (Symmetry: A)
8. 592.6233 cm-1 (Symmetry: A)
9. 712.0874 cm-1 (Symmetry: A)
10. 913.2683 cm-1 (Symmetry: A)
11. 951.3521 cm-1 (Symmetry: A)
12. 981.8287 cm-1 (Symmetry: A)
13. 1015.4825 cm-1 (Symmetry: A)
14. 1044.9853 cm-1 (Symmetry: A)
15. 1172.1464 cm-1 (Symmetry: A)
16. 1265.8560 cm-1 (Symmetry: A)
17. 1310.8807 cm-1 (Symmetry: A)
18. 1363.3932 cm-1 (Symmetry: A)
19. 1430.1135 cm-1 (Symmetry: A)
20. 1453.7185 cm-1 (Symmetry: A)
21. 1727.1453 cm-1 (Symmetry: A)
22. 2176.8890 cm-1 (Symmetry: A)
23. 3006.7547 cm-1 (Symmetry: A)
24. 3046.5726 cm-1 (Symmetry: A)
25. 3142.6994 cm-1 (Symmetry: A)
26. 3157.7330 cm-1 (Symmetry: A)
27. 3246.5790 cm-1 (Symmetry: A)
***
```

allylncs-conformerI-B3LYP-D3(BJ)/cc-pVTZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=vibrot b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	254
Electronic Energy (Eh)	-608.471207764
Sum of electronic and zero-point Energies (Eh)	-608.389479
Sum of electronic and thermal Energies (Eh)	-608.382742
Sum of electronic and enthalpy Energies (Eh)	-608.381798
Sum of electronic and thermal Free Energies (Eh)	-608.421759
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.747577       1.436623      -0.068792
H          0.694823       1.605374      -0.247343
H          2.382231       2.310195      -0.024367
C          2.252528       0.224638       0.091586
H          3.315240       0.094365       0.267966
C          1.491732      -1.072262       0.056809
H          1.627877      -1.601092       1.006390
H          1.917309      -1.721902      -0.712443
N          0.096510      -0.940621      -0.190267
C         -0.938774      -0.382696      -0.057033
S         -2.370714       0.291224       0.056640
```

__Frequencies__ (27 in total)

```
 1.      36.4295 cm-1 (Symmetry: A)
 2.      72.6578 cm-1 (Symmetry: A)
 3.     176.6449 cm-1 (Symmetry: A)
```

4. 294.3573 cm-1 (Symmetry: A)
5. 455.2577 cm-1 (Symmetry: A)
6. 464.7916 cm-1 (Symmetry: A)
7. 561.4017 cm-1 (Symmetry: A)
8. 587.4897 cm-1 (Symmetry: A)
9. 710.0982 cm-1 (Symmetry: A)
10. 906.0254 cm-1 (Symmetry: A)
11. 966.1215 cm-1 (Symmetry: A)
12. 995.6025 cm-1 (Symmetry: A)
13. 1027.2339 cm-1 (Symmetry: A)
14. 1054.3099 cm-1 (Symmetry: A)
15. 1167.9177 cm-1 (Symmetry: A)
16. 1280.3987 cm-1 (Symmetry: A)
17. 1327.9920 cm-1 (Symmetry: A)
18. 1375.6949 cm-1 (Symmetry: A)
19. 1456.0726 cm-1 (Symmetry: A)
20. 1485.1684 cm-1 (Symmetry: A)
21. 1719.2463 cm-1 (Symmetry: A)
22. 2185.9382 cm-1 (Symmetry: A)
23. 3005.8065 cm-1 (Symmetry: A)
24. 3036.3737 cm-1 (Symmetry: A)
25. 3138.6779 cm-1 (Symmetry: A)
26. 3153.8465 cm-1 (Symmetry: A)
27. 3233.0412 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/cc-pV(D+d)Z

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/gen empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	118
Electronic Energy (Eh)	-608.391068689
Sum of electronic and zero-point Energies (Eh)	-608.309592
Sum of electronic and thermal Energies (Eh)	-608.302855
Sum of electronic and enthalpy Energies (Eh)	-608.30191
Sum of electronic and thermal Free Energies (Eh)	-608.341748
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.702417       1.454879      -0.086029
H          0.641211       1.599937      -0.299635
H          2.326124       2.349682      -0.033974
C          2.231629       0.247485       0.108276
H          3.302483       0.142353       0.319034
C          1.499384      -1.070545       0.071091
H          1.617803      -1.586412       1.042868
H          1.971218      -1.730777      -0.677054
N          0.104091      -0.982195      -0.228770
C         -0.926828      -0.395339      -0.065027
S         -2.351693       0.292606       0.067518
```

__Frequencies__ (27 in total)

```
```

1. 38.7569 cm-1 (Symmetry: A)
2. 81.5630 cm-1 (Symmetry: A)
3. 175.9169 cm-1 (Symmetry: A)
4. 292.5853 cm-1 (Symmetry: A)

5. 442.5842 cm-1 (Symmetry: A)
6. 461.4479 cm-1 (Symmetry: A)
7. 554.7617 cm-1 (Symmetry: A)
8. 594.7981 cm-1 (Symmetry: A)
9. 715.7349 cm-1 (Symmetry: A)
10. 913.4670 cm-1 (Symmetry: A)
11. 950.9228 cm-1 (Symmetry: A)
12. 981.8180 cm-1 (Symmetry: A)
13. 1015.6675 cm-1 (Symmetry: A)
14. 1045.9591 cm-1 (Symmetry: A)
15. 1175.5470 cm-1 (Symmetry: A)
16. 1266.1132 cm-1 (Symmetry: A)
17. 1310.9924 cm-1 (Symmetry: A)
18. 1363.5214 cm-1 (Symmetry: A)
19. 1430.0591 cm-1 (Symmetry: A)
20. 1453.7561 cm-1 (Symmetry: A)
21. 1727.1168 cm-1 (Symmetry: A)
22. 2172.4788 cm-1 (Symmetry: A)
23. 3005.7302 cm-1 (Symmetry: A)
24. 3046.1287 cm-1 (Symmetry: A)
25. 3142.3960 cm-1 (Symmetry: A)
26. 3157.7530 cm-1 (Symmetry: A)
27. 3246.6628 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/cc-pV(T+d)Z

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/gen empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	259
Electronic Energy (Eh)	-608.473412179
Sum of electronic and zero-point Energies (Eh)	-608.39165
Sum of electronic and thermal Energies (Eh)	-608.384939
Sum of electronic and enthalpy Energies (Eh)	-608.383995
Sum of electronic and thermal Free Energies (Eh)	-608.42379
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.758641       1.431638      -0.078446
H          0.711463       1.605101      -0.283610
H          2.397928       2.301522      -0.027705
C          2.251205       0.217901       0.105679
H          3.308612       0.082097       0.308122
C          1.481841      -1.073732       0.065734
H          1.589048      -1.592394       1.024711
H          1.921938      -1.734658      -0.685254
N          0.093856      -0.933046      -0.219879
C         -0.941965      -0.378794      -0.067192
S         -2.367769       0.292974       0.065514
```

__Frequencies__ (27 in total)

```
```

1. 41.2991 cm-1 (Symmetry: A)
2. 74.5688 cm-1 (Symmetry: A)
3. 178.1001 cm-1 (Symmetry: A)
4. 294.0380 cm-1 (Symmetry: A)

5. 458.9520 cm-1 (Symmetry: A)
6. 469.4474 cm-1 (Symmetry: A)
7. 561.4006 cm-1 (Symmetry: A)
8. 589.5642 cm-1 (Symmetry: A)
9. 713.1649 cm-1 (Symmetry: A)
10. 906.2098 cm-1 (Symmetry: A)
11. 965.9498 cm-1 (Symmetry: A)
12. 996.0620 cm-1 (Symmetry: A)
13. 1027.5703 cm-1 (Symmetry: A)
14. 1054.8572 cm-1 (Symmetry: A)
15. 1168.2228 cm-1 (Symmetry: A)
16. 1280.0555 cm-1 (Symmetry: A)
17. 1328.0051 cm-1 (Symmetry: A)
18. 1375.5843 cm-1 (Symmetry: A)
19. 1455.8573 cm-1 (Symmetry: A)
20. 1485.4777 cm-1 (Symmetry: A)
21. 1719.1031 cm-1 (Symmetry: A)
22. 2178.6348 cm-1 (Symmetry: A)
23. 3004.4931 cm-1 (Symmetry: A)
24. 3038.2866 cm-1 (Symmetry: A)
25. 3138.2546 cm-1 (Symmetry: A)
26. 3153.4663 cm-1 (Symmetry: A)
27. 3232.6247 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/cc-pV(Q+d)Z

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/gen empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	489
Electronic Energy (Eh)	-608.492820158
Sum of electronic and zero-point Energies (Eh)	-608.4111
Sum of electronic and thermal Energies (Eh)	-608.404384
Sum of electronic and enthalpy Energies (Eh)	-608.40344
Sum of electronic and thermal Free Energies (Eh)	-608.44327
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.757408       1.431223      -0.079337
H          0.711516       1.604702      -0.287645
H          2.396251       2.300593      -0.027444
C          2.249459       0.217802       0.106631
H          3.305729       0.082236       0.311933
C          1.480474      -1.073712       0.065519
H          1.586368      -1.592193       1.023929
H          1.921274      -1.733878      -0.684668
N          0.093209      -0.933033      -0.221279
C         -0.941152      -0.378389      -0.067038
S         -2.365671       0.293014       0.066138
```

__Frequencies__ (27 in total)

```
```

1. 39.8155 cm-1 (Symmetry: A)
2. 74.7227 cm-1 (Symmetry: A)
3. 177.6364 cm-1 (Symmetry: A)
4. 294.4884 cm-1 (Symmetry: A)

5. 457.4856 cm-1 (Symmetry: A)
6. 468.3477 cm-1 (Symmetry: A)
7. 561.2690 cm-1 (Symmetry: A)
8. 590.3246 cm-1 (Symmetry: A)
9. 713.7388 cm-1 (Symmetry: A)
10. 906.1564 cm-1 (Symmetry: A)
11. 966.3383 cm-1 (Symmetry: A)
12. 995.2149 cm-1 (Symmetry: A)
13. 1027.3781 cm-1 (Symmetry: A)
14. 1054.7224 cm-1 (Symmetry: A)
15. 1168.1861 cm-1 (Symmetry: A)
16. 1280.4709 cm-1 (Symmetry: A)
17. 1327.3626 cm-1 (Symmetry: A)
18. 1375.5359 cm-1 (Symmetry: A)
19. 1456.1181 cm-1 (Symmetry: A)
20. 1484.6581 cm-1 (Symmetry: A)
21. 1716.1280 cm-1 (Symmetry: A)
22. 2173.6646 cm-1 (Symmetry: A)
23. 3003.5116 cm-1 (Symmetry: A)
24. 3037.5921 cm-1 (Symmetry: A)
25. 3136.9591 cm-1 (Symmetry: A)
26. 3152.0927 cm-1 (Symmetry: A)
27. 3230.9865 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/aug-cc-pVDZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/aug-cc-pvdz empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	187
Electronic Energy (Eh)	-608.403532012
Sum of electronic and zero-point Energies (Eh)	-608.322002
Sum of electronic and thermal Energies (Eh)	-608.315284
Sum of electronic and enthalpy Energies (Eh)	-608.31434
Sum of electronic and thermal Free Energies (Eh)	-608.353986
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.748701       1.442426      -0.097606
H          0.702030       1.609432      -0.349836
H          2.388737       2.321793      -0.036597
C          2.243574       0.225491       0.129300
H          3.301805       0.101951       0.377734
C          1.484955      -1.076703       0.084141
H          1.547259      -1.575931       1.065758
H          1.962543      -1.755030      -0.637929
N          0.102253      -0.951653      -0.273086
C         -0.932400      -0.384715      -0.080521
S         -2.367945       0.295023       0.080037
```

__Frequencies__ (27 in total)

```
```

1. 46.6609 cm-1 (Symmetry: A)
2. 83.2051 cm-1 (Symmetry: A)
3. 178.4209 cm-1 (Symmetry: A)
4. 292.7269 cm-1 (Symmetry: A)

5. 438.9197 cm-1 (Symmetry: A)
6. 459.5330 cm-1 (Symmetry: A)
7. 555.5002 cm-1 (Symmetry: A)
8. 594.1963 cm-1 (Symmetry: A)
9. 712.6486 cm-1 (Symmetry: A)
10. 910.6179 cm-1 (Symmetry: A)
11. 966.3247 cm-1 (Symmetry: A)
12. 984.9178 cm-1 (Symmetry: A)
13. 1011.8995 cm-1 (Symmetry: A)
14. 1043.9073 cm-1 (Symmetry: A)
15. 1161.5679 cm-1 (Symmetry: A)
16. 1263.4042 cm-1 (Symmetry: A)
17. 1315.6629 cm-1 (Symmetry: A)
18. 1358.2519 cm-1 (Symmetry: A)
19. 1439.7548 cm-1 (Symmetry: A)
20. 1466.7536 cm-1 (Symmetry: A)
21. 1714.9688 cm-1 (Symmetry: A)
22. 2153.7119 cm-1 (Symmetry: A)
23. 3015.4190 cm-1 (Symmetry: A)
24. 3061.5584 cm-1 (Symmetry: A)
25. 3148.7485 cm-1 (Symmetry: A)
26. 3160.7447 cm-1 (Symmetry: A)
27. 3247.4225 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/aug-cc-pVTZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/aug-cc-pvtz empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	395
Electronic Energy (Eh)	-608.474018208
Sum of electronic and zero-point Energies (Eh)	-608.392318
Sum of electronic and thermal Energies (Eh)	-608.385604
Sum of electronic and enthalpy Energies (Eh)	-608.38466
Sum of electronic and thermal Free Energies (Eh)	-608.424427
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.760542       1.431940      -0.078398
H          0.713719       1.605893      -0.284646
H          2.400289       2.301323      -0.027101
C          2.252793       0.217635       0.105918
H          3.309872       0.081678       0.309347
C          1.483687      -1.073740       0.065487
H          1.589142      -1.592477       1.024342
H          1.922794      -1.734428      -0.685849
N          0.095266      -0.932192      -0.220161
C         -0.940074      -0.378486      -0.066377
S         -2.371523       0.292454       0.065328
```

__Frequencies__ (27 in total)

```
```

1. 42.5753 cm-1 (Symmetry: A)
2. 75.5660 cm-1 (Symmetry: A)
3. 178.0500 cm-1 (Symmetry: A)
4. 294.4492 cm-1 (Symmetry: A)

5. 455.5288 cm-1 (Symmetry: A)
6. 466.0422 cm-1 (Symmetry: A)
7. 561.2627 cm-1 (Symmetry: A)
8. 589.2865 cm-1 (Symmetry: A)
9. 711.2206 cm-1 (Symmetry: A)
10. 906.0781 cm-1 (Symmetry: A)
11. 965.7353 cm-1 (Symmetry: A)
12. 994.5185 cm-1 (Symmetry: A)
13. 1026.2426 cm-1 (Symmetry: A)
14. 1052.9373 cm-1 (Symmetry: A)
15. 1164.6498 cm-1 (Symmetry: A)
16. 1279.8237 cm-1 (Symmetry: A)
17. 1326.1692 cm-1 (Symmetry: A)
18. 1374.8867 cm-1 (Symmetry: A)
19. 1455.8080 cm-1 (Symmetry: A)
20. 1483.9998 cm-1 (Symmetry: A)
21. 1715.3279 cm-1 (Symmetry: A)
22. 2173.9437 cm-1 (Symmetry: A)
23. 3005.5123 cm-1 (Symmetry: A)
24. 3039.9724 cm-1 (Symmetry: A)
25. 3138.2288 cm-1 (Symmetry: A)
26. 3152.9612 cm-1 (Symmetry: A)
27. 3231.5186 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/aug-cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/aug-cc-pvqz empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	714
Electronic Energy (Eh)	-608.492592701
Sum of electronic and zero-point Energies (Eh)	-608.410886
Sum of electronic and thermal Energies (Eh)	-608.404166
Sum of electronic and enthalpy Energies (Eh)	-608.403222
Sum of electronic and thermal Free Energies (Eh)	-608.44306
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.757502       1.431650      -0.079399
H          0.711536       1.604687      -0.288032
H          2.395943       2.301345      -0.027449
C          2.250187       0.218257       0.106581
H          3.306511       0.083103       0.312063
C          1.481758      -1.073574       0.065384
H          1.587282      -1.591972       1.023864
H          1.922565      -1.733631      -0.684859
N          0.094257      -0.933173      -0.221392
C         -0.940272      -0.379143      -0.067146
S         -2.367418       0.292846       0.066352
```

__Frequencies__ (27 in total)

```
```

1. 39.7376 cm-1 (Symmetry: A)
2. 74.9744 cm-1 (Symmetry: A)
3. 177.3610 cm-1 (Symmetry: A)
4. 294.5806 cm-1 (Symmetry: A)

5. 455.2512 cm-1 (Symmetry: A)
6. 466.6631 cm-1 (Symmetry: A)
7. 561.1827 cm-1 (Symmetry: A)
8. 590.0199 cm-1 (Symmetry: A)
9. 712.8019 cm-1 (Symmetry: A)
10. 906.0038 cm-1 (Symmetry: A)
11. 966.7954 cm-1 (Symmetry: A)
12. 994.5208 cm-1 (Symmetry: A)
13. 1027.6188 cm-1 (Symmetry: A)
14. 1054.7961 cm-1 (Symmetry: A)
15. 1166.8750 cm-1 (Symmetry: A)
16. 1280.4390 cm-1 (Symmetry: A)
17. 1328.2075 cm-1 (Symmetry: A)
18. 1375.3648 cm-1 (Symmetry: A)
19. 1456.8050 cm-1 (Symmetry: A)
20. 1485.1868 cm-1 (Symmetry: A)
21. 1714.7811 cm-1 (Symmetry: A)
22. 2172.4384 cm-1 (Symmetry: A)
23. 3003.8136 cm-1 (Symmetry: A)
24. 3038.0135 cm-1 (Symmetry: A)
25. 3137.2987 cm-1 (Symmetry: A)
26. 3152.2243 cm-1 (Symmetry: A)
27. 3231.2306 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/aug-cc-pV(D+d)Z

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/gen empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	192
Electronic Energy (Eh)	-608.407612814
Sum of electronic and zero-point Energies (Eh)	-608.326046
Sum of electronic and thermal Energies (Eh)	-608.319346
Sum of electronic and enthalpy Energies (Eh)	-608.318402
Sum of electronic and thermal Free Energies (Eh)	-608.357992
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.751358       1.439623      -0.102567
H          0.708362       1.608337      -0.368443
H          2.393385       2.317291      -0.038034
C          2.239462       0.222181       0.136299
H          3.294232       0.096701       0.398203
C          1.477012      -1.077632       0.088041
H          1.526450      -1.572425       1.072711
H          1.961262      -1.760495      -0.625203
N          0.098778      -0.949620      -0.286971
C         -0.935067      -0.381909      -0.084867
S         -2.360733       0.296522       0.084258
```

__Frequencies__ (27 in total)

```
```

1. 47.2859 cm-1 (Symmetry: A)
2. 84.7465 cm-1 (Symmetry: A)
3. 179.1851 cm-1 (Symmetry: A)
4. 292.4436 cm-1 (Symmetry: A)

5. 443.6197 cm-1 (Symmetry: A)
6. 464.9099 cm-1 (Symmetry: A)
7. 555.4448 cm-1 (Symmetry: A)
8. 596.5920 cm-1 (Symmetry: A)
9. 717.0970 cm-1 (Symmetry: A)
10. 910.9204 cm-1 (Symmetry: A)
11. 965.7624 cm-1 (Symmetry: A)
12. 985.0119 cm-1 (Symmetry: A)
13. 1012.0439 cm-1 (Symmetry: A)
14. 1045.0748 cm-1 (Symmetry: A)
15. 1164.3376 cm-1 (Symmetry: A)
16. 1263.4517 cm-1 (Symmetry: A)
17. 1315.6885 cm-1 (Symmetry: A)
18. 1358.1410 cm-1 (Symmetry: A)
19. 1439.5497 cm-1 (Symmetry: A)
20. 1466.9373 cm-1 (Symmetry: A)
21. 1714.7715 cm-1 (Symmetry: A)
22. 2147.6210 cm-1 (Symmetry: A)
23. 3014.4066 cm-1 (Symmetry: A)
24. 3061.7960 cm-1 (Symmetry: A)
25. 3148.4915 cm-1 (Symmetry: A)
26. 3160.7022 cm-1 (Symmetry: A)
27. 3247.4684 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/aug-cc-pV(T+d)Z

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/gen empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	400
Electronic Energy (Eh)	-608.4762175449999
Sum of electronic and zero-point Energies (Eh)	-608.394509
Sum of electronic and thermal Energies (Eh)	-608.387794
Sum of electronic and enthalpy Energies (Eh)	-608.38685
Sum of electronic and thermal Free Energies (Eh)	-608.426654
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.759304       1.431678      -0.078755
H          0.712671       1.605721      -0.285777
H          2.399210       2.300930      -0.027351
C          2.251182       0.217317       0.106247
H          3.308133       0.081328       0.310347
C          1.481824      -1.073935       0.065723
H          1.586954      -1.592403       1.024784
H          1.921440      -1.734847      -0.685123
N          0.093643      -0.932628      -0.220744
C         -0.941778      -0.378349      -0.067053
S         -2.367944       0.292962       0.065710
```

__Frequencies__ (27 in total)

```
```

1. 40.8607 cm-1 (Symmetry: A)
2. 75.2268 cm-1 (Symmetry: A)
3. 177.7780 cm-1 (Symmetry: A)
4. 294.1809 cm-1 (Symmetry: A)

5. 457.4854 cm-1 (Symmetry: A)
6. 468.0587 cm-1 (Symmetry: A)
7. 561.1853 cm-1 (Symmetry: A)
8. 589.7191 cm-1 (Symmetry: A)
9. 712.5830 cm-1 (Symmetry: A)
10. 906.1468 cm-1 (Symmetry: A)
11. 965.5411 cm-1 (Symmetry: A)
12. 994.4654 cm-1 (Symmetry: A)
13. 1026.2997 cm-1 (Symmetry: A)
14. 1053.5265 cm-1 (Symmetry: A)
15. 1166.3038 cm-1 (Symmetry: A)
16. 1279.8457 cm-1 (Symmetry: A)
17. 1326.1793 cm-1 (Symmetry: A)
18. 1374.8375 cm-1 (Symmetry: A)
19. 1455.7424 cm-1 (Symmetry: A)
20. 1483.9235 cm-1 (Symmetry: A)
21. 1715.2961 cm-1 (Symmetry: A)
22. 2172.9115 cm-1 (Symmetry: A)
23. 3005.1578 cm-1 (Symmetry: A)
24. 3039.7503 cm-1 (Symmetry: A)
25. 3138.1456 cm-1 (Symmetry: A)
26. 3153.0571 cm-1 (Symmetry: A)
27. 3231.6314 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerI-B3LYP-D3(BJ)/aug-cc-pV(Q+d)Z

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/gen empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	719
Electronic Energy (Eh)	-608.493832786
Sum of electronic and zero-point Energies (Eh)	-608.41211
Sum of electronic and thermal Energies (Eh)	-608.405402
Sum of electronic and enthalpy Energies (Eh)	-608.404458
Sum of electronic and thermal Free Energies (Eh)	-608.444225
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          1.753633       1.431818      -0.082803
H          0.709208       1.602868      -0.300452
H          2.390651       2.302401      -0.028438
C          2.246122       0.219595       0.111238
H          3.300928       0.086626       0.325776
C          1.479830      -1.073359       0.067774
H          1.580220      -1.589632       1.027983
H          1.926693      -1.734115      -0.678221
N          0.093559      -0.936284      -0.228663
C         -0.939847      -0.379967      -0.069477
S         -2.362565       0.293583       0.068350
```

__Frequencies__ (27 in total)

```
```

1. 41.6051 cm-1 (Symmetry: A)
2. 76.2678 cm-1 (Symmetry: A)
3. 177.4752 cm-1 (Symmetry: A)
4. 294.4970 cm-1 (Symmetry: A)

5. 457.3329 cm-1 (Symmetry: A)
6. 469.0178 cm-1 (Symmetry: A)
7. 561.2215 cm-1 (Symmetry: A)
8. 591.8490 cm-1 (Symmetry: A)
9. 714.1908 cm-1 (Symmetry: A)
10. 906.1402 cm-1 (Symmetry: A)
11. 966.5631 cm-1 (Symmetry: A)
12. 994.5222 cm-1 (Symmetry: A)
13. 1027.6387 cm-1 (Symmetry: A)
14. 1055.0828 cm-1 (Symmetry: A)
15. 1167.6048 cm-1 (Symmetry: A)
16. 1280.4762 cm-1 (Symmetry: A)
17. 1328.2370 cm-1 (Symmetry: A)
18. 1375.4306 cm-1 (Symmetry: A)
19. 1456.7731 cm-1 (Symmetry: A)
20. 1485.2647 cm-1 (Symmetry: A)
21. 1714.7676 cm-1 (Symmetry: A)
22. 2167.7145 cm-1 (Symmetry: A)
23. 3003.4704 cm-1 (Symmetry: A)
24. 3038.2151 cm-1 (Symmetry: A)
25. 3137.1923 cm-1 (Symmetry: A)
26. 3152.3344 cm-1 (Symmetry: A)
27. 3231.3792 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerII-B3LYP-D3(BJ)/cc-pVTZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=vibrot b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	254
Electronic Energy (Eh)	-608.470641093
Sum of electronic and zero-point Energies (Eh)	-608.389116
Sum of electronic and thermal Energies (Eh)	-608.382283
Sum of electronic and enthalpy Energies (Eh)	-608.381338
Sum of electronic and thermal Free Energies (Eh)	-608.422246
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C         -2.606601       1.094021       0.002180
H         -1.728771       1.723709      -0.050625
H         -3.570272       1.582229       0.028373
C         -2.506602      -0.224858       0.033179
H         -3.395355      -0.843704       0.085917
C         -1.223271      -1.001069       0.001224
H         -1.226490      -1.678248      -0.859648
H         -1.151464      -1.632128       0.893566
N         -0.063575      -0.171345      -0.073563
C          1.114578      -0.056293      -0.025037
S          2.678047       0.198547       0.021755
```

__Frequencies__ (27 in total)

```
  1.     16.0030 cm-1 (Symmetry: A)
  2.     62.5432 cm-1 (Symmetry: A)
  3.    185.4850 cm-1 (Symmetry: A)
  4.    254.5698 cm-1 (Symmetry: A)
```

5. 459.8943 cm-1 (Symmetry: A)
6. 486.2614 cm-1 (Symmetry: A)
7. 528.4780 cm-1 (Symmetry: A)
8. 565.6808 cm-1 (Symmetry: A)
9. 766.9370 cm-1 (Symmetry: A)
10. 915.8921 cm-1 (Symmetry: A)
11. 963.7951 cm-1 (Symmetry: A)
12. 993.2084 cm-1 (Symmetry: A)
13. 1029.8188 cm-1 (Symmetry: A)
14. 1066.9698 cm-1 (Symmetry: A)
15. 1147.9189 cm-1 (Symmetry: A)
16. 1261.6986 cm-1 (Symmetry: A)
17. 1328.1969 cm-1 (Symmetry: A)
18. 1382.1244 cm-1 (Symmetry: A)
19. 1449.6406 cm-1 (Symmetry: A)
20. 1474.6316 cm-1 (Symmetry: A)
21. 1719.9311 cm-1 (Symmetry: A)
22. 2178.8460 cm-1 (Symmetry: A)
23. 2996.8595 cm-1 (Symmetry: A)
24. 3019.7925 cm-1 (Symmetry: A)
25. 3143.9756 cm-1 (Symmetry: A)
26. 3154.4152 cm-1 (Symmetry: A)
27. 3231.8356 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerII-B3LYP-D3(BJ)/cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt=tight freq=vibrot b3lyp/cc-pvqz geom=connectivity empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	484
Electronic Energy (Eh)	-608.4909570490001
Sum of electronic and zero-point Energies (Eh)	-608.409473
Sum of electronic and thermal Energies (Eh)	-608.402639
Sum of electronic and enthalpy Energies (Eh)	-608.401694
Sum of electronic and thermal Free Energies (Eh)	-608.442633
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C         -2.619013       1.085194      -0.000000
H         -1.746715       1.723699      -0.000010
H         -3.587352       1.563442       0.000005
C         -2.507146      -0.232919       0.000006
H         -3.390680      -0.860416       0.000016
C         -1.216184      -0.996389      -0.000001
H         -1.176114      -1.649859      -0.877304
H         -1.176103      -1.649858       0.877303
N         -0.062690      -0.155296      -0.000010
C          1.116767      -0.049376      -0.000003
S          2.679328       0.195063       0.000003
```

__Frequencies__ (27 in total)

```
1.  15.4681 cm-1
2.  62.1943 cm-1
3.  185.5506 cm-1
4.  253.5512 cm-1
```

5. 460.0697 cm-1
6. 487.3694 cm-1
7. 529.2161 cm-1
8. 565.7992 cm-1
9. 769.5526 cm-1
10. 916.1388 cm-1
11. 964.5059 cm-1
12. 992.5465 cm-1
13. 1029.3048 cm-1
14. 1067.2494 cm-1
15. 1148.0198 cm-1
16. 1261.3416 cm-1
17. 1327.5783 cm-1
18. 1382.0818 cm-1
19. 1449.7112 cm-1
20. 1473.4617 cm-1
21. 1716.8199 cm-1
22. 2171.6722 cm-1
23. 2995.0381 cm-1
24. 3018.2308 cm-1
25. 3142.6803 cm-1
26. 3152.4298 cm-1
27. 3229.8550 cm-1

```
***
# allylncs-conformerII-MP2/cc-pVTZ


__Requested operations__

Run with Gaussian 16revisionB.01.

# opt freq=(vibrot,noraman) mp2/cc-pvtz output=pickett

__Relevant magnitudes__


| Datum | Value |
|:---|---:|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C4H5NS |
| Number of Basis Functions | 254 |
| Electronic Energy (Eh) | -606.411430383 |
| Sum of electronic and zero-point Energies (Eh) | -607.338858 |
| Sum of electronic and thermal Energies (Eh) | -607.332026 |
| Sum of electronic and enthalpy Energies (Eh) | -607.331082 |
| Sum of electronic and thermal Free Energies (Eh) | -607.371972 |
| Number of Imaginary Frequencies | 0 |
```

| Mean of alpha and beta Electrons | 26 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -2.569821     1.108802     0.001724
H       -1.670969     1.706526    -0.047210
H       -3.522094     1.616467     0.025691
C       -2.506291    -0.220709     0.031207
H       -3.411872    -0.812981     0.079952
C       -1.233974    -1.011293     0.001533
H       -1.233811    -1.681734    -0.861417
H       -1.161293    -1.635851     0.895351
N       -0.080591    -0.172688    -0.070463
C        1.113301    -0.067109    -0.022489
S        2.671556     0.197390     0.020564
```

__Frequencies__ (27 in total)

```
 1.     15.3436 cm-1 (Symmetry: A)
 2.     68.0384 cm-1 (Symmetry: A)
 3.    180.9478 cm-1 (Symmetry: A)
 4.    259.3815 cm-1 (Symmetry: A)
 5.    450.9846 cm-1 (Symmetry: A)
 6.    479.2079 cm-1 (Symmetry: A)
 7.    527.5402 cm-1 (Symmetry: A)
 8.    564.2499 cm-1 (Symmetry: A)
 9.    773.7180 cm-1 (Symmetry: A)
10.    935.8266 cm-1 (Symmetry: A)
11.    953.0007 cm-1 (Symmetry: A)
12.    998.9439 cm-1 (Symmetry: A)
13.   1028.3849 cm-1 (Symmetry: A)
14.   1065.9840 cm-1 (Symmetry: A)
15.   1175.8633 cm-1 (Symmetry: A)
16.   1268.0489 cm-1 (Symmetry: A)
17.   1319.8325 cm-1 (Symmetry: A)
18.   1385.4814 cm-1 (Symmetry: A)
19.   1453.8853 cm-1 (Symmetry: A)
20.   1487.9598 cm-1 (Symmetry: A)
21.   1707.6375 cm-1 (Symmetry: A)
22.   2144.5949 cm-1 (Symmetry: A)
23.   3059.5745 cm-1 (Symmetry: A)
24.   3104.5165 cm-1 (Symmetry: A)
25.   3189.9779 cm-1 (Symmetry: A)
26.   3208.2480 cm-1 (Symmetry: A)
27.   3293.5067 cm-1 (Symmetry: A)
```

***

allylncs-conformerII-MP2/cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=vibrot mp2/cc-pvqz geom=connectivity output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	484
Electronic Energy (Eh)	-606.429933435
Sum of electronic and zero-point Energies (Eh)	-607.424378
Sum of electronic and thermal Energies (Eh)	-607.417537
Sum of electronic and enthalpy Energies (Eh)	-607.416593
Sum of electronic and thermal Free Energies (Eh)	-607.458075
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C         -2.558240       1.110520       0.001591
H         -1.656822       1.703116      -0.048183
H         -3.507229       1.622509       0.025786
C         -2.501273      -0.216931       0.031781
H         -3.408824      -0.804843       0.081453
C         -1.234082      -1.011370       0.001957
H         -1.236819      -1.682542      -0.859286
H         -1.162253      -1.634218       0.895968
N         -0.079785      -0.179056      -0.072265
C          1.110928      -0.069457      -0.023013
S          2.664153       0.198300       0.021014
```

__Frequencies__ (27 in total)

```
1.      8.0663 cm-1 (Symmetry: A)
2.     67.1977 cm-1 (Symmetry: A)
3.    184.3457 cm-1 (Symmetry: A)
4.    260.7499 cm-1 (Symmetry: A)
```

5. 450.3909 cm-1 (Symmetry: A)
6. 479.1152 cm-1 (Symmetry: A)
7. 528.5107 cm-1 (Symmetry: A)
8. 564.3173 cm-1 (Symmetry: A)
9. 775.4338 cm-1 (Symmetry: A)
10. 936.7455 cm-1 (Symmetry: A)
11. 954.1532 cm-1 (Symmetry: A)
12. 999.1604 cm-1 (Symmetry: A)
13. 1027.2482 cm-1 (Symmetry: A)
14. 1066.1649 cm-1 (Symmetry: A)
15. 1177.2680 cm-1 (Symmetry: A)
16. 1267.7456 cm-1 (Symmetry: A)
17. 1319.1968 cm-1 (Symmetry: A)
18. 1385.3567 cm-1 (Symmetry: A)
19. 1450.3838 cm-1 (Symmetry: A)
20. 1487.3380 cm-1 (Symmetry: A)
21. 1706.4803 cm-1 (Symmetry: A)
22. 2145.7735 cm-1 (Symmetry: A)
23. 3059.6949 cm-1 (Symmetry: A)
24. 3105.9061 cm-1 (Symmetry: A)
25. 3189.3000 cm-1 (Symmetry: A)
26. 3207.0663 cm-1 (Symmetry: A)
27. 3293.6876 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerII-B3LYP-D3(BJ)/aug-cc-pVTZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/aug-cc-pvtz output=pickett empiricaldispersion=gd3bj

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	395
Electronic Energy (Eh)	-608.473412404
Sum of electronic and zero-point Energies (Eh)	-608.391938
Sum of electronic and thermal Energies (Eh)	-608.385105
Sum of electronic and enthalpy Energies (Eh)	-608.384161
Sum of electronic and thermal Free Energies (Eh)	-608.42496
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C         -2.608394       1.093980       0.002164
H         -1.731880       1.725589      -0.048691
H         -3.573161       1.579808       0.027456
C         -2.506516      -0.225442       0.032020
H         -3.394769      -0.844937       0.082900
C         -1.223186      -1.000878       0.001419
H         -1.224804      -1.677706      -0.859413
H         -1.151160      -1.630653       0.894358
N         -0.062996      -0.171521      -0.072781
C          1.114692      -0.056326      -0.024745
S          2.678573       0.198784       0.021732
```

__Frequencies__ (27 in total)

```
  1.     18.0229 cm-1 (Symmetry: A)
  2.     62.8767 cm-1 (Symmetry: A)
  3.    185.6809 cm-1 (Symmetry: A)
  4.    253.7565 cm-1 (Symmetry: A)
```

5. 458.0709 cm-1 (Symmetry: A)
6. 484.5584 cm-1 (Symmetry: A)
7. 527.7950 cm-1 (Symmetry: A)
8. 565.9550 cm-1 (Symmetry: A)
9. 766.2454 cm-1 (Symmetry: A)
10. 915.7272 cm-1 (Symmetry: A)
11. 963.8621 cm-1 (Symmetry: A)
12. 991.8844 cm-1 (Symmetry: A)
13. 1027.9612 cm-1 (Symmetry: A)
14. 1065.5024 cm-1 (Symmetry: A)
15. 1146.3778 cm-1 (Symmetry: A)
16. 1261.8603 cm-1 (Symmetry: A)
17. 1326.2133 cm-1 (Symmetry: A)
18. 1381.0411 cm-1 (Symmetry: A)
19. 1449.4595 cm-1 (Symmetry: A)
20. 1472.7933 cm-1 (Symmetry: A)
21. 1715.3816 cm-1 (Symmetry: A)
22. 2174.5559 cm-1 (Symmetry: A)
23. 2997.7052 cm-1 (Symmetry: A)
24. 3020.8365 cm-1 (Symmetry: A)
25. 3143.9273 cm-1 (Symmetry: A)
26. 3153.9885 cm-1 (Symmetry: A)
27. 3230.9160 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerII-B3LYP-D3(BJ)/aug-cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) b3lyp/aug-cc-pvqz output=pickett empiricaldispersion=gd3bj

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	714
Electronic Energy (Eh)	-608.491993685
Sum of electronic and zero-point Energies (Eh)	-608.410513
Sum of electronic and thermal Energies (Eh)	-608.403678
Sum of electronic and enthalpy Energies (Eh)	-608.402734
Sum of electronic and thermal Free Energies (Eh)	-608.443804
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C         -2.615739       1.086826       0.002607
H         -1.743353       1.723384      -0.046825
H         -3.582908       1.566865       0.027437
C         -2.505432      -0.231366       0.031194
H         -3.389114      -0.856786       0.080574
C         -1.216318      -0.997321       0.001055
H         -1.212746      -1.673639      -0.859647
H         -1.141076      -1.627282       0.893103
N         -0.062653      -0.159060      -0.071404
C          1.115863      -0.050881      -0.024298
S          2.677346       0.196083       0.021365
```

__Frequencies__ (27 in total)

```
1. 13.0210 cm-1 (Symmetry: A)
2. 64.2220 cm-1 (Symmetry: A)
3. 185.9398 cm-1 (Symmetry: A)
4. 253.8765 cm-1 (Symmetry: A)
```

5. 458.9191 cm-1 (Symmetry: A)
6. 486.9843 cm-1 (Symmetry: A)
7. 529.8552 cm-1 (Symmetry: A)
8. 566.0100 cm-1 (Symmetry: A)
9. 769.4580 cm-1 (Symmetry: A)
10. 915.9711 cm-1 (Symmetry: A)
11. 965.0428 cm-1 (Symmetry: A)
12. 992.1282 cm-1 (Symmetry: A)
13. 1029.6166 cm-1 (Symmetry: A)
14. 1067.5089 cm-1 (Symmetry: A)
15. 1147.8743 cm-1 (Symmetry: A)
16. 1261.7456 cm-1 (Symmetry: A)
17. 1328.2752 cm-1 (Symmetry: A)
18. 1381.5704 cm-1 (Symmetry: A)
19. 1450.4989 cm-1 (Symmetry: A)
20. 1473.8299 cm-1 (Symmetry: A)
21. 1715.2322 cm-1 (Symmetry: A)
22. 2168.6240 cm-1 (Symmetry: A)
23. 2995.3952 cm-1 (Symmetry: A)
24. 3018.5461 cm-1 (Symmetry: A)
25. 3142.8950 cm-1 (Symmetry: A)
26. 3152.5471 cm-1 (Symmetry: A)
27. 3230.1578 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerII-MP2/aug-cc-pVTZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) mp2/aug-cc-pvtz output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	395
Electronic Energy (Eh)	-606.4137622760002
Sum of electronic and zero-point Energies (Eh)	-607.358256
Sum of electronic and thermal Energies (Eh)	-607.351438
Sum of electronic and enthalpy Energies (Eh)	-607.350494
Sum of electronic and thermal Free Energies (Eh)	-607.390964
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C         -2.580040       1.103467      -0.000004
H         -1.682996       1.707467      -0.000126
H         -3.536607       1.605194       0.000060
C         -2.508764      -0.226955       0.000077
H         -3.411934      -0.826338       0.000211
C         -1.231156      -1.008630      -0.000014
H         -1.189361      -1.655695      -0.880669
H         -1.189216      -1.655691       0.880635
N         -0.081380      -0.160348      -0.000120
C          1.114779      -0.062437      -0.000049
S          2.675679       0.194676       0.000042
```

__Frequencies__ (27 in total)

```
```

1. 24.0534 cm-1 (Symmetry: A)
2. 67.3513 cm-1 (Symmetry: A)
3. 185.4738 cm-1 (Symmetry: A)
4. 258.2428 cm-1 (Symmetry: A)

5. 446.1266 cm-1 (Symmetry: A)
6. 476.5304 cm-1 (Symmetry: A)
7. 525.9562 cm-1 (Symmetry: A)
8. 564.7659 cm-1 (Symmetry: A)
9. 773.2978 cm-1 (Symmetry: A)
10. 934.3716 cm-1 (Symmetry: A)
11. 952.6533 cm-1 (Symmetry: A)
12. 997.5233 cm-1 (Symmetry: A)
13. 1024.1850 cm-1 (Symmetry: A)
14. 1061.5406 cm-1 (Symmetry: A)
15. 1171.1085 cm-1 (Symmetry: A)
16. 1268.4823 cm-1 (Symmetry: A)
17. 1315.8810 cm-1 (Symmetry: A)
18. 1384.7984 cm-1 (Symmetry: A)
19. 1449.0091 cm-1 (Symmetry: A)
20. 1491.4995 cm-1 (Symmetry: A)
21. 1700.5636 cm-1 (Symmetry: A)
22. 2132.3676 cm-1 (Symmetry: A)
23. 3053.6725 cm-1 (Symmetry: A)
24. 3098.5368 cm-1 (Symmetry: A)
25. 3181.7695 cm-1 (Symmetry: A)
26. 3199.8120 cm-1 (Symmetry: A)
27. 3285.0314 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerIII-B3LYP-D3(BJ)/cc-pVTZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=vibrot b3lyp/cc-pvtz geom=connectivity empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	254
Electronic Energy (Eh)	-608.470146926
Sum of electronic and zero-point Energies (Eh)	-608.388465
Sum of electronic and thermal Energies (Eh)	-608.381625
Sum of electronic and enthalpy Energies (Eh)	-608.380681
Sum of electronic and thermal Free Energies (Eh)	-608.421371
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          2.878700      -0.885723      -0.271459
H          3.334335      -0.372623      -1.109538
H          3.279851      -1.856512      -0.015335
C          1.878823      -0.348347       0.409753
H          1.424807      -0.881149       1.237928
C          1.297644       1.002474       0.108264
H          1.795035       1.450985      -0.751948
H          1.443614       1.680810       0.953928
N         -0.113880       0.942806      -0.159684
C         -1.116492       0.313064      -0.076491
S         -2.507033      -0.444373      -0.013603
```

__Frequencies__ (27 in total)

```
  1.      24.0156 cm-1 (Symmetry: A)
  2.      75.0972 cm-1 (Symmetry: A)
  3.     119.9051 cm-1 (Symmetry: A)
  4.     343.3762 cm-1 (Symmetry: A)
```

5. 409.4243 cm-1 (Symmetry: A)
6. 460.8406 cm-1 (Symmetry: A)
7. 512.6906 cm-1 (Symmetry: A)
8. 632.9032 cm-1 (Symmetry: A)
9. 728.3101 cm-1 (Symmetry: A)
10. 928.0869 cm-1 (Symmetry: A)
11. 955.1639 cm-1 (Symmetry: A)
12. 974.1707 cm-1 (Symmetry: A)
13. 1030.6817 cm-1 (Symmetry: A)
14. 1118.1072 cm-1 (Symmetry: A)
15. 1162.7924 cm-1 (Symmetry: A)
16. 1276.6591 cm-1 (Symmetry: A)
17. 1325.8721 cm-1 (Symmetry: A)
18. 1359.7543 cm-1 (Symmetry: A)
19. 1459.4917 cm-1 (Symmetry: A)
20. 1490.6334 cm-1 (Symmetry: A)
21. 1713.3951 cm-1 (Symmetry: A)
22. 2156.6543 cm-1 (Symmetry: A)
23. 3019.3286 cm-1 (Symmetry: A)
24. 3071.8028 cm-1 (Symmetry: A)
25. 3134.3536 cm-1 (Symmetry: A)
26. 3151.0264 cm-1 (Symmetry: A)
27. 3219.8386 cm-1 (Symmetry: A)

```
***
# allylncs-conformerIII-B3LYP-D3(BJ)/cc-pVQZ


__Requested operations__

Run with Gaussian 16revisionB.01.

# opt freq=vibrot b3lyp/cc-pvqz geom=connectivity empiricaldispersion=gd3bj output=pickett

__Relevant magnitudes__


| Datum | Value |
|:---|---:|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C4H5NS |
| Number of Basis Functions | 484 |
| Electronic Energy (Eh) | -608.4905671979999 |
| Sum of electronic and zero-point Energies (Eh) | -608.408902 |
| Sum of electronic and thermal Energies (Eh) | -608.402074 |
| Sum of electronic and enthalpy Energies (Eh) | -608.40113 |
| Sum of electronic and thermal Free Energies (Eh) | -608.44176 |
| Number of Imaginary Frequencies | 0 |
```

| Mean of alpha and beta Electrons | 26 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       2.869973    -0.888940    -0.270806
H       3.330848    -0.374635    -1.104512
H       3.265749    -1.861942    -0.017139
C       1.869799    -0.350351     0.408511
H       1.410456    -0.884571     1.232142
C       1.295725     1.003849     0.110328
H       1.797190     1.452859    -0.746399
H       1.441932     1.678210     0.958255
N      -0.115274     0.950733    -0.162028
C      -1.114478     0.316422    -0.077214
S      -2.497836    -0.446934    -0.013316
```

__Frequencies__ (27 in total)

```
 1.    24.5700 cm-1
 2.    77.3896 cm-1
 3.   119.9542 cm-1
 4.   343.7099 cm-1
 5.   410.4391 cm-1
 6.   461.1982 cm-1
 7.   514.9887 cm-1
 8.   635.1638 cm-1
 9.   729.2605 cm-1
10.   928.4768 cm-1
11.   955.2272 cm-1
12.   975.3592 cm-1
13.  1030.6140 cm-1
14.  1118.0363 cm-1
15.  1163.1740 cm-1
16.  1276.7448 cm-1
17.  1325.6599 cm-1
18.  1359.7695 cm-1
19.  1460.1028 cm-1
20.  1489.9517 cm-1
21.  1710.8824 cm-1
22.  2147.6439 cm-1
23.  3018.0501 cm-1
24.  3070.9102 cm-1
25.  3132.8346 cm-1
26.  3148.7841 cm-1
27.  3217.7991 cm-1
```

***

allylncs-conformerIII-MP2/cc-pVTZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=(vibrot,noraman) mp2/cc-pvtz geom=connectivity output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	254
Electronic Energy (Eh)	-606.411033748
Sum of electronic and zero-point Energies (Eh)	-607.338292
Sum of electronic and thermal Energies (Eh)	-607.331481
Sum of electronic and enthalpy Energies (Eh)	-607.330537
Sum of electronic and thermal Free Energies (Eh)	-607.37102
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          2.935279      -0.827738      -0.279108
H          3.407604      -0.227882      -1.045320
H          3.347113      -1.806501      -0.082946
C          1.882848      -0.371891       0.399723
H          1.407103      -0.983426       1.156988
C          1.288064       0.982781       0.168391
H          1.834010       1.509726      -0.612072
H          1.332708       1.588556       1.075649
N         -0.091610       0.886612      -0.225766
C         -1.123876       0.286505      -0.092510
S         -2.536323      -0.419044      -0.005681
```

__Frequencies__ (27 in total)

```
```

1. 25.0707 cm-1 (Symmetry: A)
2. 87.1710 cm-1 (Symmetry: A)
3. 122.9428 cm-1 (Symmetry: A)
4. 344.3697 cm-1 (Symmetry: A)

5. 405.4330 cm-1 (Symmetry: A)
6. 454.0309 cm-1 (Symmetry: A)
7. 503.7702 cm-1 (Symmetry: A)
8. 639.6444 cm-1 (Symmetry: A)
9. 739.0700 cm-1 (Symmetry: A)
10. 931.5205 cm-1 (Symmetry: A)
11. 962.3931 cm-1 (Symmetry: A)
12. 968.0918 cm-1 (Symmetry: A)
13. 1027.9808 cm-1 (Symmetry: A)
14. 1150.1731 cm-1 (Symmetry: A)
15. 1175.7140 cm-1 (Symmetry: A)
16. 1284.1735 cm-1 (Symmetry: A)
17. 1318.0235 cm-1 (Symmetry: A)
18. 1359.0412 cm-1 (Symmetry: A)
19. 1464.2794 cm-1 (Symmetry: A)
20. 1502.8915 cm-1 (Symmetry: A)
21. 1699.7294 cm-1 (Symmetry: A)
22. 2127.3185 cm-1 (Symmetry: A)
23. 3079.8466 cm-1 (Symmetry: A)
24. 3144.1636 cm-1 (Symmetry: A)
25. 3183.1439 cm-1 (Symmetry: A)
26. 3205.3421 cm-1 (Symmetry: A)
27. 3284.3181 cm-1 (Symmetry: A)

```
***
```

allylncs-conformerIII-MP2/cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt freq=vibrot mp2/cc-pvqz geom=connectivity output=pickett

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	484
Electronic Energy (Eh)	-606.42962356
Sum of electronic and zero-point Energies (Eh)	-607.423803
Sum of electronic and thermal Energies (Eh)	-607.416998
Sum of electronic and enthalpy Energies (Eh)	-607.416053
Sum of electronic and thermal Free Energies (Eh)	-607.456542
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          2.907061      -0.845221      -0.277705
H          3.380375      -0.261964      -1.054900
H          3.306792      -1.826167      -0.072460
C          1.868392      -0.367752       0.402818
H          1.391016      -0.963067       1.170986
C          1.289988       0.989120       0.158919
H          1.832847       1.498148      -0.634331
H          1.351009       1.607196       1.055663
N         -0.093266       0.903522      -0.217483
C         -1.117307       0.292959      -0.090360
S         -2.518624      -0.424590      -0.006538
```

__Frequencies__ (27 in total)

```
```

1. 24.3762 cm-1 (Symmetry: A)
2. 88.0823 cm-1 (Symmetry: A)
3. 123.1141 cm-1 (Symmetry: A)
4. 344.3915 cm-1 (Symmetry: A)

5. 407.2012 cm-1 (Symmetry: A)
6. 453.8609 cm-1 (Symmetry: A)
7. 506.0983 cm-1 (Symmetry: A)
8. 641.6087 cm-1 (Symmetry: A)
9. 739.8678 cm-1 (Symmetry: A)
10. 931.4530 cm-1 (Symmetry: A)
11. 963.0316 cm-1 (Symmetry: A)
12. 969.0626 cm-1 (Symmetry: A)
13. 1027.1445 cm-1 (Symmetry: A)
14. 1150.8761 cm-1 (Symmetry: A)
15. 1176.5477 cm-1 (Symmetry: A)
16. 1282.7464 cm-1 (Symmetry: A)
17. 1317.9316 cm-1 (Symmetry: A)
18. 1358.4008 cm-1 (Symmetry: A)
19. 1462.1472 cm-1 (Symmetry: A)
20. 1502.0872 cm-1 (Symmetry: A)
21. 1699.1071 cm-1 (Symmetry: A)
22. 2125.7663 cm-1 (Symmetry: A)
23. 3080.7477 cm-1 (Symmetry: A)
24. 3144.9810 cm-1 (Symmetry: A)
25. 3182.9994 cm-1 (Symmetry: A)
26. 3204.1000 cm-1 (Symmetry: A)
27. 3285.7024 cm-1 (Symmetry: A)

```
***
# allylncs-TS-I-I-B3LYP-D3(BJ)/cc-pVQZ


__Requested operations__

Run with Gaussian 16revisionB.01.

# opt=(calcfc,ts,noeigen) freq b3lyp/cc-pvqz empiricaldispersion=gd3bj

__Relevant magnitudes__


| Datum | Value |
|:---|---:|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C4H5NS |
| Number of Basis Functions | 484 |
| Electronic Energy (Eh) | -608.491504582 |
| Sum of electronic and zero-point Energies (Eh) | -608.409913 |
| Sum of electronic and thermal Energies (Eh) | -608.404027 |
| Sum of electronic and enthalpy Energies (Eh) | -608.403082 |
| Sum of electronic and thermal Free Energies (Eh) | -608.440456 |
| Number of Imaginary Frequencies | 1 |
```

| Mean of alpha and beta Electrons | 26 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C       -1.693324      1.454244      -0.000136
H       -0.623263      1.603208      -0.000104
H       -2.309052      2.341706      -0.000205
C       -2.242510      0.251274      -0.000095
H       -3.321854      0.144263      -0.000130
C       -1.517468     -1.066083      -0.000001
H       -1.825204     -1.650120      -0.872144
H       -1.825267     -1.650029       0.872181
N       -0.100056     -0.976528       0.000046
C        0.930111     -0.398204       0.000054
S        2.359012      0.287455       0.000072
```

__Frequencies__ (27 in total)

```
 1.    -34.5364 cm-1   *
 2.     75.9320 cm-1
 3.    170.4440 cm-1
 4.    295.2205 cm-1
 5.    449.9002 cm-1
 6.    460.2933 cm-1
 7.    562.4559 cm-1
 8.    585.9597 cm-1
 9.    705.5343 cm-1
10.    906.0887 cm-1
11.    967.1567 cm-1
12.    993.5188 cm-1
13.   1027.1693 cm-1
14.   1054.1141 cm-1
15.   1171.6015 cm-1
16.   1282.3533 cm-1
17.   1327.7755 cm-1
18.   1375.9930 cm-1
19.   1457.3963 cm-1
20.   1482.7776 cm-1
21.   1717.1051 cm-1
22.   2192.1846 cm-1
23.   3010.0840 cm-1
24.   3024.6604 cm-1
25.   3135.9719 cm-1
26.   3152.0519 cm-1
27.   3231.0265 cm-1
```

***

allylncs-TS-II-I-B3LYP-D3(BJ)/cc-pVQZ

__Requested operations__

Run with Gaussian 16revisionB.01.

opt=(calcfc,ts,noeigen) freq b3lyp/cc-pvqz empiricaldispersion=gd3bj

__Relevant magnitudes__

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H5NS
Number of Basis Functions	484
Electronic Energy (Eh)	-608.49094833
Sum of electronic and zero-point Energies (Eh)	-608.409454
Sum of electronic and thermal Energies (Eh)	-608.403553
Sum of electronic and enthalpy Energies (Eh)	-608.402609
Sum of electronic and thermal Free Energies (Eh)	-608.440026
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	26

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          2.550998        1.122563       -0.000446
H          1.662680        1.719139       -0.153842
H          3.494626        1.642966        0.071143
C          2.488100       -0.195342        0.095068
H          3.387730       -0.779892        0.248240
C          1.234795       -1.015991        0.009816
H          1.109599       -1.596687        0.929108
H          1.330119       -1.739298       -0.805847
N          0.061629       -0.234308       -0.212441
C         -1.103861       -0.080526       -0.072134
S         -2.652272        0.213107        0.062779
```

__Frequencies__ (27 in total)

```
 1.    -16.1074 cm-1   *
 2.     71.3102 cm-1
 3.    186.5896 cm-1
```

4. 257.9124 cm-1
5. 458.7948 cm-1
6. 486.0957 cm-1
7. 531.3010 cm-1
8. 566.6567 cm-1
9. 763.2775 cm-1
10. 914.5105 cm-1
11. 964.9752 cm-1
12. 994.7239 cm-1
13. 1029.3276 cm-1
14. 1065.6907 cm-1
15. 1149.8040 cm-1
16. 1264.3305 cm-1
17. 1327.3205 cm-1
18. 1379.9602 cm-1
19. 1449.7797 cm-1
20. 1475.8378 cm-1
21. 1716.3188 cm-1
22. 2173.9516 cm-1
23. 2997.3319 cm-1
24. 3021.2409 cm-1
25. 3142.6596 cm-1
26. 3152.2374 cm-1
27. 3230.0009 cm-1

```
***
# allylncs-TS-III-II-B3LYP-D3(BJ)/cc-pVQZ


__Requested operations__

Run with Gaussian 16revisionB.01.

# opt=(calcfc,ts,noeigen) freq b3lyp/cc-pvqz empiricaldispersion=gd3bj

__Relevant magnitudes__


| Datum | Value |
|:---|---:|
| Charge | 0 |
| Multiplicity | 1 |
| Stoichiometry | C4H5NS |
| Number of Basis Functions | 484 |
| Electronic Energy (Eh) | -608.487227943 |
| Sum of electronic and zero-point Energies (Eh) | -608.405812 |
| Sum of electronic and thermal Energies (Eh) | -608.399691 |
| Sum of electronic and enthalpy Energies (Eh) | -608.398746 |
| Sum of electronic and thermal Free Energies (Eh) | -608.437425 |
```

| Number of Imaginary Frequencies | 1 |
| Mean of alpha and beta Electrons | 26 |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C 1.827628 1.422688 0.204250
H 1.155388 1.530037 1.046091
H 2.267583 2.329563 -0.184520
C 2.085413 0.243683 -0.339673
H 2.750589 0.172175 -1.190901
C 1.483029 -1.056051 0.148601
H 1.738851 -1.227359 1.196640
H 1.883473 -1.896776 -0.413868
N 0.048246 -1.094186 0.038096
C -0.939134 -0.436897 0.002143
S -2.304702 0.356945 -0.050752
```

__Frequencies__ (27 in total)

```
 1.  -144.7562 cm-1   *
 2.    46.8940 cm-1
 3.    67.5962 cm-1
 4.   296.6541 cm-1
 5.   451.4966 cm-1
 6.   467.2769 cm-1
 7.   516.2208 cm-1
 8.   634.5001 cm-1
 9.   737.1252 cm-1
10.   922.5126 cm-1
11.   937.7993 cm-1
12.   980.7953 cm-1
13.  1016.7873 cm-1
14.  1095.8132 cm-1
15.  1158.1757 cm-1
16.  1272.6790 cm-1
17.  1333.3961 cm-1
18.  1376.9718 cm-1
19.  1453.9123 cm-1
20.  1498.9954 cm-1
21.  1705.2303 cm-1
22.  2143.0322 cm-1
23.  3027.7376 cm-1
24.  3084.8851 cm-1
25.  3135.2569 cm-1
26.  3155.8810 cm-1
27.  3219.9439 cm-1
```

```
***
# allylncs-TS-III-III-B3LYP-D3(BJ)/cc-pVQZ


__Requested operations__

Run with Gaussian 16revisionB.01.

# opt=(calcfc,ts,noeigen) freq b3lyp/cc-pvqz empiricaldispersion=gd3bj

__Relevant magnitudes__


| Datum                                          | Value                  |
|:-----------------------------------------------|-----------------------:|
| Charge                                         |           0            |
| Multiplicity                                   |           1            |
| Stoichiometry                                  |         C4H5NS         |
| Number of Basis Functions                      |          484           |
| Electronic Energy (Eh)                         |     -608.487565126     |
| Sum of electronic and zero-point Energies (Eh) |      -608.406418       |
| Sum of electronic and thermal Energies (Eh)    |      -608.400232       |
| Sum of electronic and enthalpy Energies (Eh)   |      -608.399287       |
| Sum of electronic and thermal Free Energies (Eh) |      -608.438277       |
| Number of Imaginary Frequencies                |           1            |
| Mean of alpha and beta Electrons               |          26            |

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          3.134962      -0.730684       0.000003
H          3.879123       0.056282       0.000019
H          3.501980      -1.746546      -0.000004
C          1.837677      -0.470360      -0.000006
H          1.114848      -1.276537      -0.000021
C          1.264731       0.929587       0.000004
H          1.610380       1.483970      -0.874528
H          1.610365       1.483951       0.874554
N         -0.165297       0.949749      -0.000008
C         -1.169017       0.318695      -0.000003
S         -2.560609      -0.433300       0.000003
```

__Frequencies__ (27 in total)

```
 1.   -131.6338 cm-1   *
 2.     39.1287 cm-1
```
```

3. 61.9796 cm-1
4. 314.0967 cm-1
5. 423.1487 cm-1
6. 456.9908 cm-1
7. 548.3989 cm-1
8. 559.3461 cm-1
9. 712.7508 cm-1
10. 909.6471 cm-1
11. 952.4164 cm-1
12. 989.0807 cm-1
13. 1027.4430 cm-1
14. 1123.2650 cm-1
15. 1157.2931 cm-1
16. 1271.0056 cm-1
17. 1330.1445 cm-1
18. 1354.7369 cm-1
19. 1453.8613 cm-1
20. 1486.8797 cm-1
21. 1704.4909 cm-1
22. 2158.3447 cm-1
23. 3028.2592 cm-1
24. 3048.8409 cm-1
25. 3131.1634 cm-1
26. 3159.0932 cm-1
27. 3217.7751 cm-1

```

***
```