

# Non bonding interactions and internal dynamics in CH<sub>2</sub>F<sub>2</sub>⋯H<sub>2</sub>CO. A rotational and model calculations study

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## SUPPLEMENTARY INFORMATION

Table 1S: Experimental transition frequencies ( $\nu$ /MHz) and (observed – calculated) values ( $\Delta\nu$ /kHz) of the DFM⋯H<sub>2</sub>CO isotopologues

$J'(K'_a, K'_c) - J''(K''_a, K''_c)$	CH <sub>2</sub> F <sub>2</sub> -HCOH				<sup>13</sup> CH <sub>2</sub> F <sub>2</sub> -HCOH(0')		CH <sub>2</sub> F <sub>2</sub> -H <sup>13</sup> COH(0')	
	0 <sup>+</sup>		0 <sup>-</sup>		$\nu$ /MHz	$\Delta\nu$ /kHz	$\nu$ /MHz	$\Delta\nu$ /kHz
	$\nu$ /MHz	$\Delta\nu$ /kHz	$\nu$ /MHz	$\Delta\nu$ /kHz				
3(0, 3) – 2(0, 2)	9881.3947	0.1	9879.7330	0.0	9847.6324	-0.5	9673.0600	-3.7
3(1, 3) – 2(1, 2)	9620.9220	-0.1	9619.9886	-2.9	9588.7496	-10.7	9423.0362	8.1
3(1, 2) – 2(1, 1)	10154.8923	2.8	10152.4327	-0.3	10119.4174	5.1	9935.0735	-2.7
3(2, 2) – 2(2, 1)	9888.7558	0.0	9887.0600	-3.7				
3(2, 1) – 2(2, 0)	9896.6124	-6.4	9894.8891	2.2				
4(0, 4) – 3(0, 3)	13165.7636	-0.7	13163.5946	-1.6	13120.8331	2.2	12888.7225	-1.0
4(1, 4) – 3(1, 3)	12825.3980	0.0	12824.1695	1.5	12782.5447	4.8	12561.7259	-3.0
4(1, 3) – 3(1, 2)	13537.2428	4.5	13533.9748	-0.6	13489.9604	-0.1	13244.3525	1.7
4(2, 3) – 3(2, 2)	13183.2209	1.1	13180.9757	5.3				
4(2, 2) – 3(2, 1)	13202.8641	-0.6	13200.5158	-0.3				
5(0, 5) – 4(0, 4)	16442.0865	-3.7	16439.4532	-2.8	16386.0559	-1.2	16096.9643	1.3
5(1, 5) – 4(1, 4)	16027.7759	2.3	16026.2548	1.6	15974.2420	2.2	15698.4859	-1.6
5(1, 4) – 4(1, 3)	16917.3041	-2.0	16913.2474	-0.2	16858.2461	-3.4	16551.5191	1.1
5(2, 4) – 4(2, 3)	16476.1514	-0.5	16473.3519	0.8				
5(2, 3) – 4(2, 2)	16515.3949	1.9	16512.3964	2.3				
5(3, 3) – 4(3, 2)	16486.0720	4.6	16483.2343	-2.3				
5(3, 2) – 4(3, 1)	16486.3478	-4.2	16483.5185	-0.7				
1(1, 1) – 0(0, 0)	15284.5950	0.7	15278.5222	3.0				
1(1, 0) – 1(0, 1)	12166.1094	1.9	12160.0878	-3.1				
2(1, 1) – 2(0, 2)	12345.9939	0.6	12339.4587	-0.7				
3(1, 2) – 3(0, 3)	12619.4851	-3.0	12612.1598	0.4				
4(1, 3) – 4(0, 4)	12990.9604	-1.7	12982.5378	-0.8				
5(1, 4) – 5(0, 5)	13466.1796	1.6	13456.3314	1.2				