Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

On the weak O-H···Halogen Hydrogen Bond. A rotational study of $CH_3CHClF\cdots H_2O$

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Electronic Supplementary Information

- Table of MP2/6-311++G(d, p) calculated principal axes coordinates (Å) of CFE-W.
- Table of transitions of all the observed isotopologues.

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

Conform I				Conform II				Conform III			
Atom	X	Y	Z	Atom	X	Y	Z	Atom	X	Y	Z
C	-0.0926	-0.1356	0.1312	C	0.4556	-0.4464	0.2022	C	0.5647	0.7549	0.2179
Cl	-1.8232	0.2334	0.2699	Cl	0.1574	1.2650	-0.2149	C	-0.0925	1.3402	-1.0030
F	0.4546	0.7270	-0.8085	F	1.7330	-0.5417	0.7080	Cl	1.4034	-0.7638	-0.1501
H	0.3712	0.1014	1.0862	H	-0.2441	-0.6961	0.9959	F	-0.3995	0.4901	1.1814
C	0.1401	-1.5568	-0.3040	H	0.5446	-2.3596	-0.7149	O	-2.6624	-0.7174	-0.3022
H	-0.2886	-2.2419	0.4299	C	0.3145	-1.3314	-1.0063	H	1.2942	1.4163	0.6836
H	1.2159	-1.7301	-0.3737	H	1.0080	-1.0120	-1.7867	H	-0.6032	2.2646	-0.7209
H	-0.3328	-1.7296	-1.2727	H	-0.7105	-1.2854	-1.3750	H	-0.8209	0.6350	-1.4062
O	2.9451	0.1682	0.4778	O	-2.6315	-0.4447	0.3595	H	0.6641	1.5632	-1.7576
H	2.6038	0.7591	-0.1997	H	-2.5906	0.5087	0.2452	H	-2.0858	-0.5652	0.4525
H	3.8144	0.5208	0.6801	H	-3.5422	-0.6103	0.6143	H	-2.9809	-1.6127	-0.1697

Table S2: Transitions of all the observed isotopomers

$J'_{Ka'Kc'}$	F'	$J''_{Ka''Kc''}$	F''	normal	^{37}Cl-H_2O	H_2O^{18}	HOD	DOD	DOH
3_{03}	3	2_{02}	2	9207.6883	9024.9998	8730.8263	8820.4358	8652.7665	9020.4499
3_{03}	2	2_{02}	1	9207.7173	9025.0028	8730.8581	8820.4658	8652.7963	9020.4630
3_{03}	4	2_{02}	3	9211.6299	9028.1173	8734.7624	8824.3694	8656.7023	9024.4005
3_{03}	5	2_{02}	4	9211.6559	9028.1405	8734.7919	8824.4054	8656.7350	9024.4262
3_{13}	3	2_{12}	2	9003.5238	8828.4709	8548.3547	8632.7994	8467.1568	8818.7231
3_{13}	4	2_{12}	3	9003.7612	8828.6525	8548.5909	8633.0133	8467.3979	8818.9479
3_{13}	2	2_{12}	1	9007.4855	8831.5966		8636.7029		
3_{13}	5	2_{12}	4	9007.7401	8831.7988	8552.5518	8636.9676	8471.3537	8822.9130
3_{12}	4	2_{11}	3	9434.6379	9242.3308	8931.5698	9027.4156	8857.2555	
3_{12}	3	2_{11}	2	9434.6576	9242.3423	8931.5920	9027.4346	8857.2702	
3_{12}	2	2_{11}	1	9438.6184	9245.4713		9031.3682	8861.2007	
3_{12}	5	2_{11}	4	9438.6316	9245.4819	8935.5316	9031.3886	8861.2110	
4_{04}	4	3_{03}	3	12265.1645	12022.1348	11632.4798	11751.2571	11528.0109	12015.9482
4_{04}	3	3_{03}	2	12265.1867	12022.1529	11632.5073	11751.2844	11528.0198	12015.9766
4_{04}	5	3_{03}	4	12267.0054	12023.5922	11634.3198	11753.0897	11529.8402	12017.7806
4_{04}	6	3_{03}	5	12267.0318	12023.6184	11634.3424	11753.1159	11529.8671	12017.8093
4_{14}	4	3_{13}	3	12002.7480	11769.2441	11396.6181	11509.0105	11288.2572	11756.4140
4_{14}	5	3_{13}	4	12003.6238	11769.9410	11397.4922	11509.8860	11289.1466	11757.3052
4_{14}	3	3_{13}	2	12004.3340	11770.5007	11398.1956	11510.5850		11758.0039
4_{14}	6	3_{13}	5	12005.2244	11771.2027	11399.0814	11511.4733	11290.7294	11758.8960
4_{13}	4	3_{12}	3	12577.2070		11907.2709	12034.8853	11808.1036	12323.7119
4_{13}	5	3_{12}	4	12577.9650		11908.0234	12035.6412	11808.8468	12324.4633
4_{13}	3	3_{12}	2	12578.7834	12322.0040			11809.6712	12325.2878
4_{13}	6	3_{12}	5	12579.5648	12322.6239	11909.6172	12037.2307	11810.4356	12326.0574
5_{05}	5	4_{04}	4	15309.0720	15006.9158				14998.1961
5_{05}	4	4_{04}	3	15309.1000	15006.9444				14998.2216
5_{05}	6	4_{04}	5	15310.1587	15007.7719				14999.2838
5_{05}	7	4_{04}	6	15310.1918	15007.7918				14999.3141
5_{15}	5	4_{14}	4	14998.4973					
5_{15}	6	4_{14}	5	14999.2204					
5_{15}	4	4_{14}	3	14999.2735					
5_{15}	7	4_{14}	6	15000.0358					
6_{16}	6	5_{15}	5	17990.2788	17640.8364	17084.2063		16921.3410	17621.2343
6_{16}	5	5_{15}	4	17990.7698	17641.2168	17084.6879		16921.8354	17621.7198
6_{16}	7	5_{15}	6	17990.8660	17641.2949	17084.7874		16921.9347	17621.8190
6_{16}	8	5_{15}	7	17991.3071	17641.6497	17085.2252	17253.0767	16922.3671	17622.2605
4_{23}	5	3_{22}	4	12291.6118	12046.8896				
4_{23}	4	3_{22}	3	12293.8681	12048.6548				
4_{23}	6	3_{22}	5	12297.9811	12051.9167				
4_{23}	3	3_{22}	2	12300.1778					
4_{22}	5	3_{21}	4	12322.6238	12075.4300				
4_{22}	4	3_{21}	3	12324.8401	12077.1834				
4_{22}	6	3_{21}	5	12328.9500	12080.4338				
4_{22}	3	3_{21}	2	12331.1739	12082.1910				
5_{14}	5	4_{13}	4	15715.9536	15395.7088				15399.2712
5_{14}	6	4_{13}	5	15716.6297	15396.2495				15399.9472
5_{14}	4	4_{13}	3	15716.7712	15396.3593				15400.0913
5_{14}	7	4_{13}	6	15717.4183	15396.8694		15040.5802		15400.7319
5_{24}	6	4_{23}	5	15363.5009					
5_{24}	5	4_{23}	4	15363.9380					
5_{23}	6	4_{22}	5	15425.2655					
5_{23}	5	4_{22}	4	15425.7341					
5_{23}	7	4_{22}	6	15428.4280					
5_{23}	4	4_{22}	3	15428.8714					
6_{06}	7	5_{05}	6			17402.3210			17966.2612
6_{06}	8	5_{05}	7			17402.3507			17966.2933
6_{06}	6	5_{05}	5			17401.5972		17243.2250	17965.5394
6_{06}	5	5_{05}	4			17401.6292		17243.2595	17965.5735
3_{21}	5	2_{20}	4				8849.2830		9052.7342
3_{22}	5	2_{21}	4						9040.6624