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Molecular and Electronic Structures of Acryloyl isothiocyanate, $CH_2CHC(O)NCS$: A Joint Experimental and Theoretical Study

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Supporting Information

Table S1. Experimental and calculated vibrational wavenumbers (cm^{-1}) of CH_2=CHC(O)NCS[a] using the B3LYP/6-311++G(3df,3pd) level of theory

Mode	Mode descriptions	Experimental		Calculated[b]	
		IR	Raman	B3LYP/6-311++G(3df,3pd) tc	cc
ν_1	CH_2 antisym. str.		3109	3240(3.3)	3242(0.7)
ν_2	C-H str.		3071	3194(1.1)	3186(2.0)
ν_3	CH_2 sym. str.		3034	3150(2.1)	3149(4.0)
ν_4	NCS antisym. str.	1989	1984	2040(1767.3)	2034(1875.8)
ν_5	C=O str.	1733	1701	1753(317.2)	1758(247.8)
ν_6	C=C str.	1629	1622	1679(33.3)	1678(82.0)
ν_7	CH_2 def.	1406	1392	1443(55.0)	1442(135.0)
ν_8	CH in-plane bend			1313(2.4)	1328(26.7)
ν_9	C-C str.	1233	1275	1257(517.2)	1181(551.5)
ν_{10}	CH_2 twist	1156	1121	1074(22.7)	1091(1.5)
ν_{11}	CH out-of-plane bend		1039	1034(10.0)	1026(26.2)
ν_{12}	CH_2 rock	973	967	1017(39.4)	1025(20.7)
ν_{13}	CH_2 twist	923	914	933(153.0)	944(205.2)
ν_{14}	CC(O)N out-of-plane bend			815(21.1)	807(25.3)
ν_{15}	C-N str.	711	689	711(7.2)	749(40.9)
ν_{16}	C-C(O)N in-plane bend.	573	567	584(107.8)	639(55.5)
ν_{17}	C=C-C in-plane bend			528(12.9)	514(0.2)
ν_{18}	C-N=C out-of-plane bend			514(0.3)	484(0.5)
ν_{19}	NCS out-of-plane bend	450	461	478(0.2)	470(3.0)
ν_{20}	NCS in-plane bend			459(12.2)	397(29.8)
ν_{21}	CCN in-plane bend			239(0.1)	265(0.1)
ν_{22}	C=C-C out-of-plane bend			129(0.9)	132(0.1)
ν_{23}	C-N=C in-plane bend			77(0.9)	78(1.6)
ν_{24}	NCS torsion			68(0.6)	51(0.9)

[a] Calculated frequencies for the tc and cc conformers of CH_2=CHC(O)NCS. [b] In parentheses relative band strength.

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Table S2. Natural population analysis of CH_2=CHC(O)NCO and CH_2=CHC(O)NCS[a]

Atom	No	X=O	X=S
C	1	-0.26402	-0.26782
C	2	-0.27899	-0.27036
H	3	0.20106	0.19467
H	4	0.19464	0.19980
H	5	0.21542	0.21405
C	6	0.65562	0.65259
O	7	-0.54312	-0.52933
N	8	-0.64694	-0.53259
C	9	0.91457	0.24879
X	10	-0.44824	0.09020

[a] Calculated at the B3LYP/6-311++G(3df,3pd) approach, for atom numbering, see Fig. 2.