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Supplementary materials

Competition between weak hydrogen bonds: C-H···Cl is preferred to C-H···F in CH_2ClF-H_2CO, as revealed by rotational spectroscopy

Content:

Table S1. MP2/6-311++G(d,p) principal axes coordinates (Å) of CFM-formaldehyde.

Atom	Conform I			Conform II			Conform III		
	X	Y	Z	X	Y	Z	X	Y	Z
C	-0.8714	-0.7070	-0.5924	-0.8617	-0.6493	0.0	-0.4823	0.2487	0.0007
Cl	-1.3692	0.8440	0.0919	-0.6720	1.1105	0.0	-2.2472	0.2010	0.0005
F	-0.3462	-1.5025	0.3946	-2.1930	-0.9725	0.0	0.0172	-1.0308	-0.0019
H	-1.7512	-1.2019	-0.9982	-0.4017	-1.0450	-0.9007	-0.1429	0.7493	0.9030
H	-0.0970	-0.5210	-1.3304	-0.4017	-1.0450	0.9007	-0.1427	0.7530	-0.8994
O	2.1311	0.2130	-0.6332	2.2669	-0.8884	0.0	2.5150	0.7981	-0.0021
C	2.3192	0.4038	0.5518	2.8198	0.1935	0.0	3.1062	-0.2637	0.0025
H	3.3365	0.5292	0.9628	2.2458	1.1365	0.0	2.5665	-1.2250	0.0040
H	1.4847	0.4596	1.2699	3.9204	0.2806	0.0	4.2094	-0.3109	0.0056

Table S2: Transitions frequencies (ν, MHz) and discrepacies between experimental and calculated values (Δν, kHz) of all the observed isotopomers

$J'_{Ka'Kc'}$	F'	$J''_{Ka''Kc''}$	F''	^{35}Cl (0$^-$)		^{35}Cl (0$^+$)		^{37}Cl (0$^-$)		^{37}Cl (0$^+$)	
				ν/MHz	Δν/kHz	ν/MHz	Δν/kHz	ν/MHz	Δν/kHz	ν/MHz	Δν/kHz
3_{13}	3	2_{12}	2	8107.6739	-1	8108.7865	0	8052.7914	-1		0
3_{13}	5	2_{12}	4	8109.1265	4	8110.2362	0	8053.9360	-6	8055.0377	-2
3_{13}	4	2_{12}	3	8110.7724	0	8111.8867	2	8055.2307	0	8056.3296	-2
3_{13}	2	2_{12}	1	8106.0208	-1	8107.1426	8	8051.4956	-6		
3_{03}	3	2_{02}	2	8539.7040	-4	8541.5385	0	8488.8632	-1		
3_{03}	5	2_{02}	4	8538.7793	-1	8540.6164	2	8488.1736	-4		
3_{03}	4	2_{02}	3	8537.3562	0	8539.1865	-1	8486.9917	0	8488.7998	2
3_{03}	2	2_{02}	1	8541.1298	-1	8542.9601	-4	8490.0436	-5		
3_{03}	4	2_{02}	4	8544.1798	1						
3_{03}	3	2_{02}	3	8534.8404	-5						
3_{12}	3	2_{11}	2	9088.6604	0	9091.6156	4	9050.4853	-5	9053.4314	2
3_{12}	5	2_{11}	4	9083.5442	0	9086.4984	1	9046.4584	-3	9049.4000	1
3_{12}	4	2_{11}	3	9085.1789	0	9088.1320	2	9047.7336	-1	9050.6770	2
3_{12}	2	2_{11}	1	9087.0206	3	9089.9726	1	9049.2052	-6	9052.1501	2
4_{14}	3	3_{13}	2	10792.2039	-2	10793.6242	-2	10717.4607	-3	10718.8616	-1
4_{14}	4	3_{13}	3	10792.5686	0	10793.9907	3	10717.7318	0	10719.1331	2
4_{14}	6	3_{13}	5	10793.2326	1	10794.6538	1	10718.2672	-1	10719.6653	-1
4_{14}	5	3_{13}	4	10793.5860	-1	10795.0064	0	10718.5305	-1	10719.9287	-2
4_{04}	3	3_{03}	2	11307.5120	-4	11309.6905	-7	11234.1585	-3	11236.2913	-4
4_{04}	4	3_{03}	3	11305.6899	-1	11307.8714	2	11232.6438	-4	11234.7762	-3
4_{04}	6	3_{03}	5	11306.2486	-1	11308.4308	0	11233.1456	-4	11235.2777	-4
4_{04}	5	3_{03}	4	11304.4150	-1	11306.5934	-1	11231.6284	-1	11233.7611	1
4_{04}	5	3_{03}	5	11309.8178	3						
4_{04}	4	3_{03}	4	11303.1772	-3						
4_{13}	3	3_{12}	2	12092.6271	-4	12096.4912	0	12040.8097	-10	12044.6486	-7
4_{13}	4	3_{12}	3	12092.9162	-1	12096.7769	0	12041.0199	-1	12044.8554	-1
4_{13}	6	3_{12}	5	12090.5560	-1	12094.4193	2	12039.1731	-3	12043.0105	0
4_{13}	5	3_{12}	4	12090.8358	-2	12094.6987	1	12039.3685	-4	12043.2078	0
4_{13}	4	3_{12}	4	12084.1549	1						
5_{15}	5	4_{14}	4	13461.8702	1	13463.5517	1	13366.3256	2		
5_{15}	4	4_{14}	3	13461.9871	2	13463.6670	0	13366.4322	-3		
5_{15}	6	4_{14}	5	13462.3401	1	13464.0186	-1	13366.6907	0	13368.3358	-5
5_{15}	7	4_{14}	6	13462.4623	3	13464.1414	0	13366.8027	-3	13368.4544	-1
5_{05}	5	4_{04}	4	14011.0458	2	14013.3865	1	13912.0817	1		
5_{05}	4	4_{04}	3	14013.1660	-1	14015.5082	-4	13913.8310	2		
5_{05}	6	4_{04}	5	14010.1938	-1	14012.5369	1	13911.4043	2	13913.6678	1
5_{05}	7	4_{04}	6	14012.3323	0	14014.6777	1	13913.1604	0	13915.4253	-1
5_{14}	5	4_{13}	4	15077.7387	0	15082.4312	1	15010.1703	3		
5_{14}	4	4_{13}	3	15078.0279	5	15082.7194	4	15010.4300	4		
5_{14}	6	4_{13}	5	15076.3539	3	15081.0442	3	15009.0694	4	15013.7230	6

5_{14}	7	4_{13}	6	15076.6359	-2	15081.3308	0	15009.3261	0	15013.9784	0
6_{16}	6	5_{15}	5	16114.5297	6	16116.4166	-1				
6_{16}	7	5_{15}	6	16114.7832	1						
6_{16}	8	5_{15}	7	16115.1382	8	16117.0271	1	15997.8796	9	15999.7284	7
6_{16}	5	5_{15}	4	16114.8570	-12						
6_{06}	6	5_{05}	5	16652.3433	1						
6_{06}	7	5_{05}	6	16651.7236	2	16654.0655	1				
6_{06}	8	5_{05}	7	16654.0112	3	16656.3507	-2	16526.2601	6	16528.4990	5
6_{06}	5	5_{05}	4	16654.5823	0	16656.9238	-3				
6_{15}	6	5_{14}	5	18034.9530	3	18040.3661	-3				
6_{15}	7	5_{14}	6	18033.9397	0	18039.3516	-7				
6_{15}	8	5_{14}	7	18034.5950	4	18040.0101	-1	17948.9840	2		
6_{15}	5	5_{14}	4	18035.5983	0						
3_{22}	5	2_{21}	4	8605.4568	1	8607.5257	-1				
3_{22}	3	2_{21}	2	8607.6770	-2	8609.7527	4				
3_{22}	4	2_{21}	3	8613.2374	-2	8615.3083	3				
3_{21}	5	2_{20}	4	8674.3832	3	8676.6919	4				
3_{21}	3	2_{20}	2	8677.5967	3	8679.9039	2				
3_{21}	4	2_{20}	3	8683.5848	-2	8685.8925	0				
4_{23}	6	3_{22}	5	11462.1066	0						
4_{23}	4	3_{22}	3	11463.9822	-2	11466.7035	7				
4_{23}	5	3_{22}	4	11464.9860	0	11467.6956	-2				
4_{22}	6	3_{21}	5	11632.8306	-5	11636.1242	-3				
4_{22}	4	3_{21}	3	11636.1684	-5	11639.4603	-6				
4_{22}	5	3_{21}	4	11637.5465	-4	11640.8396	-4				
6_{25}	8	5_{24}	7	17132.7616	-9						
6_{25}	5	5_{24}	4	17135.8662	1						
6_{25}	7	5_{24}	6	17135.9365	3						
6_{24}	6	5_{23}	5	17698.6201	3						
6_{24}	8	5_{23}	7	17696.0810	-1						
6_{24}	5	5_{23}	4	17695.9199	2						
6_{24}	7	5_{23}	6	17698.7764	0						
1_{11}	2	0_{00}	2	7240.9448	0	7242.8924	-2	7067.7755	-2		-1
1_{11}	3	0_{00}	2	7258.0559	0	7260.0064	0	7081.2857	0		1
1_{11}	1	0_{00}	2	7271.7614	0	7273.7129	0				
2_{12}	3	1_{01}	2	9785.6341	4						
2_{12}	2	1_{01}	2	9792.3050	-8						
2_{12}	3	1_{01}	3	9793.4146	-1						
2_{12}	4	1_{01}	3	9802.7276	0	9804.7569	2				
2_{12}	2	1_{01}	1	9806.3221	-1						
2_{12}	1	1_{01}	1	9815.6685	-1						
3_{13}	4	2_{02}	3	12176.4089	-5						
3_{13}	3	2_{02}	3	12180.0063	7						
3_{13}	5	2_{02}	4	12190.8982	0	12192.7179	0				

4_{04}	6	3_{13}	5	7654.1296	-1	7656.3294	2
5_{05}	7	4_{14}	6	10873.2327	1	10876.3469	-4
5_{05}	5	4_{14}	4	10879.0126	0		
5_{05}	6	4_{14}	5	10881.9636	-2		