

# On the Cl $\cdots$ C halogen bond: a rotational study of CF<sub>3</sub>Cl $\cdots$ CO

## Electronic Supplementary Information

**Content:**

Table of transition frequencies.

**Table 1:** Experimental transition frequencies ( $\nu$ ) and discrepancies between observed and calculated frequencies ( $\Delta\nu$ ) of the  $\text{CF}_3^{35}\text{Cl-CO}$  and  $\text{CF}_3^{37}\text{Cl-CO}$  complexes.

$J''$	$K''$	$F''$	$F'$	$\text{CF}_3^{35}\text{Cl-CO}$		$\text{CF}_3^{37}\text{Cl-CO}$	
				$\nu_{\text{obs}}/\text{MHz}$	$\Delta\nu/\text{kHz}$	$\nu_{\text{obs}}/\text{MHz}$	$\Delta\nu/\text{kHz}$
6	0	6	5	7449.0078	0.8	7448.2707	0.8
6	0	5	4	7449.0078	-2.7	7448.2707	-1.5
6	0	7	6	7449.8916	0.3	7448.9674	-1.3
6	0	8	7	7449.8916	-0.9	7448.9674	-2.1
7	0	7	6	8690.6060	0.6	8689.6885	1.0
7	0	6	5	8690.6060	-1.4	8689.6885	-0.3
7	0	8	7	8691.2401	1.1	8690.1872	-1.0
7	0	9	8	8691.2401	0.2	8690.1872	-1.6
8	0	8	7	9932.0489	1.3	9930.9641	-0.3
8	0	7	6	9932.0489	0.0	9930.9641	-1.1
8	0	9	8	9932.5256	0.6	9931.3397	-2.0
8	0	10	9	9932.5256	0.0	9931.3497	7.6
9	0	9	8	11173.3560	0.3	11172.1146	-1.0
9	0	8	7	11173.3560	-0.5	11172.1146	-1.6
9	0	10	9	11173.7302	1.4	11172.4091	-1.4
9	0	11	10	11173.7302	1.0	11172.4091	-1.6
10	0	10	9	12414.5314	-2.3	12413.1423	0.4
10	0	9	8	12414.5344	0.0	12413.1423	-0.0
10	0	11	10	12414.8360	2.3	12413.3801	1.2
10	0	12	11	12414.8360	2.0	12413.3801	1.0
11	0	11	10	13655.5768	-1.7	13654.0370	-1.1
11	0	10	9	13655.5768	-2.1	13654.0370	-1.4
11	0	12	11	13655.8257	0.8	13654.2333	0.5
11	0	13	12	13655.8257	0.5	13654.2333	0.3
12	0	12	11	14896.4822	-0.3		
12	0	11	10	14896.4822	-0.7		
12	0	13	12	14896.6881	-0.6		
12	0	14	13	14896.6881	-0.8		
13	0	13	12	16137.2354	-1.4		
13	0	12	11	16137.2354	-1.7		
13	0	14	13	16137.4113	-0.6		
13	0	15	14	16137.4113	-0.7		
14	0	14	13	17377.8308	-0.4		
14	0	13	12	17377.8308	-0.6		
14	0	15	14	17377.9808	-1.0		
6	1	6	5	7448.6297	-1.2	7447.9259	2.3
6	1	5	4	7449.1768	-0.7	7448.3565	-0.0
6	1	7	6	7449.2920	-1.0	7448.4438	-3.5
7	1	7	6	8690.2267	-0.0	8689.3304	-0.9
7	1	6	5	8690.5666	-2.1	8689.6019	-0.2
7	1	8	7	8690.7438	0.7	8689.7374	-2.2
7	1	9	8	8691.0889	0.4	8690.0106	-1.9
8	1	8	7	9931.6553	-1.0	9930.5926	2.3
8	1	7	6	9931.8848	0.3	9930.7704	-0.5
8	1	9	8	9932.0660	0.1	9930.9142	0.0
8	1	10	9	9932.2968	0.7	9931.0950	-1.0
9	1	9	8	11172.9429	-0.7	11171.7168	-0.2
9	1	8	7	11173.1042	0.7	11171.8432	-0.4
9	1	10	9	11173.2747	-0.0	11171.9771	-1.7
9	1	11	10	11173.4367	0.8	11172.1150	8.8
10	1	10	9	12414.0970	1.5	12412.7153	0.7
10	1	9	8	12414.2122	0.4	12412.8075	0.8
10	1	11	10	12414.3692	1.2	12412.9318	1.8
11	1	11	10	13655.1121	2.0	13653.5766	-2.2
11	1	10	9	13655.1975	0.1	13653.6482	0.2
11	1	12	11	13655.3360	-1.9	13653.7579	-1.0
11	1	13	12	13655.4257	-0.0	13653.8268	-1.6
7	3	8	7	8686.7761	-3.3		
7	2	7	6	8689.0908	0.1		
7	2	8	7	8689.2549	-1.0		
7	3	9	8	8689.8725	-3.1		
7	2	6	5	8690.4502	-3.4		
7	2	9	8	8690.6320	-1.9		
8	3	9	8	9928.3960	1.0		
8	3	8	7	9928.5231	-2.1		
8	3	10	9	9930.4570	-2.2		
8	2	8	7	9930.4847	2.2		
8	2	9	8	9930.6886	-0.3		

8	2	7	6	9931.3925	0.7		
8	2	10	9	9931.6065	-0.8		
9	3	10	9	11169.6451	1.0		
9	3	11	10	11171.0909	1.8		
9	2	9	8	11171.7086	0.9		
9	2	10	9	11171.9143	1.1		
9	2	8	7	11172.3442	-0.3		
9	2	11	10	11172.5578	1.9		
10	2	10	9	12412.7836	3.0		
10	2	11	10	12412.9726	1.4		
10	2	9	8	12413.2470	2.9		
10	2	12	11	12413.4403	1.8		