

Table S1

Observed transition frequencies (MHz) of ^{13}C and d_3 species for *cis*-acetyl isocyanate in the ground vibrational state

Transition						$^{13}\text{CH}_3\text{C}(\text{O})\text{NCO}$				$\text{CD}_3\text{C}(\text{O})\text{NCO}$		
J'	K_a'	K_c'	J''	K_a''	K_c''	A-level		E-level		A-level		
						Obsd	O - C ^a	O - C ^b	Obsd	O - C ^b	Obsd	O - C ^a
7	0	7	6	0	6	27469.98	-0.09	-0.09				
7	1	7	6	1	6	26683.35	-0.24	0.23				
7	1	6	6	1	5	29104.60	-0.07	0.03				
7	2	6	6	2	5	27950.89	0.23	0.28	27960.00	0.36		
7	2	5	6	2	4	28513.23	-0.16	-0.06			26795.55	0.06
7	3	5	6	3	4	28108.24	0.17	0.24				
7	3	4	6	3	3	28133.09	-0.01	0.06				
7	4	4	6	4	3	28084.00	-0.13	-0.07				
7	5	3	6	5	2	28068.50	0.23	0.29				
7	6	2	6	6	1	28059.09	-0.15	-0.09				
8	0	8	7	0	7	31219.70	-0.24	-0.25			29365.05	-0.05
8	1	8	7	1	7	30451.49	-0.20	-0.22			28668.02	-0.03
8	1	7	7	1	6	33197.70	-0.26	-0.16	33197.00	-0.54	31175.49	0.01
8	2	7	7	2	6	31908.20	0.17	0.21	31911.27	-1.32	29998.36	-0.10
8	2	6	7	2	5	32724.23	-0.19	-0.06	32719.90	-0.17	30749.85	-0.28
8	3	6	7	3	5	32139.50	0.26	0.34			30211.40	0.03
8	3	5	7	3	4	32189.09	0.07	0.15			30257.54	-0.16
8	4	5	7	4	4	32110.28	0.20	0.90			30184.15	0.19
8	5	4	7	5	3	32086.20	-0.08	-0.02			30162.24	-0.20
8	6	3	7	6	2	32073.16	-0.03	0.03			30150.04	-0.13
8	7	2	7	7	1	32064.76	0.05	0.11			30143.00	0.21
9	0	9	8	0	8	34923.47	-0.14	-0.19			32853.86	0.05
9	1	9	8	1	8	34206.30	-0.10	-0.14			32853.86	-0.09
9	1	8	8	1	7	37261.32	-0.07	0.03	37260.90	0.03	34992.79	-0.28
9	2	8	8	2	7	35851.57	0.16	0.21	35853.64	-0.16	33707.10	0.00
9	2	7	8	2	6	36966.40	-0.20	-0.05	36963.36	-1.08	34733.15	-0.08
9	3	7	8	3	6	36173.38	0.13	0.21			34003.51	0.09
9	3	6	8	3	5	36263.96	0.22	0.31			34087.54	-0.09
9	5	5	8	5	4	36107.50	-0.11	-0.04			33943.10	0.19
9	6	4	8	6	3	36089.20	-0.14	-0.07			33925.95	0.11
9	7	3	8	7	2	36077.52	-0.19	-0.12			33914.91	0.07
9	8	2	8	8	1	36069.60	0.20	0.27			33907.06	0.20
10	0	10	9	0	9	38590.28	0.05	-0.02			36309.14	0.07
10	1	10	9	1	9	37947.27	-0.09	-0.14			35728.32	0.00
10	1	9	9	1	8	41289.16	0.20	0.29			38777.77	0.05
10	2	9	9	2	8						37401.63	0.04
10	2	8	9	2	7	41228.57	-0.08	0.10			38734.27	0.10
10	3	8	9	3	7						37796.83	0.04
10	3	7	9	3	6						37939.36	-0.02
10	4	6	9	4	5						37771.65	-0.24
10	5	6	9	5	5	40132.88	0.22	0.30			37727.14	0.17
10	6	5	9	6	4	40108.22	0.25	0.32			37703.87	-0.08
10	7	4	9	7	3	40092.20	-0.25	-0.18			37689.25	-0.08
10	8	3	9	8	2	40081.27	-0.27	-0.21			37678.74	-0.19
10	9	2	9	9	1	40073.30	0.14	0.21			37669.30	-0.25
11	0	1	10	0	10						39741.25	0.21

Table S1. (continued)

Transition						CD ₃ C(:O)NCO	
<i>J'</i>	<i>K_a'</i>	<i>K_c'</i>	<i>J''</i>	<i>K_a''</i>	<i>K_c''</i>	Obsd	O - C ^a
11	1	11	10	1	10	39240.55	0.24
15	1	14	15	0	15	35881.10	0.40
9	2	8	9	1	9	30901.85	-0.17
10	2	9	10	1	10	32576.00	0.11
11	2	10	11	1	11	34415.60	-0.06
17	2	15	17	1	16	28326.25	0.23
18	2	16	18	1	17	31062.85	-0.28
19	2	17	19	1	18	34147.15	-0.26
20	2	18	20	1	19	37535.46	-0.28
13	3	10	13	2	11	33405.46	0.00
14	3	11	14	2	12	32374.45	-0.02
15	3	12	15	2	13	31433.43	-0.11
16	3	13	16	2	14	30651.15	-0.07
17	3	14	17	2	15	30092.65	-0.05
18	3	15	18	2	16	29816.45	-0.15
19	3	16	19	2	17	29872.98	-0.17
20	3	17	20	2	18	30303.55	-0.22
21	3	18	21	2	19	31141.10	-0.14
22	3	19	22	2	20	32409.50	-0.20
23	3	20	23	2	21	34123.85	0.09
24	3	21	24	2	22	36287.10	0.29
25	3	22	25	2	23	38889.10	0.22
25	4	21	25	3	22	39847.90	0.28
26	4	22	26	3	23	39408.75	0.05
27	4	23	27	3	24	39368.40	0.15
28	4	24	28	3	25	39768.71	-0.17

a. Obsd. - Calcd. (Fitting for the *A*-state transition frequencies)b. Obsd. - Calcd. (Fitting for the *A*- and *E*-states transition frequencies)